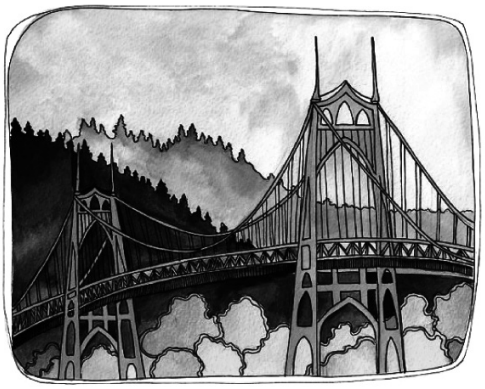
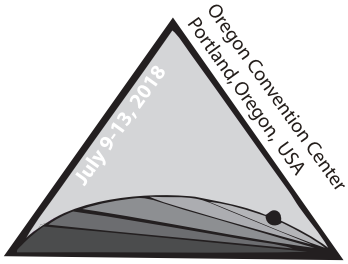
AN18-MS18-ED18 Abstracts

2018 SIAM **Annual Meeting**



July 9–13, 2018
Oregon Convention Center (OCC)
Portland, Oregon, USA



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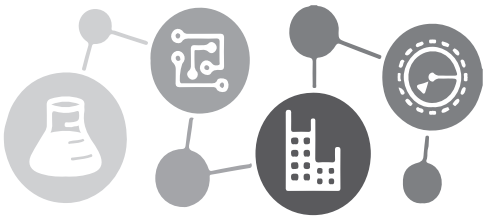
Mathematical Aspects of Materials Science



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3600 Market Street, 6th Floor
Philadelphia, PA 19104-2688 USA
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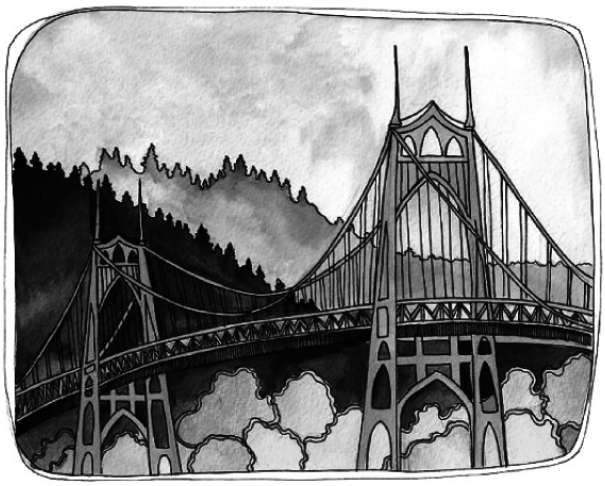
AN18 Abstracts

2018 SIAM **Annual Meeting**



July 9–13, 2018
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IP1

Bridging Scales

One fascinating aspect of probability theory is the universal aspect of the objects it allows us to construct. The most well-known example of this phenomenon is the central limit theorem: for a very large class of collections of random variables, additive functionals that only depend weakly on any one element of the collection exhibit Gaussian behaviour in the limit. When taking time evolution into account, it turns out that in certain cross-over regimes the large-scale behaviour of a number of stochastic systems can formally be described by an ill-posed stochastic PDE.

Martin Hairer
Imperial College London, United Kingdom
m.hairer@imperial.ac.uk

IP2

Algebraic Vision

Algebraic Vision is an emerging viewpoint of problems in computer vision that aims to examine polynomial models in vision through the lens of algebra. A key problem in computer vision is the estimation of the three-dimensional shape of a world scene from images and the parameters (position, orientation, etc.) of the cameras that captured them. This problem, studied under the name structure-from-motion or multiview geometry, has its origins in photogrammetry and perspective drawings. The modeling language for these problems is projective geometry, which naturally leads to polynomial models with rich and beautiful structure that beg for algebraic tools. In this talk I will show some of the surprising structure, properties, and algorithmic successes that have emerged from this algebraic viewpoint.

Rekha Thomas
University of Washington
rrthomas@uw.edu

IP3

Structure and Randomness in Encrypted Computation

Homomorphic encryption allows anyone to compute arbitrary functions on data while it remains encrypted, without the secret decryption key. This makes cloud computing compatible with privacy, even against the cloud. A naive attempt at homomorphic encryption is to make decryption (the map from "ciphertexts" to "plaintexts") a ring homomorphism. Then, adding and multiplying ciphertexts induces addition and multiplication of plaintexts, from which arbitrary functions can be built. The naive attempt fails (as far as we know) because an attacker can efficiently derive the secret homomorphism from a list of plaintext-ciphertext pairs, unless the encryption scheme itself is inefficient. Currently, all efficient and plausibly secure homomorphic encryption schemes are "noisy" variants of the naive attempt, where decryption involves removing some small "noise" or "error" from the ciphertext (think error-correcting codes) before applying a ring homomorphism. This noise hides the underlying structure; indeed, these schemes are provably secure if there are no algorithms that can efficiently solve certain computational problems, such as the approximate shortest vector problem over lattices. In this talk, I will review state-of-the-art homomorphic encryption schemes, discuss some interesting failed attempts, and possibly discuss related notions such as cryptographic program obfuscation.

Craig Gentry
IBM T. J. Watson Research Center
cbgentry@us.ibm.com

IP4

Automatic Behavioral Analysis for Computational Psychiatry at Home

According to the Centers for Disease Control and Prevention, autism affects 1 in 68 children. Autism can be diagnosed at 18 months of age, but the current average diagnosis age in the United States is 5 years old. Waiting time to see a specialist in leading hospitals in the U.S. can be up to 18 months. About 70% of counties in North Carolina lack a specialist. South Saharan Africa has an estimated half billion children served by only about 50 specialists. Current medical practices simply dont scale to address these challenges of developmental and mental health screening, diagnosis, and monitoring; we need a revolution. Since behavioral observation is the gold standard, there is a need then to develop mathematical and computational tools, which can work on smart phones, to automatically analyze behaviors and make medical practice available to the general population. This calls for an interdisciplinary teaming to design the right stimuli to evoke the appropriate behaviors that can be properly understood by mathematics and algorithms, all integrated into mobile devices, enabling personalized and at-home screening, diagnosis, and tracking of developmental and mental health disorders. We will present advances obtained by our team in the design of apps for developmental and mental health, currently being used in pediatric clinics and downloadable from iTunes. Our work has already produced the largest dataset of child behavior recorded in their natural environments.

Guillermo Sapiro
Duke University
guillermo.sapiro@duke.edu

IP5

Challenges for Numerical Analysis in Large-Scale Simulation

Finite elements are among the most popular approaches to approximate the solution of partial differential equations. Traditionally the assembling of finite element matrices and the computation of many a posteriori error estimators is obtained by local operators and thus regarded as cheap and of optimal order complexity. In many legacy codes, the solver for the arising huge systems is the bottleneck and does not scale very well. However optimal order complexity is not necessarily equivalent to short run-times, and memory traffic may slow down the execution considerably. Here we discuss several ingredients for efficient approximations of coupled multi-physics problems where Stokes type systems are involved. Surrogate finite element operators allow for a fast on-the-fly computation of the stiffness matrix entries in a matrix free setting. A variational crime analysis then yields two-scale a priori estimates. To balance the dominating components, the scheme is enriched by an adaptive steering of the polynomial order based on a hierarchical decomposition of the residual. To further improve the performance in large scale simulations, we use an all-at-once multigrid solver for the flow part. Node-wise defined Uzawa type smoothers guarantee level independent convergence rates for the variable V-cycle. All theoretical results are illustrated by a series of simulations reflecting

cost and accuracy.

Barbara Wohlmuth
M2, Centre for Mathematical Sciences,
Technische Universität München, Germany
wohlmuth@ma.tum.de

IP6

Recent Advances in Dimensionality Reduction with Provable Guarantees

This talk focuses on dimensionality reduction in the form of low-distortion embeddings into low-dimensional normed spaces. Applications include high-dimensional computational geometry, signal processing, and algorithms for linear algebra problems, to name a few. A cornerstone result is the "Johnson-Lindenstrauss (JL) lemma", which states that for any $\varepsilon > 0$ and $n > 1$, any n-point subset of Euclidean space embeds into m-dimensional Euclidean space for $m = O(\varepsilon^{-2} \log n)$ while preserving all pairwise distances multiplicatively up to $1 + \varepsilon$. Since the introduction of the JL lemma, and its use in computer science applications starting in the mid-1990s, a variety of questions concerning it have been asked as well as recently answered either optimally or near-optimally, including the optimal dimension m that can be achieved in terms of ε, n, and whether embedding above can be chosen so that any point's image can be computed quickly. In addition, new generalizations of the JL lemma and applications have been found, such as speeding up low-rank approximation computations for PCA, in addition to other large-scale linear algebra problems such as approximate least squares regression. These have been achieved via a generalization of the JL lemma known as subspace embeddings as pioneered by Sarlos. These developments will be the focus of this talk.

Jelani Nelson
Harvard
minilek@seas.harvard.edu

IP7

Nonlinear Patterns and Waves: From Spectra to Stability and Dynamics

Patterns and waves are all around us. Stripes and hexagonal patterns can be observed on animal coats, as water waves on lakes, on sand dunes in deserts, or in cloud patterns in the sky. Besides being aesthetically pleasing, patterns and waves often serve important beneficial or detrimental functions. For instance, coherent structures organize transport and mixing in geophysical fluid flows and help facilitate spatial differentiation during the early development of organisms, but they can also lead to tachycardia via reentrant cardiac arrhythmias. Patterns and waves appear in many different systems and on vastly different scales in both time and space, and their dynamic behavior is similar across these systems. Mathematical techniques can help identify the origins and common properties of patterns and waves across different applications. Understanding the ways in which such structures are created can help experimentalists identify the mechanisms that generate them in specific systems. Despite many advances, understanding patterns and waves still poses significant mathematical challenges. I will show how a combination of geometric dynamical-systems ideas combined with PDE approaches can shed light on the existence, stability, and dynamical properties of nonlinear waves and will also discuss applications and open problems.

Bjorn Sandstede
Division of Applied Mathematics
Brown University
bjorn_sandstede@brown.edu

IP8

Understanding Network Structure and Function in the Human Brain

The human brain is a complex organ characterized by a heterogeneous pattern of structural connections that supports long-range functional interactions. New non-invasive imaging techniques now allow for these patterns to be carefully and comprehensively mapped in individual humans, paving the way for a better understanding of how the complex network architecture of structural wiring supports our thought processes. While a large body of work now focuses on descriptive statistics to characterize these wiring patterns, a critical open question lies in how the organization of these networks constrains the potential repertoire of brain dynamics. In this talk, I will describe an approach for understanding how perturbations to brain dynamics propagate through complex wiring patterns, driving the brain into new states of activity. Drawing on a range of disciplinary tools from graph theory to network control theory and optimization I will identify control points in brain networks, characterize trajectories of brain activity states following perturbation to those points, and propose a mechanism for how network control evolves in our brains as we grow from children into adults. Finally, I will describe how these approaches can be used to better understand how the brain controls its own dynamics and how we can inform stimulation devices to control abnormal brain dynamics.

Danielle S. Bassett
School of Engineering and Applied Science
University of Pennsylvania
dsb@seas.upenn.edu

IP9

American Mathematical Society (AMS) Invited Address – Snow Business: Computational Elastoplasticity in the Movies and Beyond

Hyperelastic constitutive models describe a wide range of materials. Examples include biomechanical soft tissues like muscle, tendon, skin etc. Elastoplastic materials consisting of a hyperelastic constitutive model combined with a notion of stress constraint (or feasible stress region) describe an even wider range of materials. A very interesting class of these models arise from frictional contact considerations. I will discuss some recent results and examples in computer graphics and virtual surgery applications. Examples include simulation of granular materials like snow in Walt Disney's "Frozen" as well as frictional contact between thin elastic membranes and shells for virtual clothing simulation. I will also discuss practical simulation of these materials with some recent algorithmic modifications to the Particle-In-Cell (PIC) technique, the Material Point Method (MPM).

Joseph Teran
UCLA

jteran@math.ucla.edu

IP10

Connections and Reconnections: A Link Between Mathematics, Physics and DNA

Flexible circular chains appear often in nature, from microscopic DNA plasmids to macroscopic loops in solar corona. Such chains entrap rich geometrical and topological complexity which can give insight into the processes underlying their formation or modification. In the case of DNA, knotted and interlinked states are believed to be undesired in the cellular environment. However, non-trivial topologies occur frequently. Reconnection processes involving one or two cleavages are used to simplify the topology of DNA. Examples include the action of type II topoisomerases and DNA recombination. In physics, local reconnection events of knotted vortices in fluid flow have been observed, and their study reveals similar patterns of topology simplification as those observed after DNA recombination. DNA replication of a circular chromosome yields two interlinked chromosomes. We here investigate pathways of unlinking of newly replicated links by local reconnection. We use techniques from knot theory and low-dimensional topology, aided by computational tools to identify minimal unlinking pathways. These results point to a universal property relevant to any local reconnection event between two sites along one or two circles. The results presented, and the numerical methods proposed are not restricted to the biological example and are applicable to any local reconnection process.

Mariel Vazquez
University of California, Davis, USA
'mrlvazquez@ucdavis.edu'

IP11

The Future of Scientific Computation

Computational science is at a particularly challenging crossroads. Steady improvements in mathematical models, algorithms, codes and computer hardware have enabled simulations of remarkable detail and insight. More and more scientific fields are embracing the power of simulation, and critical business, policy, and national security decisions depend upon it. But Moore's Law is sputtering to an end which will have significant, but currently unknown, implications for future computers. In the midst of so much change, predicting the future of scientific computing would seem reckless if not downright foolish. But paradoxically, our simulations themselves show that highly accurate prediction is sometimes possible. At the heart of the power of mathematical models is the identification of conservation laws: temporal invariants that greatly constrain the systems possible future evolution. Although less rigorous than conservation of mass, might there be invariants that constrain the evolution of scientific fields? In this talk, I will argue that for computational science the answer is "yes". Leveraging this perspective, I will rashly make some predictions about the future of scientific computing.

Bruce Hendrickson
Lawrence Livermore National Laboratory, USA
hendrickson6@llnl.gov

IP12

Seeing Through Rock: Mathematics of Inverse Wave Propagation

Physics based interpretation of remote sensing data, such as seismic records, naturally leads to *inversion* problems: that is, construction of continuum physics models that predict the data in detail. Inversion was first suggested as a physically consistent approach to interpretation of seismic data in the 1980's, but at that time was computationally out of reach at field scale. The first feasible algorithms required another 20 years of computational and mathematical advances, and have now inspired a very active research area known as Full Waveform Inversion with branches in industrial and academic seismology. The computational needs are obvious consequences of the earth's three-dimensional structure. The mathematical issues are more surprising: they stem from the simple observation that perturbation of wave speed effectively differentiates the waveform. Combined with the nonlinearity of the elastic wavefield as a function of the coefficients (including wave velocities) in the (linear) wave equation, this hypersensitivity can lead to stagnation of local optimization, that is, failure to converge to a useful elastic model of the earth, *no matter how many Pflops are expended*. I will illustrate the stagnation phenomenon using simple examples. I will also review some of the (many) ideas advanced to overcome this obstacle, and catalog some of their successes and challenges.

William Symes
Rice University
symes@caam.rice.edu

SP1

The AWM-SIAM Sonia Kovalevsky Lecture: Learning and Efficiency of Outcomes in Games

Selfish behavior can often lead to suboptimal outcome for all participants, a phenomenon illustrated by many classical examples in game theory. Over the last two decades our community developed good understanding on how to quantify the impact of strategic user behavior on the overall performance in many games by analyzing Nash equilibria of these games (including traffic routing as well as online auctions). Learning outcomes emerged in recent years as an attractive alternative to Nash equilibrium, modeling players who havent reached a stable equilibrium, but rather use algorithmic learning. We propose that learning is a good model of behavior in games where the systems has high economic value overall, but where stakes of individual items are low, which makes exploring and learning a good behavior. Such games include both Internet packet routing as well as online auctions. In this talk we consider a few closely related questions: What are broad classes of learning behaviors that guarantee high social welfare in games, are these results robust to situations when the game or the population of players is dynamically changing, and does data from such games suggest that learning is indeed a good behavioral model of the participants.

Eva Tardos
Cornell University
Department of Computer Science
eva@cs.cornell.edu

SP2

The John Von Neumann Lecture: Untangling Random Polygons and Other Things

Suppose we are given a random polygon $\mathcal{P}_0$ with vertices

$(x_1, y_1), \ldots, (x_n, y_n)$ that have centroid (0,0). If we connect the midpoints of its edges, then we obtain a new polygon. Assume that the x-values and y-values are scaled after each update so that we always have $\|x\|_2 = 1$ and $\|y\|_2 = 1$. This update process can obviously be repeated to produce a sequence of polygons $\{\mathcal{P}_k\}$. No matter how "criss-crossy' the initial polygon $\mathcal{P}_0$, the $\mathcal{P}_k$ eventually "untangle' and their vertices head towards an ellipse with a 45-degree tilt. Why? It turns out that the sequence of x and y vectors that are produced by this iteration are the result of a power method process that involves a shifted version of the n-by-n downshift matrix S_n. That fact plus a slick SVD analysis of a certain 2-by-2 matrix explains everything. In this talk I will step through the matrix computations that explain the untangling. I will also discuss how I came across this problem and why it is a great metaphor of matrix-based computational science.

Charles F. Van Loan
Cornell University
Department of Computer Science
cv@cs.cornell.edu

SP3

Julian Cole Lectureship: Modeling of Complex Fluids: Wormlike Micellar Solutions, Polymers and Mucins

Complex and viscoelastic fluid properties arise due to immersed mesoscale structures. These structures may be small particles, long chain molecules, or transiently connected networks. This talk will cover elements of macroscale, and of stochastic mesoscale, modeling and simulation of transiently networked fluids; fluids typified by wormlike micellar solutions, polymers and mucins.

L. Pamela Cook
Department of Mathematical Sciences
University of Delaware
cook@math.udel.edu

SP4

W.T. and Idalia Reid Prize Lecture: Modeling, Simulation, and Control of Differential-Algebraic Port-Hamiltonian Systems

Complex multi-physics, multi-scale systems are at the heart of almost all modern technology developments. A highly relevant example is the real time control of modern energy systems that have to integrate different energy sources (fossil and renewables) and large networks of producers and consumers. To obtain a systematic approach for modeling, simulation, optimization and control of such complex systems, the concept of port-Hamiltonian systems is ideal. The structure is close to the underlying physics, the interconnection, Galerkin discretization and model reduction preserves the structure and there are nice algebraic properties of the equations and geometric properties of the resulting flow. When such systems contain constraints (such as e.g. Kirchhoff's laws in networks) then the resulting model is best described by (partial) differential-algebraic systems of port-Hamiltonian structure. The analysis, numerical solution, and control of this class of systems will be discussed, new mathematical and computational challenges will be described and the success of the approach will be demonstrated for the synchronization of power networks.

Volker Mehrmann
Technische Universität Berlin
mehrmann@math.tu-berlin.de

SP5

I.E. Block Community Lecture: How Paradoxes Shape Mathematics and Give Us Self-Verifying Computer Programs

A paradox is a seeming contradiction. The liar's paradox is one of the best known: "This statement is a false." If the statement is true, then it is false; if it is false, then it is true. Paradoxes can be so amusing that we might think that paradoxes are nothing more than a game. However, paradoxes triggered a crisis in math a century ago when a paradox similar to the barber paradox was found: a barber named Bertie shaves exactly those who do not shave themselves. Does Bertie shave himself? If he does, then he doesn't; if he doesn't, then he does. Other clever paradoxes show us the disturbing limits of computation and mathematics. These results are mathematical bombshells. Today, we design computer programs that check that other computers programs have no bugs. Can computer programs be fed into themselves to check their own correctness? Or does paradox stop us in our tracks? And can we know that beneficial artificial intelligence will not turn evil when it starts to modify its own computer code?

Thomas Hales
University of Pittsburgh
hales@pitt.edu

JP1

The Mathematics of Wrinkles and Folds

The wrinkling and folding of thin elastic sheets is very familiar: our skin wrinkles; a crumpled sheet of paper has folds; and a flat sheet stretched over a round surface must wrinkle or fold. What kind of mathematics is relevant? The stable configurations of a sheet are local minima of a variational problem involving its elastic energy – which consists of a nonconvex *membrane energy* (favoring isometry) plus a small coefficient times *bending energy* (penalizing curvature). The bending term is a *singular perturbation*; its small coefficient is the sheet thickness squared. The patterns and defects seen in thin sheets arise from energy minimization – but not in the same way that minimal surfaces arise from area minimization. Rather, the analysis of wrinkles and folds involves the *asymptotic character* of minimizers as the sheet thickness tends to zero. What kind of methods are useful? It has been fruitful to focus on the *energy scaling law*, in other words the dependence of the minimum energy upon the thickness of the sheet. Optimizing within an ansatz gives an *upper bound*. A key mathematical challenge is to obtain ansatz-free *lower bounds*. When the lower and upper bounds are close to agreement they demonstrate the adequacy of the ansatz, and the underlying arguments help to explain why certain configurations are preferred.

Robert V. Kohn
Courant Institute of Mathematical Sciences
New York University
kohn@cims.nyu.edu

JP2

Applied and Computational Mathematics: A New Curriculum for 21st Century Discovery and Inno-

vation

We present BYU's undergraduate Applied and Computational Math program, which provides students with a rigorous foundation in mathematics, statistics, and computation. This program was designed from the ground up with the hopes of attracting top employers and graduate programs and thus becoming a national model for applied math education. This program runs as a two-year upper-division lockstep curriculum consisting of 32 credit hours, spread out evenly over four semesters. In addition, students select an area of specialization in one of over 25 areas in the pure and applied sciences and take additional coursework to fulfill a concentration requirement. The first year of the program is devoted to the design, analysis, and optimization of algorithms, and gives students an arsenal of mathematical and statistical tools to explore the performance, complexity, and accuracy of algorithms. The second year focuses on the art and science of mathematical modeling, which gives students the ability to connect the real world with abstract mathematics and numerical simulation. At every stage of the program, students integrate theory with application and computation and data-enabled discovery. At the close of its 5th year in service, we have learned a lot about how to build a program, how to adapt to the needs of the students and the changes in technology, and how to adjust the program in real time to serve the needs of employers and other stakeholders.

Jeffrey Humpherys
Brigham Young University
jeffh@math.byu.edu

CP1

Generalized Geodesic Approach for Nonlinear Dimensionality Reduction with the Aid of Matrix Completion

Nonlinear dimensionality reduction schemes approximate distances on underlying manifolds and embed higher dimensional data into low dimensional representations. However, approximated geodesic distances on manifolds involve high error at far apart points. Thus, we rely on nearby geodesic distances and treat far apart geodesic distances on the manifold as unknowns. We formulate the distance matrix (D) of geodesics on the manifold such that it has missing entries for far apart points. Then, we utilize Matrix Completion (MC) techniques with extra constraints to recover this corrupted distance matrix. These extra constraints assure that the inner product matrix corresponds to the distance matrix is positive semi-definite. MC assures that the recovered D is low rank, thus the singular value decomposition of recovered D provides the low dimensional representation of the data. We validate the performance of this approach using synthetic datasets.

Kelum Gajamannage, Randy Paffenroth
Worcester Polytechnic Institute
kdgajamannage@wpi.edu, rcpaffenroth@wpi.edu

CP1

Sobol' Indices for Correlated Variables

When performing global sensitivity analysis (GSA), it is often assumed, for the sake of simplicity, for lack of information, or for sheer expediency, that uncertain variables in the model are independent. It is intuitively clearand easily confirmed through simple examplesthat applying a GSA method designed for independent variables to a set of correlated variables generally leads to results that hard to interpret, at best. We generalize the probabilistic framework for GSA pioneered by Sobol to problems with correlated variables; this is done by reformulating his indices in terms of approximation errors rather than variance analysis. The implementation of the approach and its computational complexity are discussed and illustrated on synthetic examples.

Joseph L. Hart
North Carolina State University
jlhart3@ncsu.edu

Pierre Gremaud
Department of Mathematics
North Carolina State University
gremaud@ncsu.edu

CP1

Quantifying Uncertainty in Reduced Models for Discrete Fracture Networks

Reduced modeling is becoming increasingly necessary to yielding fast results for complicated, expensive models. Although many models rely on a similar modeling methodology for reduction, ie taking a matrix system and reducing it while maintaining of the same properties as the larger system, there are other avenues. A large-scale computational model for transport was developed at Los Alamos National Laboratory that uses discretized meshes for the forward solution. A reduced model was created using graph networks to simplify the problem. We propose to model the uncertainty in quantities of interest, such as pressure, by using the graph model. We propose to test our uncertainties against well-established results of the high-fidelity model as proof of trust for use in larger and unknown transport problems.

Jaime A. Lopez-Merizalde
TULANE UNIVERSITY
jlopez8@tulane.edu

CP2

Image Segmentation and its Effects on Patient Specific Fluid Modeling

Patient specific models of hemodynamics are important in analyzing and understanding the progression of cardiovascular disease. Medical imaging is often used to obtain a patient specific geometry, which creates a more accurate domain for the model. Segmentation techniques, such as global thresholding, are not perfect and introduce uncertainty into the geometric parameters that guide model prediction. This talk focuses on the propagation of geometric uncertainty into a one-dimensional (1D) fluid dynamical model in a network of pulmonary blood vessels. Micro-CT images from C57BL6/J mice (Jackson Laboratory, Bar Harbor, ME) pulmonary networks are segmented and skeletonized to give vessel centerlines and radius estimates. Each terminal vessel is connected to a three element windkessel. The segmentation parameters used in the initial stages of this process ultimately affect the estimated length and radius of each vessel, which then propagates to nominal estimates of model and boundary condition parameters. This shows that model parameters and predictions are sensitive to the measured geometry used for the model.

Mitchel J. Colebank, Muhammad U. Qureshi

North Carolina State University
mjcoleba@ncsu.edu, muquresh@ncsu.edu

Naomi Chesler
University of Wisconsin, Madison
chesler@engr.wisc.edu

Laura Ellwein
Virginia Commonwealth University
lellwein@vcu.edu

Mette Olufsen
North Carolina State University
msolufse@ncsu.edu

CP2

Evaluating Dosimetric Changes Caused by Positional Errors of Savi Applicator used for Breast Cancer Treatment

Breast cancer is the most frequently detected cancer in women in developed countries and is generally diagnosed with women while rarely in men. The research focused on High-Dose-Rate Brachytherapy technique that is an accepted and effective internal radiation to reduce the number of malignant tumor cells. This research investigated the effects of dosimetric changes which are depend upon geometric positioning errors of the radiation source dwell positions. This technique is done by implanting a SAVI applicator to daily deliver a prescribed dose twice for five days. Prior to each administration of the radiation, the SAVI implanted device is inspected to ensure that there is no change such as rotational or translational offset. Source positional errors can typically cause enormous positional changes of the radiation source inside the SAVI catheters which can result in an inaccurate radiation dose. Usually, the inspection of applicator insertion is achieved by CT scan or other imaging devices. It falls into the clinicians and staffs to determine if the changes are clinically significant enough to warrant re-planning the radiation treatment. These changes were compared with previous patients data. Dose Volume Histogram (DVH) has been used to extract the results and evaluate the delivered doses in different organs close to breast tissues. According to the NASBP PROTOCOL B-39, the maximum dose of skin, chest wall, PTV EAVL for V90, V100, V150 and V200 will be evaluated.

Abbas M. Jammali
Ball State University
amjammali@bsu.edu

Andrew Bergan
Ball Memorial Hospital
abergan@iuhealth.org

CP2

The Influence of Tear Supply and Drainage on Tear Film Dynamics During a Realistic Blink

We simulate the tear film dynamics on a realistic blinking eye-shaped domain to examine the influence of the tear supply and drainage on the tear dynamics. During a blink, tear fluid supplied from the lacrimal gland is distributed from the upper meniscus region onto the ocular surface to form a stable tear film, and tear fluid is drained through the puncta and into the nose. Because the current state-of-the-art instrumentation does not yet have the capability to image the tear film thickness over the entire front of the eye during the blinks, especially near lids, it is not fully understood how the tear supply and drainage impacts the tear film formation, and thus subsequent tear film thinning during the interblink. Using video of a blinking eye, we create a realistic moving eye-shaped domain by fitting the computational boundary curves to lid margins in the video. The evolution equation of the tear film thickness is derived using lubrication theory and includes the effects of viscosity and surface tension. By implementing a moving overset grid method, we examine how different models of tear supply and drainage, linked to lid motion and lid speed, affect the tear formulation and subsequent tear film breakup times. Our results are compared with prior modeling results and experimental observations.

Kara L. Maki
School of Mathematical Sciences
Rochester Institute of Technology
kmaki@rit.edu

Emily Kiesel
Rochester Institute of Technology
emily.kiesel57@gmail.com

William Henshaw
Rensselaer Polytechnic Institute
wdhenshaw@gmail.com

Alex McManus
Rochester Institute of Technology
atm3702@g.rit.edu

Richard Braun
University of Delaware
rjbraun@udel.edu

Tobin Driscoll
University of Delaware
Mathematical Sciences
driscoll@udel.edu

CP2

Anomalous Diffusion on a Growing Domain

Subdiffusive transport has been observed in many physical and biological systems leading to intensive efforts to provide robust theoretical models for this phenomena. Additionally many physical and biological phenomena occur on domains which evolve with time. We have derived a diffusion equation, using a continuous time random walk, for particles on a domain that grows with time. This allows us to construct models that represent physical and biological systems which incorporate both diffusion and a domain that is growing. The resulting equations feature fractional derivatives. The implementation of the master equation is illustrated with a simple model of subdiffusing proteins in a growing membrane.

Anna V. Mcgann
UNSW
a.mcgann@unsw.edu.au

CP2

Information Flow Analysis of Genetic Regulatory Systems

We made a mathematical model of genetic regula-

tory system across multiple omics layers as a directed acyclic Bayesian network [Touchette H, Lloyd S (2000) Information-theoretic limits of control. Phys. Rev. Lett. 84:1156.]. We conducted formula analyses on the model and found loss of a control capability concurrent with loss of the mutual information among the controlled variable and the feedback signal under environmental stimuli which is similar to the observation reported in our previous work [Sakata K, Saito T, Ohyanagi H, Okumura J, Ishige K, Suzuki H, Nakamura T, Komatsu S (2016) Loss of variation of state detected in soybean metabolic and human myelomonocytic leukaemia cell transcriptional networks under external stimuli. Sci Rep. 6: 35946.]. In order to validate the model, we performed numerical experiments about a well-studied genetic regulatory system with coupled expression of regulator and effector genes [Hlavacek WS, Savageau MA (1996) Rules for coupled expression of regulator and effector genes in inducible circuits. J Mol Biol. 255:121-139.] using multiple set of system parameters including directly coupled, uncoupled, or inversely coupled patterns for both the negatively and positively controlled systems. In this talk, we will introduce the modeling and formulation, and demonstrate the numerical experiments.

Katsumi Sakata
Maebashi Institute of Technology
ksakata@maebashi-it.ac.jp

Toshiyuki Saito
NIRS
saito.toshiyuki@qst.go.jp

Hajime Ohyanagi
KAUST
hajime.ohyanagi@kaust.edu.sa

Sho Asahi, Daiki Sato, Yuta Morikawa
Maebashi Institute of Technology
m1461001@maebashi-it.ac.jp,
m1461020@maebashi-it.ac.jp,
m1461044@maebashi-it.ac.jp

Setsuko Komatsu
University of Tsukuba
komatsu.setsuko.fu@u.tsukuba.ac.jp

CP2

Controlling Period-2 Electrical Activity in a Cardiac Cell Model

This study focused on the control of a dynamic behavior called alternans, exhibited by cells responding to stimuli. Electrical alternans, the beat-to-beat alternations of cellular action potentials and/or intracellular calcium concentration, is a state that precedes life-threatening arrhythmia. Arrhythmia is characterized by irregular propagation of electrical waves and is the leading cause of sudden cardiac death. Previous efforts at alternans control have utilized mathematical models that primarily exhibited voltage-driven alternans; we considered the impact of intracellular calcium mechanisms. We used the Shiferaw-Fox et al. cardiac action potential model [Coupled dynamics of voltage and calcium in paced cardiac cells], which is capable of both voltage- and calcium-driven alternans, for single cells (0D) and cables of cells (1D). Control schemes were applied to four different combinations of driving mechanisms. The control schemes include a constant-diastolic-interval(DI) method, a voltage-feedback method, a calcium-feedback method, and an early-stimulus method. The results showed differences depending on the alternans mechanism; calcium-driven alternans were more difficult to control. In 0d, the calcium-feedback method eliminated alternans regardless of driving mechanism. In 1D, the voltage-feedback and constant-DI methods showed the most promise. The results indicate that the success of control of cardiac alternans may depend on the underlying alternans mechanism.

Mariya A. Savinov
University of Pittsburgh
Department of Mathematics
masha@pitt.edu

Elizabeth M. Cherry
Rochester Institute of Technology
School of Mathematical Sciences
excsma@rit.edu

Daniel Olszewski
Carroll College
dolszewski@carroll.edu

CP2

M-current Expands the Range of Gamma Frequency Inputs to which the Target Entrains

Theta (4 Hz - 8 Hz) and gamma (30 Hz - 80 Hz) rhythms in the brain are commonly associated with memory and learning [Kahana 2006, Quilichini et al. 2010]. The precision of co-firing between neurons and incoming inputs is critical in these cognitive functions. We consider an inhibitory neuron network with M-current under forcing from gamma pulses and a sinusoidal current of theta frequency. The M-current has a long time constant ($\sim$ 100 ms) and it has been shown to contribute to theta rhythms [Hu et al. 2002]. We have found that, in our model, a slow M-current contributes to the precise co-firing between the network and fast gamma pulses in the presence of a slow sinusoidal forcing. It expands the phase-locking frequency range of the network, counteracts the slow theta forcing, and admits bistability in some parameter range. The balancing between the M-current and the theta forcing cannot be observed if the sinusoidal current is faster than the theta frequency band. We characterize the dynamical mechanisms underlying the role of the M-current in enabling a network to be entrained to gamma frequency inputs using averaging methods, geometric singular perturbation theory, and bifurcation analysis.

Yujia Zhou
Boston University
zhouy@bu.edu

Theodore Vo
Department of Mathematics
Florida State University
vo@math.fsu.edu

Michelle McCarthy
Department of Mathematics and Statistics
Boston University
mmccart@bu.edu

Nancy Kopell
Boston University
Department of Mathematics

nk@bu.edu

CP3

Multiwavelet Design by Matrix Spectral Factorization

Given a multiscaling function with symbol $H(z)$, its lowpass product filter has the symbol $P(z) = H(z)H(z)^*$. We are interested in finding $H(z)$, given a $P(z)$ with desirable features. Unfortunately, desirable $P(z)$ cause numerical problems with the factorization algorithm. I will describe the setup of the problem, and various attempts to speed up its convergence and improve accuracy.

Fritz Keinert
Dept. of Mathematics
Iowa State University
keinert@iastate.edu

CP3

Green's Function Estimation and Correction from Strain Rate Measurements of Random Seismic Noise

By recording controlled vibration sources on a seismic sensor array, we can calculate maps of subsurface seismic velocities, but this can be expensive and logistically difficult in populated areas, so continuous subsurface monitoring is rare. We combine two methods to make frequent subsurface imaging cheaper: estimating wave equation Green's functions by cross-correlating random vibration recordings in the area of interest, and measuring vibrations as meter-scale strain rate profiles along standard fiber optic cables. Most seismic processing assumes scalar pressure or vector particle velocity data, but with fiber we measure one component of strain rate, a tensor quantity. In earthquake records we see that events are detected at the right time, but fiber data look qualitatively different from traditional particle velocity measurements. We explain how the switch from vector to tensor quantities leads to these changes. When we cross-correlate ambient noise recorded along collinear subsets of fiber, results are similar to those from velocity data. When the fiber segments are not collinear, we predict that extracted signals travel at a faster apparent velocity than the true medium velocity. We verify predictions with computational modeling and show examples from real fiber optic array data sets. From our understanding of this change from velocity to strain rates, we propose a correction to our estimated Greens function arrival times which can then be used for tomographic imaging.

Eileen R. Martin
Stanford University, Lawrence Berkeley National Lab
ermartin@sep.stanford.edu

Nate Lindsey
UC Berkeley
Lawrence Berkeley National Lab
natelindsey@berkeley.edu

Jonathan Ajo-Franklin
Lawrence Berkeley National Lab
jbajo-franklin@lbl.gov

Biondo Biondi
Geophysics Department
Stanford University
biondo@sep.stanford.edu

CP3

The Boykov-Kolmogorov Algorithm and the Three-label Problem in Liver Image Segmentation

While advancements have been made in recent decades in liver image segmentation, leading to improvements in diagnosis, planning, and assessment, it is still a challenging task due to complex image backgrounds, fuzzy boundaries, and variation among livers. In this talk, we propose a new model that starts with scalar pixels and then associates a vector with each pixel through various convolutions. We will discuss the development of an energy functional for our three-label problem and the solutions obtained using the Boykov-Kolmogorov min-cut max-flow algorithm and a gradient descent method for finding the approximate energy-minimizing segmentation.

Enrique Alvarado, Yufeng Cao, Yunfeng Hu, Michael Newsham, Laramie Paxton, Kevin R. Vixie, Yuan Wang
Washington State University
ealvarado9611@gmail.com, ycao1@hotmail.com, yunfeng.hu90@gmail.com, mike.newsham6@gmail.com, realtimemath@gmail.com, vixie@speakeasy.net, yuan.wang.stat@gmail.com

CP3

3D Image Reconstruction from Spect Compton Camera Data

In this talk, we describe the mathematical features of Compton camera imaging and the corresponding cone transform. We will present variety of inversion formulas that use overdetermined data and allow large flexibility on the geometry of detectors and relevant weight functions. They are, in particular, applicable for reconstructing from SPECT Compton camera data.

Fatma Terzioglu
Texas A&M University
fatma@math.tamu.edu

Peter Kuchment
Department of Mathematics, Texas A&M University
USA
kuchment@math.tamu.edu

Leonid A. Kunyansky
University of Arizona
Department of Mathematics
leonk@math.arizona.edu

CP3

Imagery Analysis to Investigate Oyster Reef Pattern Formation and the Interaction of Reefs with Hydrodynamics

Due to the collapse of the Eastern oyster population over the last century and its ecological and economic consequences, oyster restoration becomes of critical importance. We investigate historic oyster reefs that still remain in the Chesapeake Bay and the surrounding areas to gain insight into oyster reef morphology, and how morphology is shaped by underlying hydrodynamics, bathymetry, nutrient concentration and other factors. Two types of oyster reef imagery are available to us: aerial (used for intertidal reefs) and sonar (used for subtidal reefs). For the multispectral

aerial imagery, more conventional image classification techniques can be used, while the same methods will not be adequate for the grey-scale sonar imagery. Two main classification approaches are discussed in this talk: supervised image classification for aerial imagery and texture analysis for sonar imagery. The classified imagery will later be used to cluster the reef structures into meaningful groups in hopes of uncovering new possible reef configurations beyond what has been observed to date. The classified imagery will then be analyzed in a GIS data model to correlate reef geometry with flow, bathymetry and chlorophyll concentrations. The ultimate goal is to have a better understanding of reef morphology and inform oyster restoration efforts in determining suitable locations and configurations of artificial oyster reefs to maximize their success.

Sofya Zaytseva
The College of William and Mary
szaytseva@email.wm.edu

Leah Shaw
College of William and Mary
lbshaw@wm.edu

Rom Lipcius
Virginia Institute of Marina Science
rom@vims.edu

Donglai Gong
Virginia Institute of Marine Science
gong@vims.edu

David Bruce, Jay Lazar
NOAA Federal
david.bruce@noaa.gov, jay.lazar@noaa.gov

CP4

High-dimensional Sparse Fourier Transforms

We discuss the development of high-dimensional sparse Fourier transforms(SFT). In "Adaptive Sublinear Time Fourier Algorithm" by D. Lawlor, Y. Wang and A. Christlieb (2013), an efficient algorithm with $O(k \log k)$ runtime and $O(k)$ sampling complexities on average was developed for signals of bandwidth N, where k is the number of significant modes such that $k \ll N$. In this work we develop efficient algorithms for high-dimensional SFT for higher dimensional signals, extending some of the ideas in the paper mentioned above. Note a higher dimensional signal can always be unwrapped into a one dimensional signal, but when the dimension gets large, unwrapping a higher dimensional signal into a one dimensional array is far too expensive to be realistic. Our approach here introduces two new concepts: "partial unwrapping' and "tilting'. These two ideas allow us to efficiently compute the SFT of higher dimensional signals. Moreover, the measurements of signals often contain noise, and some signals are well approximated by a few Fourier modes. Accordingly, we propose a multiscale SFT for noisy samples which gradually improves the estimate of energetic Fourier frequencies in an entry-wise fashion when the noise is assumed to be not overwhelming.

Bosu Choi, Andrew Christlieb
Michigan State University
choibosu@math.msu.edu, christli@msu.edu

Yang Wang
Hong Kong University of Science and Technology
yangwang@ust.hk

CP4

Emergence of Heavy-tailed Skew Distributions from the Heat Equation

It is well known that the symmetric Gaussian function, called the fundamental solution, serves as the Green's function of the heat equation. In reality, on the other hand, distribution functions obtained empirically often differ from the Gaussian function. This study presents a new solution of the heat equation, satisfying localized initial conditions like the Gaussian fundamental solution. The new solution corresponds to a hetero-mixture distribution, which generalizes the Gaussian distribution function to a skewed and heavy-tailed distribution, and thus provides a candidate for the empirical distribution functions.

Byoungseon Choi
Department of Economics, Seoul National University
bschoi12@snu.ac.kr

Hyuk Kang
National Institute for Mathematical Sciences
Korea
glorious2076@gmail.com

M.Y. Choi
Department of Physics and Astronomy and Center for Theoretic
Seoul National University
mychoi@snu.ac.kr

CP4

High-order Imposition of Neumann Boundary Conditions for AES-FEM and GFD

Imposing Neumann boundary conditions can be challenging for both the finite element methods (FEM) and generalized finite difference (GFD) methods, especially for high-order methods. For FEM, it is very difficult to guarantee a good quality mesh when using high-order elements. For GFD, a normal vector at a corner or a ridge is not defined, and it may be unclear how to satisfy multiple boundary conditions meeting at a single point. We present a new approach to impose Neumann boundary conditions by introducing a new test function, whose support is contained only within the boundary of the domain. This type of test function can be used with the Adaptive Extended Stencil Finite Element Method (AES-FEM) or with GFD. AES-FEM is a generalization of the finite element method that is insensitive to mesh quality. It replaces the traditional basis functions with generalized Lagrange polynomial basis functions, which are computed using weighted least squares. It can achieve high-order accuracy using linear elements. For AES-FEM, our new approach allows using only high-order surface elements in conjunction with linear volumetric elements, which eases mesh generation. For GDF, our approach enables more robust imposition of Neumann boundary conditions at corners, where normals may be ill-defined. Numerical results demonstrate the high-order convergence of AES-FEM and GFD for 2D and 3D elliptic PDEs.

Rebecca Conley
Saint Peter's University
rconley@saintpeters.edu

Tristan Delaney, Xiangmin Jiao
Stony Brook University

tristan.delaney.88@gmail.com, xiangmin.jiao@stonybrook.edu

CP4

Existence of a Unique Solution to an Elliptic Equation with Data at an Interior Point

We consider the elliptic partial differential equation $-\nabla \cdot (a(u)\nabla u) = f - \frac{1}{|\Omega|}\int_\Omega f d\mathbf{x}$ for $\mathbf{x} \in \Omega$, subject to the condition $u(\mathbf{x}_0) = u_0$ at a given point $\mathbf{x}_0 \in \Omega$, and under the boundary condition $\mathbf{n}(\mathbf{x}) \cdot \nabla u(\mathbf{x}) = 0$ for $\mathbf{x} \in \partial\Omega$, where $\mathbf{n}(\mathbf{x})$ is the outward unit normal vector. The domain Ω is a bounded, connected, open set with a smooth boundary $\partial\Omega$. We prove the existence of a unique, classical solution $u(\mathbf{x})$. The key to the proof lies in obtaining a priori estimates for u.

Diane Denny
Texas A&M University - Corpus Christi
diane.denny@tamucc.edu

CP4

Iterated Circular Convolutions in the Binomial Options Pricing Model

This work was inspired by the observation that iterated circular convolutions can be used to express the martingale pricing algorithm in the binomial options pricing model. We use discrete Fourier analysis in this context of iterated circular convolutions to derive analytical results that could prove useful for fast real-time options pricing on algorithmic trading platforms, as well as for a deeper theoretical understanding of no-arbitrage options pricing in terms of the inverse Fourier transform of the terminal option payoff, and the Fourier transform of a special weight vector built from the risk-neutral probabilities. This work is a direct application of a surprisingly similar problem in geometry that we have investigated in the context of limiting forms of iterated circular convolutions of random skew polygons in higher-dimensional Euclidean spaces.

Boyan Kostadinov
NYC College of Technology, CUNY
NYC College of Technology, CUNY
bkostadinov@citytech.cuny.edu

CP4

Top-down Approach for ESO Portfolio Valuation under Stochastic Exercise Intensity

We present a top-down model to value multiple employee stock options (ESOs) under a stochastic exercise intensity that depends on the underlying stock price and number of options exercised. We derived the associated PDEs and solve them numerically using finite difference method (FDM), fast Fourier transform (FFT), and maturity randomization, respectively. Among our results, we find that with stochastic intensity the ESO cost increases sublinearly with respect to the number of options.

Yang Zhou
Department of Applied Mathematics
University of Washington
yzhou7@uw.edu

Tim Leung
University of Washington
timleung@uw.edu

CP5

The Vicodin Abuse Problem: A Mathematical Approach

The prescription opioid epidemic in the United States has gained attention in recent years. Vicodin is the country's mostly widely prescribed pain reliever, and it contains a narcotic component that can lead to physical and chemical dependency. The majority of Vicodin abusers were first introduced via prescription, unlike abusers of other drugs, who often initially experience the drug due to experimentation. Most abusers report obtaining their supply from a prescription, either their own or someone else's. Although the problem with prescription drug abuse is well known, there is no standard method of addressing the problem. To better understand how to do this, we develop and analyze two mathematical models of Vicodin use and abuse, considering only those patients who were initially prescribed the drug. Through sensitivity analysis, we show that focusing efforts on abuse prevention rather than treatment has greater success at reducing the population of Vicodin abusers. We further show that in our nonlinear model, the parameters associated with treatment have no effect, while the rate at which abusers seek treatment has a measurable effect in both the linear and nonlinear models. Our results demonstrate that relying solely on rehabilitation and other treatment programs is not enough to combat the prescription opioid problem in the United States. We anticipate that implementing preventative measures in both prescribers and patients will reduce the number of Vicodin abusers.

Wendy K. Caldwell
Los Alamos National Laboratory
Arizona State University
wkcaldwell@lanl.gov

CP5

Modeling Nonconvex Dose-volume Constraints for Radiation Therapy

Fluence map optimization for intensity-modulated radiation therapy treatment planning can be formulated as a large-scale inverse problem with various constraints. Unfortunately, the clinically relevant dose-volume constraints are nonconvex, adding an extra layer of difficulty to the problem. We propose a new nonconvex relaxation for handling dose-volume constraints that is amenable to efficient algorithms based on partial minimization. We present treatment plans obtained using this approach, including examples where our formulation naturally adapts to handle maximum constraints and cases of infeasibility.

Kelsey Maass, Aleksandr Aravkin
University of Washington
kmaass@uw.edu, saravkin@uw.edu

Minsun Kim
Department of Radiation Oncology
University of Washington School of Medicine
mk688@uw.edu

CP5

Modeling Ertapenem: Dosing of the Antibiotic in

Children

Ertapenem is an antibiotic commonly used to treat a broad spectrum of infections. Previously, a physiologically-based pharmacokinetic model was developed to investigate the uptake, distribution, and elimination of ertapenem following a once-a-day, single one gram dose in men and women with varying body mass index. This model has been modified to consider children ages 3 months to 17 years who were given different doses of the antibiotic based on their age and weight. Parameters in the model that were not available in the literature were estimated using an iterative weighted least squares algorithm with published data for blood concentrations of ertapenem in children. Simulations were performed to consider the distribution of the antibiotic in male and female children of differing ages and weights who were given different doses. These results could help to determine possible best dosing regimens for children in the future.

Cammey Cole Manning
Meredith College
ManningC@meredith.edu

Michele Joyner
East Tennessee State University
joynerm@mail.etsu.edu

CP5

Binarization of Spontaneous Neural Activities for Neural Ring Analysis

Typical electrophysiological experiments in neuroscience examine the neural responses to sensory stimuli. That is, within the stimulus-response framework, how accurately the neural responses reflect the sensory stimuli has been characterized information theoretically. However, it is not necessarily clear if the neural responses actually responded only to the sensory stimuli the experimenters presented. For example, the neurons can actually respond to some hidden variables of which the experimenters are unaware. So, it is desirable to know in advance how much dimensions the hidden stimulus space for a neuron spans. For that purpose, the systematic method of neural ring was proposed recently. This novel, algebraic geometry-based method could uncover the information which conventional methods like PCA neglected. Here we applied the neural ring method to the spontaneous neural activities in rat hippocampus. The issues here can be that the real data is considerably noisy and that there are many possible ways to binarize the data so that the neural ring is applicable. By trying different styles of binarization, we discovered that some aspects of results are stable and did not change significantly. This suggests that, with the appropriate use, the neural ring can be a reliable data analysis method for obtaining stable biological conclusions.

Keiji Miura
Kwansei Gakuin University
miura@kwansei.ac.jp

CP5

Modeling the Heroin Epidemic

A preliminary report will be given on the formulation of a heroin epidemic model. This model, consisting of a system of ordinary differential equations, aims to better understand the dynamics between regular prescription opioid use, opioid addictive use, heroin use and treatment.

Tricia Phillips, Christopher Strickland
University of Tennessee, Knoxville
tphill30@vols.utk.edu, cstric12@utk.edu

Suzanne M. Lenhart
University of Tennessee and
National Institute for Mathematical and Biological Synthesis
slenhart@utk.edu

Nicholas Battista
College of New Jersey
battistn@tcnj.edu

Leigh Pearcy
University of North Carolina, Chapel Hill
leighbp@live.unc.edu

CP5

Modelling the Effect of Mucin Binding in the Gut on Drug Delivery

An important part the absorption, distribution, metabolism and excretion (ADME) of an oral therapeutic is the flux rate of drug compound crossing the mucus lining of the gut. To understand this part of the absorption process we develop a mathematical model of advection, diffusion and binding of drug compounds within the mucus layer of the intestines. Analysis of this model yields simple, measurable criteria for the successful mucin layer traversal of drug compound.

Jeffrey S. Saltzman
Cottonwood Applied Mathematics
jeffsaltzman@cottonwoodam.solutions

CP6

Monitoring Depth Profile of Residual Stress via Rayleigh-wave Dispersion

In this talk, the inverse problem is to investigate the possibility of using Rayleigh waves to monitor the retention of the protective prestress during the lifetime of a structural component. The solution of the inverse problem is based on the direct problem to determine dispersion curves for Rayleigh waves propagating in various directions when the material parameters, texture coefficients, and initial stresses are given. We can infer the depth profiles of the residual stresses which are good approximations to the real ones.

Yue Chen
Louisiana State University
ychen5@aum.edu

Chi-Sing Man
University of Kentucky
cman@uky.edu

Kazumi Tanuma
Gunma University
tanuma@gunma-u.ac.jp

Christopher Kube
U.S. Army Research Laboratory
Aberdeen Proving Ground

ckube@huskers.unl.edu

CP6

A Comparison of Higher Order Regularization Operators Applied to Inverse Geosounding

Tikhonov's regularization method is the standard technique applied to obtain models of the subsurface conductivity distribution from electric or electromagnetic measurements. $U_T(m) = \|F(m) - d\|^2 + \lambda P(m)$. The second term correspond to the stabilizing functional, with $P(m) = \|\nabla m\|^2$,the usual approach and λ the regularization parameter. Due to the roughness penalizer inclusion, the model developed by Tikhonovs algorithm tends to smear discontinuities, a feature that may be undesirable. An important requirement for the regularizer is to allow the recovery of edges, and smooth the homogeneous parts. As is well known, Total Variation (TV) is now the standard approach to meet this requirement. Recently, Wang et.al. proved convergence for alternating direction method of multipliers in nonconvex, nonsmooth optimiza- tion. In this talk we present a study of several algorithms for model recovering of Geosounding data based on Infimal Convolution, and also on hybrid, TV and second order TV and nonsmooth, nonconvex regularizers, observing their performance on synthetic and real data. The algorithms are based on Bregman iteration and Split Bregman method, and the geosounding method is the low-induction numbers magnetic dipoles. Non-smooth regularizers are considered using the Legendre-Fenchel transform.

Hugo Hidalgo-Silva
CICESE-Ciencias de la Computacion
hugo.cicese@gmail.com

Enrique Gómez-Treviño
CICESE
egomez@cicese.mx

CP6

Solving Inverse Problems using Machine Learning

With data proliferation in all geosciences domains, machine learning and data analytics are emerging as important research areas in geosciences. Inverse problems have been important tools to infer the subsurface based on various geophysical measurements. However, inverse problems in geosciences are usually ill-posed due to the poor data coverage, and not to mention their expensive computational costs. In this talk, we developed novel machine learning techniques to solve traditional inverse problems, and further apply to infer and characterize subsurface structure using seismic data. We show that our novel machine learning methods can not only accurately estimate the subsurface parameters of interest, but also yield rather high efficiency. Therefore, our machine-learning-based inverse problems solution has great potential in various applications.

Youzuo Lin
Los Alamos National Laboratory
ylin@lanl.gov

CP6

Fast Algorithms for Inverse Transport Problems

We will discuss the formulation and design of fast solvers for inverse transport problems. The applications that motivate this work are in medical imaging sciences. We will consider a PDE-constrained formulation, where the PDE constraints are the transport equations for image intensities or, more generally, densities (state variable). The control variable is the velocity field. We will see that the optimality systems are complex, multiphysics operators that pose significant numerical challenges. We will discuss an effective Newton–Krylov scheme for the solution of the optimization problem. This solver has been designed to scale on supercomputing platforms. It allows us to solve problems of unprecedented scale (200 billion unknowns) and paves the way to tackle real-time applications. We will study numerical accuracy, rate of convergence, quality of the inversion, and scalability of our solver on synthetic and real-world data.

Andreas Mang
The University of Texas at Austin
The Institute for Computational Engineering and Sciences
andreas@math.uh.edu

CP6

A Convexification Method for Coefficient Inverse Problems for the Wave Equation

In this talk we consider the problem of reconstructing the refractive index of a medium using electromagnetic waves. In the time-domain, the 1-d model is described by the following equation

$$c(x)\, u_{tt} = u_{xx} + \delta(x - x^0),\ (x,t) \in \mathbf{R} \times (0,\infty), \quad (1)$$
$$u(x,0) = 0, u_t(x,0) = 0. \quad (2)$$

where $c(x)$ represents the refractive index of the medium and x^0 is a given point in $\mathbf{R}$ representing the source location. The frequency-domain model is represented by a Helmholtz equation. Assume that $0 < c_0 \leq c(x) \leq 1 + d, c(x) = 1, \forall x \notin (0,b)$ with given positive constants c_0 and d. The inverse problem to be discussed here is to reconstruct $c(x),\ x \in (0,b)$, from the measurement of the wave function at $x = 0$ for $t \in (0,\infty)$ for the time-domain problem or at multiple frequencies for the frequency-domain problem. In this talk, we discuss a convexification method for solving this inverse problem. The key idea of the method is to construct a Carleman weighted objective functional which can be proved to be globally convex. This method works for both time-domain and frequency-domain models. The performance of this method is demonstrated with numerical results.

Thanh Nguyen
Rowan University, Department of Mathematics
nguyent@rowan.edu

Michael Klibanov
University of North Carolina at Charlotte
mklibanv@uncc.edu

CP6

Anisotropic Functional Laplace Deconvolution

In the present paper we consider the problem of estimating a three-dimensional function f based on observations from its noisy Laplace convolution. Our study is motivated by the analysis of Dynamic Contrast Enhanced (DCE) imaging data. We construct an adaptive wavelet-Laguerre estimator of f, derive minimax lower bounds for the L2-risk when f belongs to a three-dimensional Laguerre-Sobolev ball and demonstrate that the wavelet-Laguerre estimator is adaptive and asymptotically near-optimal in a wide

range of Laguerre-Sobolev spaces. We carry out a limited simulations study and show that the estimator performs well in a finite sample setting. Finally, we use the technique for the solution of the Laplace deconvolution problem on the basis of DCE Computerized Tomography data. Key words: Laguerre functions basis, wavelets, Laplace deconvolution, DCE imaging

Rasika U. Rajapakshage
University of Central Florida
udara@knights.ucf.edu

Marianna Pensky
Department of Mathematics, University of central florida
marianna.pensky@ucf.edu

Rida Benhaddou
Department of Mathematics, Ohio University
benhaddo@ohio.edu

CP7

Enhanced Electroosmotic Flow and Ion Selectivity Through a Patterned Groove Nanochannel with Charge Regulated Groove Polymer Segments

Electroosmotic flow through a soft nanochannel has shown great applications such as manipulation of ion transport, developing nanofluidic and nano ionic valves and many more. In recent years, several authors studied the electroosmotic flow (EOF) through a soft nanochannel. This article deals with the modulation of electroosmotic flow through a periodic groove nanochannel where the grooves are filled with polyelectrolyte layer (PEL). The PEL of the grooves is containing both acidic and basic functional groups. The flat walls and the surface of the grooves channel are assumed to be maintained a constant surface charge density and a zero surface charge density, respectively. A nonlinear model based on the nonlinear Poisson-Nernst-Planck equation coupled with the Darcy-Brinkman equation is adopted. Going beyond the widely employed Debye-Hückel linearization, we adopt a sophisticated numerical tool to study the effect of pertinent parameters in this study. Several interesting key features, including the flow enhancement and occurrence of zero flow rate, are studied by regulating the charges entrapped within the PEL and the surface charge distributed along the flat walls. In addition, we have also demonstrated the selectivity of the mobile ions through this patterned channel. The results indicate that the channel can be cation-selective, an anion-selective as well as non-selective based on the nature of the charges within the PEL and flat walls charge.

Naren Bag
INDIAN INSTITUTE OF TECHNOLOGY KHARAGPUR
narenbag88@gmail.com

Somnath Bhattacharyya
I.I.T. Kharagpur
somnath@maths.iitkgp.ernet.in

CP7

Modeling Tracheal Angioedema for Modified Tissue Stiffness

Tracheal angioedema is a pathology of the airway caused by soft tissue swelling due to fluid leakage from the blood vessels. This pathology can suddenly change the normal tracheal luminal size and cause breathing difficulty for an medical emergency. The extra fluid accumulation inside the tissue can also alter the stiffness of the tissue, and make the luminal size change more complicated. We set up a model using continuum mechanics to understand how the angioedema swelling extent can quantitatively change the trachea luminal size particularly under the tissue stiffness modification. Interestingly, the swelling may not always shrink the tracheal lumen, and may expand it for proper parameter values. This model can assist conducting more appropriate medical treatment for tracheal angioedema.

Kun Gou
Texas A&M University-San Antonio
Department of Science and Mathematics
kgou@tamusa.edu

CP7

Modeling Vas Deferens Smooth Muscle Electrophysiology: Role of Ion Channels in Generating Electrical Activity

The Vas deferens smooth muscle (VDSM) cells contract to direct and propel sperms from the epididymis to the urethra. The coordinated firing of sympathetic nerves causes contraction of the VDSM cells to achieve this transportation task. It is well known that membrane electrical activity, particularly the action potential (AP) is an essential prerequisite for the initiation of contraction in all types of muscle cells. As the coordinated activation of a number of ion channels in the VDSM cell membrane causes AP generation, any mutation or dysfunction of any ion channel will modulate the AP generation and hence the contraction. To explore the quantitative contribution of individual active ionic current to the AP generation, a biophysically based single guinea-pig VDSM cell model is presented. The simulated ionic currents and AP show good agreement with the experimental recordings in terms of several parameters. Therefore, this electrophysiological model can be a preliminary platform to investigate the various electrical properties of VDSM cells in both normal and pathological conditions. In parallel, this model can be extended into the network level in order to establish a more robust and physiologically realistic computational model for the future investigation at the tissue level.

Chitaranjan Mahapatra, Rohit Manchanda
Indian Institute of Technology Bombay
cmahapatra97@gmail.com, rmanch@iitb.ac.in

CP7

Minimal Model of Directed Cell Motility on Patterned Substrates

Cell motility is ubiquitous in biological processes ranging from wound healing to the immune response. The study of actin driven, crawling cells has been of recent interest to biologists and mathematicians alike; even in simple settings cells may exhibit a wide range of motility modes. In particular we investigate the effect of non-homogeneous substrate patterns on the speed and direction of cell motion. We first derive a minimal differential equation model which couples cell velocity, actin distribution, adhesion site density, and substrate deformations. Our model is verified qualitatively against experimental data. By varying the substrate pattern and biophysical parameters of the cell, we subsequently capture varying behaviors. This work suggests a method for directed cell motion and cell sorting on

engineered substrates.

Matthew S. Mizuhara
The College of New Jersey
mizuharm@tcnj.edu

Igor Aranson
Pennsylvania State University
isa12@psu.edu

Leonid Berlyand
Penn State University
Eberly College of Science
lvb2@psu.edu

CP7

Modeling the Effects of Inflammation in Bone Fracture Healing

A new mathematical model is presented to study the early inflammatory effects in bone healing. It consists of a system of nonlinear ordinary differential equations that represents the interactions among macrophages, mesenchymal stem cells, and osteoblasts. A qualitative analysis of the model is performed to determine the equilibria and their corresponding stability properties. There are three equilibria which represent the successful healing, nonunion, and dead tissue. A set of numerical simulations is presented to support the theoretical results. The model is also used to numerically monitor the evolution of a broken bone for different types of fractures and to explore possible treatments to accelerate bone healing by administrating anti-inflammatory drugs.

Imelda Trejo
University of Texas at Arlington
imelda.trejo@mavs.uta.edu

CP7

Effect of Biovariability on Observed Risk of Hearing Loss

Hearing loss impacts about 360 million people worldwide (over 5 percent of the global population). One cause of hearing loss is exposure to loud sounds. We consider the hearing loss injury among subjects in a crowd with a wide spectrum of individual intrinsic injury probabilities due to biovariability. Here biovariability means that subjects in the crowd have their own individual injury probabilities. That is, some subjects are biologically less or more susceptible to hearing loss injury than others. For multiple acoustic impulses, the observed injury risk of a crowd vs the effective combined dose follows the logistic dose-response relation where the injury risk of a crowd is the average fraction of injured. We explore the possibility of interpreting the observed logistic dose-response relation in the framework of biovariability of the crowd. We derive analytically the distribution of individual injury probability that produces the observed logistic dose-response relation and prove that the derived distribution is mathematically a proper density function. Our mathematical analysis implies that the observed logistic dose-response relation can be theoretically explained in the framework of biovariability in the absence of immunity effect.

Hong Zhou
Department of Applied Mathematics
Naval Postgraduate School, Monterey, CA
hzhou@nps.edu

Hongyun Wang
Department of Applied Mathematics and Statistics
University of California, Santa Cruz
hongwang@soe.ucsc.edu

Wesley Burgei
US Department of Defense
Joint Non-Lethal Weapons Directorate
wesley.burgei@usmc.mil

CP8

Hilbert Transform, Quadrature Formulas for the Cauchy Integral in a Semi-axis, and Singular Integral Equations

New quadrature formulas for the Cauchy integral in a semi-infinite interval based on integral relations for the Laguerre polynomials and the confluent hypergeometric function are derived and tested numerically. Bounds for the reminder are obtained. Collocation method for singular integral equations in a semi-infinite interval based on these quadrature formulas is discussed. The quadrature formulas are derived on the basis of the semi-infinite Hilbert transform of the Laguerre polynomials, the confluent hypergeometric function, and the cylindrical functions. A part of these formulas are obtained by exploiting some properties of the Hermite polynomials including their Hilbert and Fourier transforms and connections to the Laguerre polynomials. The relations discovered give rise to complete systems of new orthogonal functions. Free of singular integrals exact and approximate solutions to the characteristic and complete singular integral equations in a semi-infinite interval are proposed. Another set of the Hilbert transforms in a semi-axis are deduced from integral relations with the Cauchy kernel in a finite segment for the Jacobi polynomials and the Jacobi functions of the second kind by letting some parameters involved go to infinity. These formulas lead to integral relations for the Bessel functions. Their application to a model problem of contact mechanics is given.

Yuri A. Antipov
Louisiana State University
Department of Mathematics
antipov@math.lsu.edu

Suren Mkhitaryan
Department of Mechanics of Elastic and Viscoelastic Bodies
National Academy of Sciences, Yerevan, Armenia
smkhitaryan39@rambler.ru

CP8

Zeros of Partial Sums from Combinations of the Exponential

We study the asymptotics and the limiting behavior of the zeros of the polynomials $p_n(z) = As_{an}(\alpha nz) + Bs_{bn}(\beta nz)$ where α, β, A, B are complex numbers and $1 \leq a < b$ are integers. Here $s_n(z) = \sum_{k=0}^{n} z^k/k!$ is the Taylor polynomial of e^z. Our work builds on the classical work of Szegö on $s_n(nz)$ and is related to work of Borwein-Chen-Dilcher on sections of $s_n(nz)$ and Bleher-Mallison on Taylor polynomials of linear combinations of exponentials.

Robert Boyer
Department of Mathematics
Drexel University
rboyer@mcs.drexel.edu

Joseph Erickson
Bucks County Community College
je345@drexel.edu

CP8

A New Construction of Linear Codes Including a Wide Family of MDS Codes

Let Z_p be the finite field of integers modulo p, where $p > 3$ is a prime. This paper presents a new construction of linear codes over Z_p. Based on our construction, linear codes of length $p-1$, include a wide family of MDS- codes. We shall discuss the parameters of the codes defined while describing a generator matrix for the family.

Asiyeh Rafieipour
Ohio University
ar996517@ohio.edu

Majid Mazrooei
University of Kashan
m.mazrooei@kashanu.ac.ir

CP8

Quasiconformal Extension of Meromorphic Univalent Functions with Nonzero Pole

It is well-known that the univalent functions defined in the unit disc that admit a quasiconformal extension to the extended complex plane play an important role in Teichmüller space theory. In this talk we consider meromorphic univalent functions f in the unit disc with a simple pole at $z = p \in (0, 1)$ which have a k-quasiconformal extension to the extended complex plane where $0 \leq k < 1$. We denote the class of such functions by $\Sigma_k(p)$. We first prove an area theorem for functions in this class. Next, we derive a sufficient condition for meromorphic functions in the unit disc with a simple pole at $z = p \in (0, 1)$ to belong to the class $\Sigma_k(p)$. Finally, we also provide a representation formula for functions in $\Sigma_k(p)$ and using this formula we derive an asymptotic estimate of the Laurent coefficients for the functions in this class.

Goutam Satpati
Department of Mathematics, IIT Kharagpur, Kharagpur, West Bengal, India, 721302
gsatpati@iitkgp.ac.in

Bappaditya Bhowmik
Department of Mathematics, Indian Institute of Technology
Kharagpur, India
bappaditya@maths.iitkgp.ernet.in

Toshiyuki Sugawa
Graduate School of Information Sciences, Tohoku University,
Aoba-Ku, Sendai 9808579, Japan
sugawa@math.is.tohoku.ac.jp

CP8

Some General Results in the Theory of Ordinary Fractional Differential Equations

Despite the nowadays widespread use of fractional differential equations, issues concerning the structure of the full set of solutions to fractional ordinary differential equations (fODEs) seems to have been not addressed so far. We will do it, focusing on both, homogeneous and inhomogeneous fODEs.

Renato Spigler
Dipartimento di Matematica, Universita Roma tre.
Rome (Italy)
spigler@mat.uniroma3.it

CP8

Gauss-Hermite vs Trapezoidal Quadrature

For integrals defined on the real line, there are two popular quadrature rules: the trapezoidal rule and Gauss-Hermite quadrature. Which one converges faster? The answer is not so simple because for each of these rules it is possible to map the infinite line to itself with a simple linear transformation, and that introduces free parameters. Only after optimal values of these scaling parameters have been established can one compare the two methods fairly. We investigate this question for the case when the integrand can be extended to a complex analytic function in the neighborhood of the real line.

Andre Weideman
University of Stellenbosch
South Africa
weideman@sun.ac.za

CP9

Networks of Deterministic Spiking Neurons for Label Propagation

Synchronization across large populations of neurons driven by a uniform stimulus has been used to implement label propagation on unstructured data. In this talk, we show how label propagation can be implemented with a set of fully-connected, deterministic leaky-integrate and fire neurons, driven with a sparse set of stimuli and without the use of global inhibitors. Information about strongly connected vertices is extracted from the locally correlated spike trains. We test our approach on graphs of 128 vertices with known community memberships.

Kathleen Hamilton
Oak Ridge National Laboratory
Complex Systems Division
k8hamilton@gmail.com

Neena Imam, Travis Humble
Oak Ridge National Laboratory
imamn@ornl.gov, humblets@ornl.gov

CP9

Sensitivity Analysis of Chaotic Systems using Periodic Shadowing Approximations

The sensitivity of ergodic averages of a hyperbolic chaotic system to parameter perturbations can be determined using the shadowing direction, the unique, uniformly-bounded-in-time solution of the sensitivity equations. A practical approach for finding the sensitivity is the Least-Squares Shadowing (LSS) algorithm (Q Wang, SIAM J Numer Anal 52, 156, 2014), whereby the shadowing direction is approximated by the solution the sensitivity equations with the least average norm. Here, we present an alternative, potentially simpler shadowing-based method, termed Periodic Shadowing (PS). The idea is to obtain a bounded solution of the sensitivity equations by complementing it

with periodic boundary conditions in time. We show that this is not only justifiable when the reference trajectory is itself periodic, but also possible and effective for aperiodic chaotic trajectories. We show that PS has similar convergence rates to LSS, and demonstrate the approach on the Smale-Williams map and on the Lorenz equations. Moreover, as T tends to infinity, PS sensitivities converge to the same value obtained from long unstable periodic orbits (D Lasagna, SIAM J Appl Dyn Syst, In Press). We also examine finite-difference approximations of the sensitivity and show that FD and PS converge to each other for the hyperbolic map, while convergence for the Lorenz system is more subtle, and depends on the system parameters.

Johan Meyers
KU Leuven
Department of Mechanical Engineering
johan.meyers@kuleuven.be

Davide Lasagna, Ati Sharma
University of Southampton
Aerodynamics and Flight Mechanics group
davide.lasagna@soton.ac.uk, a.sharma@soton.ac.uk

CP9

Dynamical Stability Despite Time-varying Network Structure

Dynamic processes on real-world networks are inherently time-delayed due to finite processing speeds, the need to transmit data over distances, or other interruptions in the network's dynamics. These time-delays, which correspond to bisecting edges in the network's underlying graph of interactions, can and often do have a destabilizing effect on the network's dynamics. We demonstrate that networks whose underlying graph of interactions satisfy the criteria which we refer to as *intrinsic stability* are able to maintain their stability even in the presence of time-varying time-delays. These time-varying delays can be of any form, e.g. deterministic, stochastic, etc. Furthermore, determining whether a network is intrinsically stable is straightforward and can be implemented on large-scale networks.

David Reber, Benjamin Webb
Brigham Young University
davidpreber@mathematics.byu.edu,
bwebb@math.byu.edu

CP9

Structural and Functional Robustness in Biological Networks

Several scholars of evolutionary biology have suggested that functional redundancy (also known as biological "degeneracy') is important for robustness of biological networks. Structural redundancy indicates the existence of structurally similar subsystems that can perform the same function. Functional redundancy indicates the existence of structurally different subsystems that can perform the same function. For networks with Ornstein–Uhlenbeck dynamics, Tononi et al. [Proc. Natl. Acad. Sci. U.S.A. 96, 3257–3262 (1999)] proposed measures of structural and functional redundancy that are based on mutual information between subnetworks. For a network of n vertices, an exact computation of these quantities requires $O(n!)$ time. We derive expansions for these measures that one can compute in $O(n^3)$ time. Using these expansions, we study links between information propagation in network motifs and the entropy of the coupled Ornstein–Uhlenbeck process. We compare the contributions of different types of motifs to a network's structural and functional redundancy. We compute structural and function redundancy for protein-interaction networks and find that these networks have larger functional redundancy than corresponding realisations of several random-graph models.

Alice C. Schwarze
Mathematical Institute
University of Oxford
alice.schwarze@dtc.ox.ac.uk

Mason A. Porter
University of Oxford
Mathematical Institute
mason@math.ucla.edu

Jonny Wray
E-Therapeutics plc
jonny.wray@etherapeutics.co.uk

CP9

Noise and Multistability in the Square Root Map

Analysis of recurrent mechanical real-world systems with impacts are often modelled using impact oscillators. Near low-velocity impacts the dynamics of impact oscillators can be described by a one-dimensional map known as the square root map. In this talk we will describe the complex structure of the basins of attraction of stable periodic orbits of the square root map and how this produces sensitivity to the addition of small-amplitude white noise. In particular we focus on the effects of noise of varying amplitudes on the square root map for parameter values that lead to bistability. We will show that there is a nonmonotonic relationship between noise amplitude and the proportion of time spent in each of the two periodic behaviours. The relationship can be explained by comparing approximations of steady-state distributions of trajectory deviations due to noise and the deterministic structures of the map. We will also show that bistability can be induced by the addition of noise of an appropriate amplitude and present the mechanisms behind noise-induced transitions.

Eoghan J. Staunton, Petri T. Piiroinen
School of Mathematics, Statistics and Applied Mathematics
National University of Ireland, Galway
eoghan.staunton@nuigalway.ie,
petri.piiroinen@nuigalway.ie

CP9

Sensitivity Analysis for Dynamical Systems with Optimization Problems Embedded

Sensitivity analysis is presented for dynamical systems with optimization problems embedded. More specifically, parametric sensitivity functions are obtained for differential-algebraic equations (DAEs) with nonlinear programs (NLPs) embedded. The system is rewritten as differential-algebraic equations with optimality criteria (DAEOs), by replacing the NLP with its KKT conditions. The resulting DAEO system exhibits nonsmoothness, because of active set changes in the NLP, but is shown to be well-posed and possesses a sensitivity theory under appropriate regularity assumptions. This is accomplished using recent results in nonsmooth DAEs (including a generalization of the notion of differentiation index) and a generalized sensitivity analysis for NLPs. This theoretical framework

allows for practically implementable methods to be developed, and the sensitivity information furnished from this approach can be supplied to dedicated nonsmooth numerical methods (e.g. equation-solving or local optimization methods). This work has application in systems biology and atmospheric chemistry, where a DAEO system is used to model physical problems with incomplete information (i.e. an underdetermined DAE system).

Peter Stechlinski
Process Systems Engineering Laboratory
Massachusetts Institute of Technology
peter.stechlinski@maine.edu

CP9

Tipping Points in Stochastically Perturbed Filappov Systems

Motivated by a recent energy flux model of Arctic sea ice thickness, this project explores the tipping time of periodically forced, piecewise smooth systems perturbed by weak additive noise. The goal of this study is to determine the most probable time of escape between basins of attraction for two metastable states as a function of the deterministic and stochastic parameters in the problem. For the parameter regimes in which the geometry of the flow clearly partitions the domains of attraction, tipping time can be directly estimated using martingale estimates. In other regimes, because of the piecewise nature of the vector field, the null-clines intersect the unstable limit cycle. Therefore, in these regimes there are sliding regions about the unstable orbit at the discontinuity. Because tipping events are affected by this change in the geometry of the vector field, standard methods for calculating exit time are not sufficient. However, by studying local minimizers of the Onsager-Machlup functional, we provide a framework for calculating the most probable transition paths.

Jessica Zanetell
Wake Forest University
zanej16@wfu.edu

John Gemmer
Wake Forest University
Department of Mathematics and Statistics
gemmerj@wfu.edu

CP10

Dynamics of Discrete-time Host-parasitoid Models

We present a systematic comparison and analysis of a suite of discrete-time host-parasitoid models. These models were selected to compare different combinations of standard functional forms for density dependent growth of the host species and the effects of parasitism. Additionally, we explicitly account for the timing of the density dependence and parasitism in the host life cycle. These models combine simple and well-understood individual components, but these particular combinations yield some unexpected dynamics and rich mathematical behavior. We consider the implications of the dynamics of these models for their use in ecological studies, particularly biological control.

Kelsey Marcinko, Mark Kot
University of Washington
kmar517@uw.edu, mark_kot@comcast.net

CP10

Parameterizing Landscape-level Models of Disease Spread using Incommensurate Data

The study of animal movement is undergoing a revolution due to the boom in availability of individual telemetry data (GPS tracking) and the increase in resolution of remotely-sensed environmental data (landscape classification from satellite imagery). This data is a time series of correlated locations embedded in landscape patches of known type and varying effect on animal movement. A long history of mathematical research describes probabilistic consequences of animal movement using partial differential equations. Solutions, with appropriate initial data, are probability density functions (PDFs) of future locations in a time series of individual telemetry data. Such a PDF can be used in a maximum likelihood estimation procedure to estimate animal movement parameters. The diffusion equation is commonly used but does not allow for variable landscape resistance to movement, spatial aggregation of populations in favorable habitats, or correlation in individual movement. All three are significant for animals like mule deer. The ecological telegrapher's equation (ETE) naturally aggregates populations in preferred habitats and accommodates both correlated movement and variable landscape resistance. We use the ETE to derive a PDF describing individual movement. Using asymptotic techniques and homogenization over short scale variation we find a closed form solution to parameterize a landscape-level population model for mule deer in Southern Utah.

Ian McGahan
Utah State University
ian.mcgahan@aggiemail.usu.edu

James Powell
Department of Mathematics and Statistics
Utah State University
powell@math.usu.edu

Molly Robinson, Thomas Edwards
Utah State University
mollyrob15@gmail.com, t.edwards@usu.edu

CP10

Reducing Mathematical Models for Wolbachia Transmission in Mosquitoes to Control Mosquito-borne Diseases

We create and analyze a reduced model for the spread of a Wolbachia bacteria infection in mosquitoes that can help predict the effectiveness of efforts to control the spread of Zika, chikungunya, dengue fever and other mosquito-borne diseases. Mosquitoes that are infected with some strains of the Wolbachia bacteria are much less effective at transmitting zoonotic diseases. The infection will persist in a wild mosquito population only if the fraction of infected mosquitoes exceeds a minimum threshold. This threshold can be characterized as a backward bifurcation for a system of nine ordinary differential equations modeling the complex vertical transmission of the bacteria infection in a heterosexual mosquito population. Although the large system of differential equations capture the detailed transmission dynamics, they are difficult to analyze. We derive a seven-equation, a four-equation and a two-equation system of differential equations that are formulated in terms of the more accurate nine-equation model and capture the

important properties of the original system. The reduced models preserve key dimensionless numbers, the ratios of infected and uninfected male and female mosquitoes, and accurately capture the backward bifurcation threshold. We use phase plane analysis to fully analyze the reduced model and characterize the sensitivity of the threshold conditions as a function of the full model parameters.

Zhuolin Qu, James Hyman
Tulane University
zqu1@tulane.edu, mhyman@tulane.edu

CP10

Noise Induced Mixed-mode Oscillations in a Singularly Perturbed Predator-prey Model

We study the effect of stochasticity, in the form of Gaussian white noise, in a three species predator-prey model with two distinct timescales. The interactions between the three species is modeled by a system of slow-fast Itô stochastic differential equations. For a suitable parameter regime, the deterministic drift part of the model admits a folded node singularity and exhibits a singular Hopf bifurcation. We transform the stochastic model into its normal form near the folded node, which can be then used to understand the interplay between deterministic and stochastic small amplitude oscillations. The stochastic model admits several kinds of noise driven mixed-mode oscillations that capture the intermediate dynamics between two cycles of population outbreaks of the prey. We perform numerical simulations to study the distribution of the random number of small oscillations between two large oscillations, which can be related to the return time between the outbreaks. Depending on the noise intensity and the distance to the Hopf bifurcation, we find that the distributions of the small oscillations resemble the 1200 years record on the return times of larch budmoth outbreak events in the subalpine larch forests in the European Alps.

Susmita Sadhu
Georgia College and State University
susmita.sadhu@gcsu.edu

Christian Kuehn
Technical University of Munich
ckuehn@ma.tum.de

CP11

Loss of Hyperbolicity in Mixed-type PDEs, with Applications to Geophysics

In a first course on PDEs, it is shown that linear equations can be consistently classified according to the existence of characteristic solutions. In this classification, they can be either hyperbolic, elliptic or parabolic. When it comes to nonlinear PDEs however, this classification does not hold in general as most equations may admit the transition from one type to another: in this case, the equations are called *mixed type*, with examples ranging from geometry to fluid mechanics. In this talk, we will introduce and address this class of equations, highlighting some of the main results and challenges in the area. As an important example, we will formulate and discuss the problem of density stratified interfacial flows in the shallow water limit, a type of flow that occurs in nature with the atmosphere and ocean being prime examples.

Francisco De Melo Virissimo
University of Bath
fdmv20@bath.ac.uk

Paul A. Milewski
Dept. of Mathematical Sciences
University of Bath
p.a.milewski@bath.ac.uk

CP11

An A-stable Method for the 2D Wave Equation Based on the Method of Lines Transpose

In this paper, we will present a high order A-stable scheme based on the method of lines transpose (MOL^T) to solve the high dimensional wave equation. This is based on the previous work of Causley and Christlieb (2014). The previous work relies on an alternating direction implicit (ADI) scheme, while here we employ a dimension-by-dimension strategy. This leads to much simpler implementation of the methods and better computational efficiency. Moreover, the new proposed scheme is superior in dealing with non-periodic boundary conditions. A collection of numerical examples are presented to demonstrate high resolution and robustness of the method.

Pierson Guthrey
Iowa State University
Department of Mathematics
piersonguthrey@gmail.com

CP11

Exploration of Characteristics Governing Dynamics of Whirlwinds: Application to Dust Devils

It is intended to model mathematically an ideal whirlwind which characterizes this geo-physical phenomenon and eventually helps us decode the inherent dynamics. A dense cylindrical aerial mass is taken into consideration surrounding a rarer aerial region in order to keep a radial favorable gradient of pressure to sustain a rotational motion. It has been concluded that the whirlwind will survive as long as the low pressure region exits. The vertical pressure gradient also plays an equally important role. Since it is not connected to any cloud and the axial velocity is in the vertically upward direction, the momentary vertical gradient of pressure is required for its growth and survival. Horizontal ambient winds that rush towards low pressure zone, crush the air in the buffer zone and turn vertically upward, may also take the dust carried with them visibly to some height. It is considered that the angular azimuthal velocity varies within the annulus. An inference is that no whirlwind without a low pressure region within it can survive. This may be termed as the fundamental characteristic of whirlwind. It is further concluded that if the radial pressure difference between the outermost and innermost layers is larger, the whirlwind is thicker and consequently, it will last longer. Moreover, another conclusion arrived at is that the angular velocity will vanish if the inner radius is zero.

Jagdish P. Maurya, Sanjay Pandey
Indian Institute of Technology (BHU), Varanasi
jpmaurya.rs.apm12@itbhu.ac.in,
skpandey.apm@itbhu.ac.in

CP11

Mathematical Modelling of the Hydration Process

in Contact Lens Production

In this talk we present a mathematical model of an industrially motivated problem, which arises in the production of soft contact lenses using a cast-moulding technique. This project arises from a collaboration with Johnson and Johnson Vision Care, who produce contact lenses in Limerick, Ireland. The first step of the manufacturing process involves casting a liquid monomer along with an inert diluent between two moulds which define the shape of the lens. The hydration process follows, during which unwanted chemicals, impurities or unreacted monomers are removed from the lenses. The hydration process is the rate limiting step on the production line, and optimising this stage is of particular interest to Johnson and Johnson Vision Care. We focus on modelling the removal of the chemical diluent (CD) in the process. This is removed by washing the lenses with an organic solvent (OS), which is subsequently removed by washing with deionised water. We model this CD removal using a coupled set of Partial Differential Equations, which describe volume fractions of both the CD and the OS. The problem is posed as a Stefan problem, which is a particular type of boundary value problem in which the phase boundaries can move with time. We solve the system numerically using a front tracking method, and also discuss some interesting asymptotic approaches as well as comparisons with experimental data.

Niall Mcinerney
University of Limerick
niall.mcinerney@ul.ie

Stephen O'Brien
MACSI
University of Limerick
stephen.obrien@ul.ie

Sarah Mitchell
University of Limerick
Ireland
sarah.mitchell@ul.ie

Kevin Moroney
University of Limerick
kevin.moroney@ul.ie

William Lee
University of Huddersfield
w.lee@ud.ac.uk

CP11

Mathematical Model of Particle-droplet Interaction for Dust Control

In mining operations, dust control is a critical problem affecting workers' health. A common method for controlling dust is a water spray system. Choosing an optimal spray nozzle is often driven by prior experience, and current systems do not allow for calibration of a nozzle design in response to various environmental properties. In order to arrive at a proper design for such a system, we propose a mathematical model that describes the interaction between a water droplet and a dust particle. Using the incompressible Navier-Stokes equations with finite Reynolds number (larger than 1), we solve for a stream function that describes the flow around a spherical water droplet. Initially, dust particles far away from the water droplet will have constant speed, and as they approach the droplet, they cross different streamlines. Solutions for the stream function are obtained numerically using a Galerkin method, and the pathline for a dust particle is obtained consequently using a Runge-Kutta method. The model identifies the starting initial height of a dust particle needed to be captured by a water droplet. This allows for a measure of the single sphere efficiency which can be used to determine the overall capture efficiency of a system. Numerical simulations of the particle-droplet collisions demonstrate the impact of the uniform fluid velocity, water droplet size, dust particle size, and dust particle density on the single sphere capture efficiency.

Cristina Negoita
Arizona State University
cristina.negoita@oit.edu

John-Glen Swanson
Hochschule Magdeburg-Stendal
jswanson@gmx.net

CP11

Uniform Estimate for Maxwell's Equations in a Heterogeneous Medium

We present a uniform estimate for Maxwell's equations in a periodic heterogeneous medium. The existence and the uniqueness of the solution of the Maxwells equations are well-known. However, not many results can be found in the literature for the uniform estimate for the solution of Maxwells equations in highly heterogeneous media, which has applications in photonic crystal fibers, metamaterials, electrical conductivity of fibre-reinforced composites. It is known that the behavior of the material with respect to electromagnetic waves is characterized by its electric permittivity and its magnetic permeability. In general, the two quantities are complex, bounded, and piecewise smooth functions. Let $\delta \in (0, 1]$ denote the periodic size of the periodic material and let $\tau^2 \in (0, 1]$ denote the minimal value of the electric permittivity (or the magnetic permeability). We derive a L^p gradient estimate uniformly in δ and τ^2 for the magnetic field H and the electric field E.

Li-Ming Yeh
Department of Applied Mathematics
National Chiao Tung University, Taiwan
liming@math.nctu.edu.tw

CP12

A Chebyshev Spectral Collocation Method Based Series Approach for Boundary Layer Flow and Heat Transfer in a Micropolar Fluid Past a Permeable Flat Plate

In this paper, we demonstrate the applicability of the large parameter spectral perturbation method (LSPM) on a coupled system of partial differential equations that cannot be solved exactly. The LSPM is a numerical method that employs the Chebyshev spectral collocation method in the solution of a sequence of ordinary differential equations (ODEs) that are derived from decomposing coupled systems of nonlinear partial differential equations (PDEs) using series expansion about a large parameter. The validity of the LSPM is investigated on the problem of boundary layer flow and heat transfer in a micropolar fluid past a permeable flat plate in the presence of heat generation and thermal radiation. The coupled nature of the PDEs that define the problem under investigation precludes the option of using series based methods that seek to generate analytical solutions even in the presence of small or large pa-

rameters. The present study demonstrates that the LSPM can easily overcome this limitation while giving very accurate results in a computationally efficient manner. The results of this study are validated against known results from literature and against results obtained using other numerical methods. Further accuracy validation is demonstrated using residual error and solution error analysis on the governing PDEs and their underlying solutions.

Titilayo M. Agbaje
University of Kwazulu-Natal, South Africa.
titilayoagbaje@gmail.com

CP12

An Ale Method for Large Structural Displacements in Fluid-structure Interaction Simulations of Venous Valves

Veins are blood vessels subjected to very low blood pressures and they rely on muscle contractions and one-way valves to push blood back to the heart. The main contribution of venous valves is to prevent backflow. In fluid-structure interaction (FSI) simulations of venous valves, the large structural displacements may lead to mesh deterioration and entanglements, causing instabilities of the solver and, consequently, the numerical solution to diverge. In this talk, I will present an Arbitrary Lagrangian-Eulerian (ALE) scheme for FSI simulations that aims to solve these instabilities. A monolithic formulation for the FSI problem is considered and, due to the complexity of the operators, the exact Jacobian matrix is evaluated using automatic differentiation tools. The scheme relies on the introduction of a mesh velocity in the formulation to improve the accuracy and on fictitious springs to model the elastic contact of the valve leaflets. Unlike existing strategies for large structural displacements, no remeshing procedure is necessary with the proposed method. Numerical results are shown for a 2D and a 3D model of a venous valve.

Sara Calandrini
Texas Tech University
sara.calandrini@ttu.edu

Eugenio Aulisa
Department of Mathematics and Statistics.
Texas Tech University
eugenio.aulisa@ttu.edu

CP12

The Divergence-conforming Immersed Boundary Method

The divergence-conforming immersed boundary (DCIB) method is presented to tackle a long-standing issue of immersed boundary (IB) methods for fluid-structure interaction, namely, the challenge of accurately imposing the incompressibility constraint at the discrete level [H. Casquero, Y. J. Zhang, C. Bona-Casas, H. Gomez, Non-body-fitted fluid-structure interaction: Divergence-conforming B-splines, fully-implicit dynamics, and variational formulation, under review, 2018]. The DCIB method follows up on our previous work [H. Casquero, C. Bona-Casas, H. Gomez, A NURBS-based immersed methodology for fluid-structure interaction. CMAME, 284, 943-970, 2015], where we discretized the mathematical model proposed by the IB method using NURBS. In the DCIB method, the Eulerian velocity-pressure pair is discretized using divergence-conforming B-splines, which leads to *inf-sup* stable, H^1-conforming, and *pointwise* divergence-free Eulerian solutions. The DCIB method is fully implicit in time, which is key to impose accurately the no-penetration and no-slip conditions at the fluid-solid interface. Two- and three-dimensional problems are solved performing mesh-independence studies, comparisons with other methods, and measurement of convergence rates. The DCIB method leads to completely negligible incompressibility errors at the Eulerian level and various orders of magnitude of increased accuracy at the Lagrangian level compared to other IB methods.

Hugo Casquero
Carnegie Mellon University
hugocp@andrew.cmu.edu

Yongjie Zhang
Department of Mechanical Engineering
Carnegie Mellon University
jessicaz@andrew.cmu.edu

Carles Bona-Casas
Universitat de les Illes Balears
carles.bona@uib.es

Hector Gomez
Purdue University
hectorgomez@purdue.edu

CP12

Water Wave Interaction with two Submerged Unequal Plates of Non-uniform Permeability

In this study, we analyze the effect of two unequal submerged permeable plates in the propagation of water waves under the assumptions of linear water wave theory. The permeability of the plates varies along the depth of submergence of the plates. The plates are present in the water of uniform depth. The velocity potential is expanded by using Havelocks expansion of water wave potential. Employing Havelocks inversion formula together with conditions on the permeable plates the boundary value problem is reduced to two coupled Fredholm type integral equations. A multi-term Galerkin approximation in terms of Chebyshev polynomials is used to solve the vector integral equations and to obtain numerical estimates for the reflection and the transmission coefficients. The effects of the depth of submergence of the plates, the permeability of the plates and the separation length between them on the reflection coefficient are depicted graphically. The present results are validated against the known results for the case of two identical impermeable plates and for a single permeable plate.

Sourav Gupta
Indian Institute of Technology Kharagpur
gupta.sourav12@gmail.com

Rupanwita Gayen
Indian Institute of Technology Kharagpur,
Kharagpur-721302
West Bengal, India
rupanwita.gayen@gmail.com

CP12

Scattering of Water Waves by an Inclined Thin

Plate in a Two-layer Fluid of Finite Depth

The problem of water wave scattering by an inclined thin plate submerged in the lower layer of a two-layer fluid is investigated here using linear theory. In a two-layer fluid, for a prescribed frequency, incident waves propagate with two different wavenumbers. Thus we determine the reflection and the transmission coefficients and the hydrodynamic force for both the wavenumbers. This leads to two separate problems. These problems are reduced to hypersingular integral equations for the potential difference across the plate which are solved by an expansion-collocation method. Several numerical results are presented graphically in a number of figures for the physical quantities varying the inclination, depth, and length of the plate. Making suitable adjustment of the parameters published results for a vertical plate submerged in a single layer fluid are recovered. In addition, the energy identities are used as a partial check on the correctness of the numerical results.

Najnin Islam
Indian Institute of Technology Kharagpur,
Kharagpur-721302
West Bengal, India
najnin.islam92@gmail.com

Rupanwita Gayen
Indian Institute of Technology Kharagpur,
Kharagpur-721302
West Bengal, India
rupanwita.gayen@gmail.com

CP13

More About Visual Geometries - Visual Structural Equations

This paper is devoted to a new perspective to the visual geometries and their intrinsic invariants. It presents our approach to determine visual invariants, Frenet-Serret frames and formulas, as well as visual angles and drawing visual normals. We also introduce visual Structural theorem indicating that each regular smooth curve in a visual geometry satisfies a unique 3rd order differential equation.

Reza Aghayan
University of Texas at San Antonio
reza.aghayan@utsa.edu

CP13

Graph Reduction by Edge Deletion and Contraction

How might one 'compress' a graph? That is, generate a reduced graph that approximately preserves the structure of the original? Spielman and collaborators developed the concept of spectral graph sparsification, i.e. deleting a fraction of the edges and reweighting the rest so as to approximately preserve the Laplacian quadratic form. Interestingly, for a planar graph, edge deletion corresponds to edge contraction in its planar dual (and more generally, for a graphical matroid and its dual). This duality suggests a way to further reduce a graph. Indeed, with respect to the dynamics induced by the Laplacian (e.g. diffusion), deletion and contraction are physical manifestations of two opposite limits: edge weight of 0 and ∞, respectively. In this work, we propose a measure of edge importance with respect to these two operations. Based on this measure, we provide a unifying framework by which one can systematically preserve large-scale structure of a graph while reducing its size, not only in the number of edges, but also in the number of nodes.

Gecia Bravo Hermsdorff
Princeton University
geciah@princeton.edu

Lee M. Gunderson
Princeton University
Plasma Physics Laboratory
leeg@princeton.edu

CP13

Randomized Incremental Construction of Net-trees

Har-Peled & Mendel introduced the net-tree as a linear-size data structure that efficiently solves a variety of (geo)metric problems such as approximate nearest neighbor search, well-separated pair decomposition, spanner construction, and others. More recently, such data structures have been used in efficient constructions for topological data analysis. Net-trees are similar to several other data structures that store points in hierarchies of metric nets (subsets satisfying some packing and covering constraints) arranged into a tree or DAG. The extensive literature on such data structures can be partitioned into two disjoint groups: those that are easy to implement and those that can be constructed in $O(n \log n)$ time for doubling metrics. In this talk, we present an algorithm that is both simple and asymptotically efficient. We combine several ideas already present in the literature with a randomized incremental approach. The challenge is relegated to the analysis, where the usual tricks for randomized incremental algorithms do not apply to net-trees, mostly because they are not canonically defined by a point set.

Mahmoodreza Jahanseir, Donald Sheehy
University of Connecticut
mahmoodreza.jahanseirroodsari@uconn.edu,
don.r.sheehy@gmail.com

CP13

The Application of Regularized Optimization to Optical Design

One way of posing an optical design problem is to assign a geometric distribution and its associated vector field, which we will denote $\mathbf{W}$, to the problem. Then the solution to the design problem is a surface, σ, tangent to the distribution or perpendicular to the vector field. If the solution is exact, then the unit normal vectors to the surface, $\hat{n}$, will be in the same direction as the vector field. If the solution is not exact, there will be a difference in the directions of some or all of the vectors. If no exact solution exists, one way of finding an approximate solution is to find a surface that minimizes the difference between $\mathbf{W}$ and the normal vectors, in other words, minimize the quantity $|\mathbf{W} - \hat{n}|^2$ over possible surfaces. We want to measure the difference over the entire surface, so we use a surface integral to calculate the cost, $\mathfrak{F}[\sigma]$, of a particular surface σ

$$\mathfrak{F}[\sigma] = \int\int_{\sigma} |\mathbf{W} - \hat{n}|^2 \, dA.$$

The Euler-Lagrange equation of this cost functional yields a partial differential equation that can be solved for a surface σ. This functional, variations on the functional, the difficulty of boundary value problem, and the addition of

regularization to make the problem well-posed will all be discussed. Finally, the application of this method to the passenger-side vehicle mirror problem will be shown.

Sarah G. Rody, Andrew Hicks
Drexel University
sarahgotwalsrody@gmail.com, rah29@drexel.edu

Gideon Simpson
Department of Mathematics
Drexel University
grs53@drexel.edu

Ronald Perline
Drexel University
perlinrk@drexel.edu

CP13

Isogeometric Analysis of Geometric Flows on Surfaces with Application to Mesh Processing

Geometric flows represent a class of problems by which differential geometric entities, such as mean and Gaussian curvatures, are advected across a manifold. We present a novel solution method for a broad range of geometric flows over NURBS geometries. In this talk, we will focus on Isogeometric solutions to Ricci Flow, Willmore Flow and Mean Curvature Flow. These flows offer significant value in geometric processing, and we will discuss specific implications to finite element mesh processing, including shape optimization and targeted freeform geometric deformation.

Corey L. Wetterer-Nelson
University of Colorado Boulder
corey.nelson@colorado.edu

CP14

Fisher Information for Discrete Stochastic Models of Gene Expression

RNA and protein expression are discrete, stochastic processes, where single molecules can determine the fate of a cell or organism. Modern experiments measure single-cell and single-molecule dynamics and provide highly informative data for these stochastic processes. The finite state projection (FSP) approach solves the chemical master equation to precisely analyze these stochastic dynamics. We are introducing the FSP-based Fisher information matrix (FSP-FIM), which uses the FSP formalism to estimate the expected information from potential experiments. The FSP-FIM differs from previous analyses in that it makes no assumptions about the distribution shape of single-cell data, and it does not require precise measurement of high-order statistical moments. We validate the FSP-FIM against well-known Fisher information results for simple distributions, and we show that the FSP-FIM can optimize more complex single-cell experiments that yield non-Gaussian fluctuations. We validate optimal experiments determined using the FSP-FIM with Markov Chain Monte-Carlo, and we contrast these to experiments chosen by analyses that assume Gaussian fluctuations or use the central limit theorem. By systematically designing experiments to use all of the measurable fluctuation information, our method can improve co-design of experiments and quantitative models.

Zachary Fox
School of Biomedical Engineering
Colorado State University, Fort Collins
zrfox@rams.colostate.edu

CP14

Deterministic Methodology for Comparison of Stochastic Models

Model comparison techniques are well developed for deterministic models. In this talk, we extend those techniques to three different classes of stochastic models: continuous time Markov chains (CTMC), stochastic differential equations (SDE), and random differential equations (RDE). For nested models, we extend the statistically-based ideas and techniques developed previously for deterministic differential equation models. We then illustrate how the Akaike information criterion (AIC) under the framework of least squares estimation can be extended for comparison of non-nested stochastic models. The effectiveness and limitations of the model comparison techniques are explored using simulated data as well as algae longitudinal growth data.

Michele Joyner
East Tennessee State University
joynerm@etsu.edu

H.T. Banks
North Carolina State University
htbanks@ncsu.edu

CP14

Detecting Causal Relationships in Cerebral Autoregulation by Convergent Cross Mapping

The convergent cross mapping is an effective method in determining the causal networks, which has been widely applied on epidemiology and financial regulation. Cerebral autoregulation plays an important role in maintaining appropriate blood flow, which is critical to the functioning of brain. Changes occur during disease or brain injury. Understanding the physiology of blood flow control is very important in clinical intervention to optimize patient outcome. We apply the convergent cross mapping to study the causal relationships of inter-beat intervals, blood pressure, cerebral blood flow velocities and tissue oxygenation index. The results are obtained by analyzing data collected in resting state, task performing state and under treatment. The statistical significance of the results is also estimated. The study will help us better understand how the physiological systems work and provide evidence for medicine intervention.

Sijie Shen
The University of Texas at Dallas
sxs143631@utdallas.edu

Yan Cao
The University of Texas at Dallas
Department of Mathematical Sciences
yan.cao@utdallas.edu

Rong Zhang, Takashi Tarumi
University of Texas Southwestern Medical Center
rongzhang@texashealth.org,
takashitarumi@texashealth.org

CP14

Convergence Theorems for Sums of Dependent

Moving Windows

The concept of strong convergence theorems for the sums of dependent moving windows problems with fix length are explored. A sequence of dependent Bernoulli random variables with equal probabilities has considered. A general class of dependent probabilistic model is being used to obtain the asymptotic results. Some properties of the sums of moving windows are derived. Furthermore, the strong law of large numbers, central limit theorem and the law of iterated logarithms are established for the sums based on standard martingale limit theories.

Deepak Singh, Somesh Kumar
Indian Institute of Technology Kharagpur
deepak.singh@maths.iitkgp.ernet.in,
smsh@maths.iitkgp.ernet.in

CP15

A Class of Modified Gram-Schmidt Algortihms and their Analysis

We develop a class of block modified Gram-Schmidt (BMGS) algorithms to factor a full column rank m-by-n matrix X, into an m-by-n left orthogonal matrix Q and an n-by-n upper triangular R such that

$$X = QR.$$

The BLAS-3 algorithm builds upon block Householder representation of Schreiber and Van Loan [R. Schreiber and C.F. Van Loan, A storage-efficient WY representation for products of Householder transformations,SIAM J. Sci. Stat. Computing,10:53–57,1989] and an observation by Charles Sheffield analyzed by Paige [C.C. Paige, A useful form of unitary matrix from any sequence of unit 2-norm n-vectors, SIAM J. Matrix Anal. Appl., 31(2):565–583, 2009] about the relationship between modified Gram-Schmidt and Householder QR factorization. Using the Sheffield framework, we show that the BMGS has a similar relationship to Householder QR factorization and thus has similar error analysis properties to modified Gram-Schmidt.

Jesse L. Barlow
Penn State University
Dept of Computer Science & Eng
barlow@cse.psu.edu

CP15

Scalable Linear Solvers for Ill-conditioned Matrices

I will present a parallel hierarchical solver for general sparse linear systems on distributed-memory machines. Large-scale sparse linear systems arise in many science and engineering fields, e.g., computational fluid dynamics, ice sheet modeling, structural mechanics and etc. For these large linear systems, our fully algebraic algorithm is faster and more memory-efficient than sparse direct solvers because it exploits the low-rank structure of fill-in blocks. Depending on the accuracy of low-rank approximations, the hierarchical solver can be used either as a direct solver or as a general-purpose pre-conditioner. The parallel algorithm is based on data decomposition and requires only local communication for updating boundary data on every processor. Moreover, the computation-to-communication ratio of the parallel algorithm is approximately the volume-to-surface-area ratio of the subdomain owned by every processor. Various numerical results and related work will also be discussed.

Chao Chen, Leopold Cambier
Stanford University
cchen10@stanford.edu, lcambier@stanford.edu

Eric F. Darve
Stanford University
Mechanical Engineering Department
darve@stanford.edu

Siva Rajamanickam, Raymond Tuminaro
Sandia National Laboratories
srajama@sandia.gov, rstumin@sandia.gov

Erik G. Boman
Center for Computing Research
Sandia National Labs
egboman@sandia.gov

CP15

Recycling Preconditioners and Subspaces

Preconditioners are generally essentially for fast convergence in the iterative solution of linear systems of equations. The computation of a good preconditioner can be expensive and so it can be advantageous to recycle (update and reuse) preconditioners when solving a sequence of many systems. We discuss a simple and effective method for updating preconditioners that is independent of the preconditioner type and quality, which we refer to as the Sparse Approximate Map, or SAM, update. Recycling Krylov subspaces from previous systems is a complementary method for reducing computational cost. Rather than discarding the spaces generated for one system, we can select a subspace (or the recycle space) to use for another, closely related system in order to speed up convergence. We examine recycling preconditioners along with recycling subspaces. Applications include hydraulic tomography, topology optimization, quantum Monte Carlo, and the nonlinear convection-diffusion equation.

Arielle K. Grim-McNally, Eric De Sturler
Virginia Tech
arielle5@vt.edu, sturler@vt.edu

CP15

Preconditioners for Nonsymmetric Linear Systems with Low-rank Skew-symmetric Part

To solve large and sparse linear systems $Ax = b$ by an iterative method a good preconditioner is desirable. If A is nonsymmetric, but its skew symmetric part can be well approximated with a skew-symmetric low-rank matrix one can compute a preconditioner for the symmetric part of A and then update it to get a good preconditioner. To be precise if $A = H+K$ where H and K are the symmetric and skew-symmetric parts of A, respectively; $K = FCF^T + E$ where $F \in R^{n\times s}$ is a full-rank rectangular matrix, $C \in R^{s\times s}$ is a nonsingular skew-symmetric matrix with s even, $s \ll n$ and $\| E \| \ll 1$. Then an incomplete factorization of the block matrix

$$\begin{bmatrix} H+E & F \\ F^T & -C^{-1} \end{bmatrix}$$

is computed. Some approximation and spectral properties of the preconditioner will be presented as well as some numerical results. This work was supported by Spanish Min-

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Jose Mas
Institut de Matematica Multidisciplinar
Universitat Politecnica de Valencia
jmasm@imm.upv.es

Juana Cerdán
Instituto de matemática multidisciplinar
Universitat Politècnica de València
jcerdan@imm.upv.es

Danny Joel Guerrero
Departamento de Ciencias Matemáticas
Universidad Pedagógica Nacional Francisco Morazán
danguefl@doctor.upv.es

José Marín
Instituto de matemática multidisciplinar
Universitat Politècnica de València
jmarinma@imm.upv.es

CP16

High Order Hybrid Hermite-discontinuous Galerkin Overset Grid Methods for the Wave Equation

We present efficient and high order hybrid Hermite-discontinuous Galerkin methods for the wave equation on complex domains. The hybridization combines efficient Herimite methods on Cartesian grids with geometrically flexible Galerkin methods curvilinear grids coupled through overset grid technology. Although both methods are probably stable on single grids the interpolation between the overset grids may cause instabilities. We demonstrate that for many combinations the dissipation from the Hermite interpolation in the Hermite method and the upwind fluxes is sufficient to supress weak instabilities. For stronger instabilities, appearing when the grid sizes of different grids are very different, we add high order artificial viscosity. By an extensive study of the spectrum of the discretization we conclude that it is always possible to stabilize the hybrid method. Numerical experiments demonstrating the efficiency and accuracy of the method will be presented. Experiments will include convergence and efficiency studies as well as more applied examples.

Oleksii Beznosov
University of New Mexico
obeznosov@unm.edu

Daniel Appelo
Department of Applied Mathematics
University of Colorado Boulder
daniel.appelo@colorado.edu

CP16

Energy-Conserving Finite Difference Discretization of Acoustic Wave Equations on Nonconforming Staggered Grids

We consider the numerical simulation of acoustic wave equations arising from seismic applications, for which staggered grid finite difference methods are popular choices due to their simplicity and efficiency. We relax the uniform grid restriction on finite difference methods and allow the grids to be block-wise uniform with nonconforming interfaces. In doing so, variations in wave speeds of the subterranean media can be accounted for more efficiently. Staggered grid finite difference operators satisfying the summation-by-parts property are devised to approximate the spatial derivatives appearing in the acoustic wave equations. These operators are applied within each block independently. The coupling between blocks is achieved through simultaneous approximation terms, which impose the interface conditions weakly, i.e., by penalty. Ratios of the grid spacing of neighboring blocks are allowed to be rational numbers, for which special interpolation formulas are designed. These interpolation formulas constitute key pieces of the simultaneous approximation terms. The overall discretization is shown to be energy-conserving and examined on test cases of both theoretical and practical interests, delivering accurate and stable simulation results.

Longfei Gao
KAUST
longfei.gao@kaust.edu.sa

David C. Del Rey Fernandez
University of Toronto Institute For Aerospace Studies
dcdelrey@gmail.com

Mark H. Carpenter
NASA Langley Research Center
mark.h.carpenter@nasa.gov

David E. Keyes
KAUST
david.keyes@kaust.edu.sa

CP16

A Comparison of Nodal Discontinuous Galerkin Schemes for Hypersonic Flow over a Blunt Object

In this talk, we will discuss the use of a family of compact discontinuous Galerkin (DG) methods to simulate unsteady hypersonic inviscid flow over a blunt body. The presence of discontinuities such as shocks/small-scale flow features make such simulations problematic for numerical simulation. In particular, we assess a high-order DG scheme's performance for standard benchmark tests while varying the shocking capturing limiter, numerical flux, and the scheme's order. In particular, we consider the classical MinMod limiter, its high-order generalization(s), and a recently introduced moment-based limiter by Moe, Rossmanith, and Seal. To couple our quadrilateral sub-domains we consider the popular Lax Friedrichs numerical flux, as well as the HLL, Roe, and Marquina numerical fluxes. The talk's focus will be to summarize the strengths and weaknesses of each flux/limiter combination for hypersonic inviscid flow over a blunt object. We will report on comparisons between some of our best performing flux/limiter combinations with a second-order structured finite-volume solver. Our simulations are carried out using a newly developed partial differential equation solver, SpECTRE[1], that combines a discontinuous Galerkin method with a task-based parallelism model. Previous work shows the code's scalability on the Blue Waters supercomputer up to the machine's full capacity of 22,380 nodes. We will briefly touch on the SpECTRE's scalability for our problem and computational resources.

Aakash Kardam
Graduate Student, Mechanical Engineering
University of Massachusetts Dartmouth, USA
akardam@umassd.edu

Scott Field
Mathematics Department, UMASS Dartmouth
Dartmouth, MA , USA
sfield@umassd.edu

Alireza Mazaheri
Aerothermodynamics Branch, NASA Langley Research Center,
Hampton, VA 23681, USA
ali.r.mazaheri@nasa.gov

CP16

Duality Principles and A Posteriori Error Estimation for DPG Methods with a View Towards Viscoelastic Fluids

A generalized duality theory for finite element methods with trial and test spaces of unequal dimension is briefly introduced and then used to derive the newly discovered DPG* methods. Motivation for this new theory is taken from a challenging problem in viscoelastic fluid flow modeling and, in particular, goal-oriented adaptive mesh refinement for the drag coefficient therein. A posteriori error estimation, for both DPG and DPG* methods, is essential in understanding such an adjoint-based, goal-oriented strategy and we will present two novel theoretical results on the subject.

Brendan Keith
The University of Texas at Austin
The Institute for Computational Engineering and Sciences
brendan@ices.utexas.edu

CP16

Eliminating Gibbs Phenomenon: A Nonlinear Petrov-Galerkin Method for Convection-dominated Problems

We consider the numerical approximation of partial differential equations whose solutions may contain sharp features, such as interior and boundary layers. One of the main challenges of designing a numerical method for these types of problems is that these sharp features can lead to non-physical oscillations in the numerical approximation, often referred to as Gibbs phenomena. The idea we are pursuing is to consider the approximation problem as a residual minimization in dual norms in L^q-type Sobolev spaces, with $1 \leq q < 2$. We then apply a non-standard, non-linear Petrov-Galerkin discretization that is applicable to reflexive Banach spaces, such that the space itself and its dual are strictly convex. Similar to discontinuous Petrov-Galerkin methods, this method is based on employing optimal test functions. Replacing the intractable optimal test space by a suitable computable approximation gives rise to a non-linear inexact mixed method for which optimal a priori estimates hold. This generalizes the Petrov-Galerkin framework developed in the context of discontinuous Petrov-Galerkin methods to more general Banach spaces. A key advantage of considering a more general Banach space setting is that the oscillations in the numerical approximation vanish as q tends to 1, as we will demonstrate using a few simple numerical examples.

Sarah Roggendorf
University of Nottingham
Sarah.Roggendorf@nottingham.ac.uk

Ignacio Muga
Pontificia Universidad Cat{ó}lica de Valpara{í}so
ignacio.muga@uvc.cl

Paul Houston
School of Mathematical Sciences
University of Nottingham, UK
Paul.Houston@nottingham.ac.uk

Kris van Der Zee
University of Nottingham
kg.vanderzee@nottingham.ac.uk

CP16

Higher-order Adaptive Finite Difference Methods for Fully Nonlinear Elliptic Equations

In this talk, we introduce generalized finite difference methods for solving fully nonlinear elliptic partial differential equations. The methods are based on piecewise Cartesian meshes augmented by additional points along the boundary. This allows for adaptive meshes and complicated geometries, while still ensuring consistency, monotonicity, and convergence. We will describe an algorithm for efficiently computing the non-traditional finite difference stencils using quadtrees. We also discuss a strategy for computing formal higher-order convergent methods. Computational examples that demonstrate the efficiency, accuracy, and flexibility of the methods will be presented.

Brittany Froese Hamfeldt
New Jersey Institute of Technology
bdfroese@njit.edu

Tiago Salvador
McGill University
saldanha@umich.edu

CP17

Realization of Port Hamiltonian Systems

Realizations allow to represent systems accurately in a state space form. In this work, we study the realization of port Hamiltonian systems from raw input/output data or from descriptor systems. Port Hamiltonian systems have been studied extensively during recent years as they exhibit a special structure and their states represent physical quantities in industrial applications. The realization presented in this work will allow to represent a system in its port Hamiltonian representation directly from its input/output data. This realization technique was implemented in MATLAB and the challenges facing this implementation are presented. Finally, some examples are presented to illustrate its use.

Karim Cherifi
institute of electrical and electronic engineering (ex INELEC) Boumerdes Algeria.
cherifikarimdz@gmail.com

Volker Mehrmann
Technische Universität Berlin
mehrmann@math.tu-berlin.de

Kamel Hariche
University of Boumerdes

khariche@yahoo.com

CP17

Stabilization of a Flying Inverted Pendulum using Controlled Lagrangians

We propose the use of Controlled Lagrangians for stabilization of a flying inverted pendulum. We see the system as a mechanical system whose vertical translational symmetry is broken due to the gravity. We combine a kinetic shaping (where symmetry is preserved) and a potential shaping (where the broken symmetry is taken into account), thereby achieving complete state-space asymptotic stabilization of the system. The purpose of this work is to extend the method of Controlled Lagrangians-which has been applied to an inverted pendulum on a tilted plane by Bloch et al.- to an inverted pendulum sitting on a flying device (such as a quadrotor) studied by Hehn and DAndrea. Our approach is different from theirs in that we do not linearize the system as well as that our closed-loop dynamics remain in Lagrangian form. By using nonlinear control methods one hopes to contribute to the improvements in robustness and efficiency in control as compared to linear methods, which neglects the rich dynamics due to nonlinearity.

Cesar Contreras, Tomoki Ohsawa
University of Texas at Dallas
cxc145430@utdallas.edu, tomoki@utdallas.edu

CP17

Structured Radius of Controllability for State Space Systems

Consider a state space system given by $\dot{x} = Ax + Bu$ where $A \in \mathbb{R}^{m\times m}$, $B \in \mathbb{R}^{m\times n}$. The distance to the nearest uncontrollable pair to (A, B), also known as the radius of controllability is a good metric to gauge the numerical robustness of the system. However, it should be noted that in many real life applications, due to physical constraints, perturbation to every parameter in system matrices A and B is not possible. Let $\mathcal{A} \subset \mathbb{R}^{m\times m}$ and $\mathcal{B} \subset \mathbb{R}^{m\times n}$ be the linear subspaces of structured matrices which represent the structure imposed on the perturbations to the system matrices. We now define the structured radius of controllability as follows:

$$SR_c = \min_{\Delta A\in\mathcal{A},\ \Delta B\in\mathcal{B}} \{\|[\Delta A \ \ \Delta B]\|_F \mid (A+\Delta A, B+\Delta B) \text{ is uncontrollable}\}$$

The problem of computing SR_c is shown to be equivalent to computing the nearest SLRA of a certain Toeplitz structured matrix. We propose to compute the nearest SLRA to this structured matrix by posing it as an optimization problem on a Stiefel manifold. The line search algorithm is implemented on the Stiefel manifold to compute the optimal solution. Several numerical examples are presented to illustrate the efficiency of the proposed method.

Tanay Saha
Indian Institute of Technology, Kharagpur, India.
sahatanay50@gmail.com

Swanand R. Khare
Department of Electrical Engineering
Indian Institute of Technology Bombay
srkhare@maths.iitkgp.ernet.in

CP17

On Exact Boundary Controllability of Second-order Boundary Feedback Systems with Memory

We are concerned with second-order boundary feedback systems with memory, which cover a number of concrete viscoelastic systems subject to boundary controls. We focus our attention in this work to the exact boundary control problem for the systems modelled by second-order integro-differential equations. We first prove that under some assumptions, the solutions of some related initial value problems form a Riesz sequence in $L^2(0, T)$, which is not only an important process for the establishment of the desired exact boundary controllability for the concerned boundary feedback systems with memory but also is useful for numerical computations of the control functions. Then, we derive a continuous dependence result for the Cauchy problem in a suitable initial datum setting, which leads to an existence and uniqueness result for solutions to the Cauchy problem for the systems with null initial data. Finally, we obtain a general exact boundary controllability theorem for these second-order boundary feedback systems with memory. Moreover, as an application of our general exact boundary controllability theorem, we show the exact boundary controllability of a concrete viscoelastic beam equation. This is joint work with Zhe Xu.

Ti-Jun Xiao
Fudan University
tjxiao@fudan.edu.cn

CP18

Uncertainty-based Active Learning for Deep Learning Networks

While much work in machine learning literature centers around a static corpus of data for use in a supervised or unsupervised task, there exist other problems that involve ongoing learning and interaction with the user where the number of samples to learn a concept can often be much lower. Sometimes in interactive machine learning it also becomes cost-prohibitive to obtain copious amounts of input data due to user fatigue; because of this, there has been much focus in industry and the academic community on how to optimally query domain experts. This work will provide a menu of techniques for the optimal query task including techniques from design of experiments as well as other techniques including expected error reduction, query by committee, and uncertainty-based sampling. Next, the work will present the model-based uncertainty method that we used to deal with the active learning problem within the context of a user-centric decision support system where stakeholders interactively design group-based environmental solutions. This technique involves determining which points the implemented model is the most uncertain about using the objective function that has been chosen as most closely tied to model performance. This work will thus have the following contributions: i) describe current techniques for dealing with active learning, and ii) describe one use case that successfully deals with the online machine-learning problem.

Andrew P. Hoblitzell
Indiana University Purdue University Indianapolis

ahoblitz@purdue.edu

CP18

An $O(n^4)$ Graphic Approach for Solving the Optimal Linear Ordering Problem

The optimal assignment of locations for a set of n machines or pins in a bi-directional line layout (BLL) is to be determined to minimize the total flow cost among these machines, where all machines have identical width. This popular layout problem is equivalent to the optimal linear ordering problem (OLO, NP-complete) when adjacent locations are at unit distance apart and only the flow among machines or the wire length among pins are considered in the optimization problem. We show that OLO and/or BLL can be transformed into a network flow problem by an augmented graph with one sink/source node at two ends of the linear layout. Based on the cut approach, an efficient polynomial time $O(n^4)$ algorithm is developed and tested to find the optimum or near optimum layout sequence. The computational study has demonstrated that the proposed heuristic is efficient and effective. The average cost deviation is less than 0.5%, when the approximate solution is compared with that in the integer programming model.

Shine-Der Lee
National Cheng Kung University
Dept. of Industrial & Information Management
sdlee@mail.ncku.edu.tw

CP18

Deep Learning for Classification of 3D LiDAR Point Cloud Data

3D LiDAR point cloud data has gained great interests in the last few years as seen in different applications (mapping, forest planning, environmental assessment, flood models, pollution models, management of coastline, transport planning, oil and exploration, mining, archeology, solar energy, etc.) LiDAR stands for light detection and ranging and it is an optical remote sensing technique that uses laser light to densely sample the surface of the earth, producing highly accurate x, y and z measurements. We first perform dimensionality reduction of the original 3D LiDAR point cloud data (extracted from the USGS Earth Explorer) using PCA and the inner layer of auto-encoders (an unsupervised learning algorithm that applies backpropagation, setting the target values to be equal to the inputs). We then aim to classify all the points of the cloud data into elementary, relevant classes, for example, according to their morphology using machine learning techniques, e.g. K-nearest neighbors or random forest. We compare the accuracy of the proposed machine learning algorithms and propose new research questions related to intrinsic dimension. This is joint work with Randy Paffenroth.

Francis P. Medina
Oregon State University
fpmedina@wpi.edu

Randy Paffenroth
Worcester Polytechnic Institute
rcpaffenroth@wpi.edu

CP18

Solution Uniqueness of Convex Piecewise Affine Functions based Optimization with Applications to Constrained ℓ_1 Minimization

In this talk, we study the solution uniqueness of an individual feasible vector of a class of convex optimization problems involving convex piecewise affine functions and subject to general polyhedral constraints. This class of problems incorporates many important polyhedral constrained ℓ_1 recovery problems arising from sparse optimization, such as basis pursuit, LASSO, and basis pursuit denoising. By leveraging the max-formulation of convex piecewise affine functions and convex analysis tools, we develop dual variables based necessary and sufficient uniqueness conditions via simple and yet unifying approaches; these conditions are applied to a wide range of ℓ_1-minimization problems under possible polyhedral constraints. An effective linear program based scheme is proposed to verify solution uniqueness conditions. The results obtained in this paper not only recover the known solution uniqueness conditions in the literature by removing restrictive assumptions but also yield new uniqueness conditions for much broader constrained ℓ_1-minimization problems.

Seyedahmad Mousavi
University of Maryland, Baltimore County
University of Maryland, Baltimore County
smousav1@umbc.edu

Jinglai Shen
University of Maryland Baltimore County
shenj@umbc.edu

CP18

Identifying Sensitive Content in Online Ad Images with Deep Learning

In online advertising, identifying potentially inappropriate content in an advertisement before it is displayed on a publisher's website is a critical quality control step in the ad serving process. This ensures that sensitive content (e.g., alcohol, tobacco ads) is not shown to the wrong audience, inappropriate ads (e.g., hate speech, porn) are not shown at all, and that online publishers can better control the quality of the content displayed on their webpage. Historically, identifying sensitive content has been performed by human auditors, which is costly and time consuming. Here we show that a deep neural network achieves better than human level performance at identifying sensitive content on a large fraction of ads. We use a pre-trained convolutional neural network to extract a representation of an ad image, concatenate this representation with data describing the landing page (the webpage that loads when the ad is clicked), and pass this through two fully connected layers to predict the probability that an ad has a sensitive category. If the probability exceeds a threshold estimated during the training process, then the model classifies the content of the ad, otherwise the ad is sent to an auditor. The model was trained on 8 million images collected on our platform and achieved an accuracy of 99.9% (human performance is 99.7%), while classifying the content on 61.2% of ads in a held-out test set.

Daniel Austin, Kannan Sankaran, Ryan Woodard, Ashutosh Sanzgiri, Amit Lissack, Sam Seljan
AppNexus
asanzgiri@appnexus.com, ksankaran@appnexus.com, rwoodard@appnexus.com, asanzgiri@appnexus.com,

alissack1@appnexus.com, sseljan@appnexus.com

CP19

Computational Advances in Optimal Reconstruction of Constitutive Relations for Porous Media Flows

Comprehensive full-physics models for flow in porous media typically involve parameters to be reconstructed from experimental data. Special complexity is seen when the reconstructed parameters are considered as state-dependent functions, e.g. the relative permeability coefficients k_{rp}. Modern petroleum reservoir simulators still use simplified approximations of k_{rp} as single variable functions of p-phase saturation s_p given in the form of tables or simple analytical expressions. This form is hardly reliable in modern engineering applications used, e.g., for enhanced oil recovery, carbon storage, modeling thermal and capillary pressure relations. Thus, the main focus of our research is on developing a novel mathematical concept for building new models where k_{rp} are approximated by multi-variable functions of fluid parameters, namely phase saturations s_p and temperature T. Reconstruction of such complicated dependencies requires advanced mathematical and optimization tools to enhance the efficiency of existing engineering procedures with a new computational framework generalized for use in various earth science applications.

Vladislav Bukshtynov
Florida Institute of Technology
Department of Mathematical Sciences
vbukshtynov@fit.edu

CP19

Double-diffusive Convection and Viscous Dissipation in a Horizontal Non-Darcy Porous Medium

The onset of double-diffusive convective instability induced by viscous dissipation in a fluid saturated porous layer of high permeability is investigated. The porous layer is infinitely long along the horizontal direction and is bounded by two rigid surfaces maintained at constant, but different solute concentrations. The lower surface is thermally insulated, whereas, the upper surface is considered to be isothermal. There is a horizontal throughflow in the medium. Darcy-Brinkman model is adopted for deriving the equations governing the flow in the medium. The instability in the base flow is considered to be induced by the non-negligible viscous heating. Disturbances in the base flow are assumed in the form of oblique rolls, where the longitudinal and the transverse rolls are at the two extreme inclinations. The disturbance functions are assumed to be of $O(1)$. It is considered that $Ge \ll 1$ and $\mid Pe \mid \gg 1$ and the eigenvalue, that is, $R = GePe^2$ is of $O(1)$. The eigenvalue problem with coupled ordinary differential equations governing the disturbances in the flow is solved numerically in Matlab. Results obtained depict that the flow is most stable in the Brinkman regime and the longitudinal rolls are the most preferred mode of instabilities. Solute concentration gradient has a linear monotonic impact on the instability of the flow in the medium.

Rashmi Dubey, P. V. S. N. Murthy
Indian Institute of Technology Kharagpur, Kharagpur, West Bengal 721302, India.
rashmirkd2012@gmail.com, pvsnm@maths.iitkgp.ernet.in

CP19

Numerical Analysis of a Generalized Cahn-Hilliard Equation with Applications in Porous Media

Here we discuss the numerical analysis of a generalized Cahn-Hilliard equation with applications in porous material. The Cahn-Hilliard equation is a 4th-order non-linear partial differential equation of the form

$$u_t = \gamma\Delta\left(f(u) - \alpha\Delta u\right),$$

where $f(u)$ is generally taken to be the derivative of a double well potential function and $\alpha, \gamma > 0$. Observe that if $\alpha = 0$, the equation reduces to the forward-backward heat equation, and becomes ill-posed. Here we analyze a generalization of this equation of the form:

$$\begin{aligned} u_t &= \nabla \cdot (\mathbf{K}\nabla w) \\ w &= f(u) - \alpha\Delta u \end{aligned}$$

where $\mathbf{K}$ is a symmetric positive definite matrix valued function of the spacial coordinates representing conductivity. We present analysis showing properties of the strong form, weak form, and a first order IMEX numerical algorithm for no forcing function. We conclude with numerical results.

Zachary J. Hilliard, Lynn Schreyer, Nikolaos Voulgarakis, Sergey Lapin
Washington State University
zachary.hilliard@wsu.edu, lynn.schreyer@wsu.edu, n.voulgarakis@wsu.edu, slapin@wsu.edu

CP19

Thermoconvective Instability of a Power Law Fluid Flow through Porous Channel with Viscous Dissipation

The convective instability of horizontal throughflow of non-Newtonian power law fluid with viscous dissipation in a horizontal porous channel is investigated in this study. The constant heat flux boundary condition is considered at the lower wall, and the upper wall has a fixed constant temperature. A basic steady state solution of the governing equation is determined for a horizontal throughflow of a power law fluid. The basic temperature profile is influenced by the presence of viscous dissipation term in energy equation. For the onset of convective instability of horizontal throughflow, the critical value of Rayleigh number corresponding to wave number is affected by the values of Péclet number (Pe), power law index (n) and Gebhart number (Ge). For numerical computation, the eigenvalue problem is solved entirely using `bvp4c` routine in Matlab and shooting method coupled with R-K method in Mathematica. It has been noticed that the effect of viscous dissipation has increased the thermal instability of power law fluid flow. The convective instability of base flow is discussed for the longitudinal rolls and transverse rolls. It is shown that the longitudinal rolls are the most unstable mode for dilatant fluid ($n > 1$) and for pseudoplastic fluid ($n < 1$) transverse rolls are the most unstable disturbance.

Seema Kumari
Indian Institute of Technology Kharagpur,
Kharagpur-721302
West Bengal, India
seemakumari151@gmail.com

P.V.S.N Murthy
Indian Institute of Technology Kharagpur,
Kharagpur-721302
West Bengal, India
pvsnm@maths.iitkgp.ernet.in

CP19

Unsteady Mixed Convection in Nanofluid Flow through a Porous Medium with Thermal Radiation using the Bivariate Spectral Quasilinearization Method

In this paper, we investigated the unsteady mixed convection flow and heat transfer in a nanofluid with buoyancy, thermal radiation and double-diffusive effects over a vertical plate which is assumed to be moving in the free stream direction in a porous medium. The plate is maintained at a constant wall temperature while the nanoparticle flux at the boundary is zero. The free stream velocity is time-dependent, an assumption that leads to non-similar differential equations. The equations are solved using the bivariate spectral quasilinearization method, a method used to solve this kind of problem for the first time. The thermal radiation parameter enhances the temperature profile, while the nanoparticle concentration profile is enhanced by the thermophoresis parameter but reduced by an increase in the Brownian motion parameter. The unsteadiness of the flow leads to an increase in the momentum boundary layer thickness and a decrease in the temperature and concentration boundary layer thickness. The skin friction coefficient is reduced by the unsteady parameter, while it increases the rate of heat transfer. We present a comparison of result with those in existing literature.

Ibukun S. Oyelakin
University of KwaZulu-Natal
Scottsville Pietermaritzburg
ibkoyus@yahoo.com

CP20

A Multivariant Partition of Unity Adaptive Refinement Chebyshev Polynomial Method

Chebyshev tensor product interpolants can provide spectral convergence for bivariate functions on squares. One setback is that the number of interpolating points grows quadratically with respect to the degree of the approximation along each dimension. One way to avoid this while still having a globally smooth operator is to divide the square into overlapping rectangles and blend the local interpolants using a partition of unity. Using recursive bisection, a simple divide-and-conquer algorithm can be used to find an overlapping splitting that is adapted to the features of the function. This method can be extend to trivariate functions on cubes by recursively splitting the domain into overlapping cuboids. Utilizing the recursive structure of the approximations, efficient methods for computation such as addition and multiplication can be developed.

Kevin W. Aiton, Tobin Driscoll
University of Delaware
Mathematical Sciences
kaiton@udel.edu, driscoll@udel.edu

CP20

Low-rank Kernel Matrix Approximation using Skeletonized Interpolation with Endo- or Exo-Vertices

We introduce a new method to compute low-rank approximations of dense kernel matrices arising in integral equations. The method relies on ideas combining interpolation and rank-revealing QR decomposition in order to build an optimal custom interpolant for a given kernel function. The resulting method is provably stable and accurate. We consider various kernel-sampling heuristics like random points, Chebyshev grids, spherical points and maximally dispersed vertices. They are compared in terms of quality (ranks obtained), accuracy and robustness on various industrial benchmarks. Overall, we show that a simple maximally dispersed vertices sampling of the mesh allows for the smallest-rank factorization for a given accuracy.

Zixi Zu, Leopold Cambier
Stanford University
zixizu@stanford.edu, lcambier@stanford.edu

Pierre LEplattenier
Livermore Software Technology
pierre@lstc.com

Francois-Henry Rouet
Livermore Software Technology Corp.
fhrouet@lstc.com

Yun Huang
Livermore Software Technology
huang@lstc.com

Cleve Ashcraft
Livermore Software Technology
Corporation
cleve@lstc.com

Eric F. Darve
Stanford University
Mechanical Engineering Department
darve@stanford.edu

CP20

Diagonalization Methods for Solving Generalized Definite Eigenvalue Problem

We derive and analyze three diagonalization methods for the generalized definite eigenvalue problem $Ax = \lambda Bx$ with complex Hermitian matrices A and B. The first one is complex Falk-Langemeyer method which is well defined for a definite pair of complex Hermitian matrices. It is characterized by the requirement that the transformation matrices have unit diagonal. The second one is the HZ method which requires that B is positive definite. This method is better understood since its global and quadratic convergence have been proved. It is characterized by the requirement that the iterated matrix B has unit diagonal. The third one is similar to the HZ method, but its algorithm is based on the Cholesky factorization of the pivot submatrix of B followed by the Jacobi step on the updated pivot submatrix of A. We call it complex Cholesky-Jacobi method. All these methods are important because on pairs of well behaved positive definite matrices they show high relative accuracy property. This makes them a good choice for the kernel algorithm of the block Jacobi methods for the generalized eigenvalue and singular value problems. On contemporary CPU and GPU computing machines, one-sided block Jacobi methods have proved to be very efficient and

accurate solvers of those problems.

Vjeran Hari
University of Zagreb
hari@math.hr

CP20

Fast Factorization of Rectangular Vandermonde Matrices with Chebyshev Nodes

The polynomial interpolation problem with distinct interpolation points and the polynomial represented in the power basis gives rise to a linear system of equations with a Vandermonde matrix. This system can be solved efficiently by using the structure of the Vandermonde matrix with the aid of the Björck–Peyrera algorithm. When the interpolation points are required to live in a specified interval, but are otherwise arbitrary, it is generally beneficial to let them be zeros of a translated Chebyshev polynomial of the first kind for this interval. This paper is concerned with polynomial least-squares approximation with polynomials in power form and Chebyshev nodes as well as Chebyshev extrema points. New fast algorithms are described and compared to an available fast method, as well as to a structure-ignoring method. The new algorithms are based on the fast computation of a QR or a QR-like factorization of a rectangular Vandermonde matrix.

Mykhailo Kuian
Kent State University
mkuian@kent.edu

CP20

Solution of the Affine Partial Quadratic Inverse Eigenvalue Problem for the Quadratic Matrix Pencil

This paper concerned with the study of the affine partial quadratic inverse eigenvalue problem (APQIEP) for the quadratic matrix pencil. APQIEP deals with finding the affine structured matrices $K \in \mathbb{R}^{n\times n}$ and $C \in \mathbb{R}^{n\times n}$ from given m (where $1 \leq m \leq 2n$) eigenpairs so that the corresponding quadratic matrix pencil $P(\lambda) = \lambda^2 M + \lambda C + K$ has the given eigenpairs as its eigenvalues and eigenvectors. A necessary and sufficient condition for the existence of solution of this problem is established in this paper. Analytical expressions for the solution K and C of the APQIEP is presented. Our proposed approach is applied on different numerical examples to illustrate the validity of our proposed approach.

Suman Rakshit
RESEARCH SCHOLAR, DEPT. OF MATHEMATICS, IIT KHRAGPUR
sumanrakshit1991@gmail.com

Swanand R. Khare
Department of Electrical Engineering
Indian Institute of Technology Bombay
srkhare@maths.iitkgp.ernet.in

CP20

Core-chasing Algorithms for the Eigenvalue Problem

Francis's implicitly-shifted QR algorithm has been one of the most important tools for eigenvalue computation for more than fifty years now, and one might think that everything that can be said about it has already been said, but this turns out not to be the case. We claim that superior implementations can be obtained by storing the upper Hessenberg (or Hessenberg-like) matrix A in QR-decomposed form: $A = QR$. The unitary factor Q is then a product of $n-1$ essentially 2×2 matrices (e.g. Givens rotators or reflectors), for which we use the generic term *core transformation*. Of course we store Q in this factored form. The standard Francis algorithm is a bulge-chasing algorithm. When we implement it on the QR-decomposed form, it chases extra core transformations (instead of a bulge) from the top to the bottom of the matrix, so we call it a *core-chasing algorithm*. There are classes of structured eigenvalue problems for which this methodology is obviously advantageous. These include the unitary and the unitary-plus-rank-one problem, which includes companion matrices. We have also used this methodology to solve polynomial eigenvalue problems. This is joint work with Jared Aurentz, Thomas Mach, Leonardo Robol, and Raf Vandebril. We will publish a monograph on this topic in the near future.

David S. Watkins
Washington State University
Department of Mathematics
watkins@math.wsu.edu

CP21

Perfectly Matched Layer Method for Acoustic Scattering Problem by a Locally Perturbed Line with Impedance Boundary Condition

In this talk, we study the two-dimensional Helmholtz scattering problem by a locally perturbed line with impedance boundary condition. Different from the problem with Dirichlet boundary condition, the Green function of the Helmholtz equation with impedance boundary condition becomes very complicated and comprises surface waves along the locally perturbed line. A uniaxial perfectly matched layer (UPML) method is proposed to truncate the half plane into a bounded computational domain. The main contribution of this paper is to prove the well-posedness of the PML problem and the exponential convergence of the approximate solution to the exact solution as either the thickness or the medium parameter of PML increases.

Xue Jiang
School of Science
Beijing University of Posts and Telecommunications
jxue@lsec.cc.ac.cn

CP21

Dynamical System Stability Analysis for Travelling Wave Propagation in Nonlinear Media

We formulate the Travelling Wave Propagation problem in nonlinear Media using coupled Maxwell's equation, and analyze the stability regimes. We show that in addition to the trivial stationary point of (0,0), the system posses additional points of stability dependent on the incident energy of the plane wave. By modelling the nonlinear polarization as a function of this energy, we define a Lyapunov energy function and show conservation, resulting in stability. Eigenvalue analysis of the system is also presented. We also perform bifurcation analysis and plot the stable and unstable points. We verify our methods by experiments on

the travelling kink soliton wave propagation.

Sandeep Koranne
Mentor Graphics Corporation
sandeep_koranne@mentor.com

Vrushali A. Bokil
Oregon State University
bokilv@math.oregonstate.edu

CP21

Numerical Simulation of Diffraction Gratings

In chirped laser pulse amplification, a pulsed laser beam is sent into a compressor consisting of diffraction gratings. Each grating reflects the incoming beam at frequency dependent angles. For perfect gratings there exists analytic expressions for computing the reflected beams. We consider gratings that are imperfect. For example, there could be small variations in line spacing. Imperfections might cause undesirable precursor pulses in the exiting beam. To compute reflection of laser light from gratings, we solve Maxwell's equations for a metallic grating, formulated as the electric field integral equation (EFIE), discretized by a boundary element method. The problem is challenging due to the wide range of scales present. The wavelength of laser light is on the order of a micron, while the grating can be of decimeter size. The discretized problem is a very large dense linear system of equations that must be solved iteratively. The fast multi-pole method (FMM), or alternatively low-rank directional expansions of the Helmholtz kernel, are used to efficiently evaluate matrix-vector products. The presentation will address practical aspects of the FMM including: * Estimates of errors in Helmholtz kernel expansions, * Efficient preconditioning of the linear system resulting from the EFIE * Handling of the near matrix, * Computed results.

Bjorn Sjogreen, Anders Petersson
Center for Applied Scientific Computing
Lawrence Livermore National Laboratory
sjogreen2@llnl.gov, andersp@llnl.gov

CP21

Multilane Traffic Flow

In this talk, we consider macroscopic fluid-like traffic flow models describing multilane traffic flow and account for lane changing effects. We start with single lane models, and consider the scalar model proposed in the 1950s (Lighthill-Whitham 1955, Richards 1956) where velocity-density closure relation is required. We propose a more realistic closure relation, based on real data fitting. We extend the single lane model to include dynamic effects of in-lane car acceleration, leading to a 2x2 hyperbolic system in the spirit of Aw-Rascle 2000, Zhang 2002, guided by microscopic particle-like acceleration models. Using the relationship between car headway and flow density, we develop an acceleration model that reflects well microscopic flow characteristics. The models are then generalized to multilane traffic flow and incorporate mass exchange terms, as well as inter-lane acceleration. Consideration for lane changing includes the potential for velocity gain, available space, as well as data-driven velocity-density closures and realistic drivers (average/probabilistic) inclination to change lanes. Using Roe-type upwind scheme, we reproduce realistic flow patterns and study the influence of lane changing and lane reduction on flow capacity, including comparisons with scalar aggregate multilane models.

Jiah Song
University of Michigan
jiahsong@umich.edu

Smadar Karni
University of Michigan
Department of Mathematics
karni@umich.edu

CP21

Fractional Laplacian Computation on Complex Geometries with Nonhomogeneous Boundary: Algorithm and Applications

We present an algorithm for computing the fractional Laplacian on finite 2D/3D complex domains with nonhomogeneous boundary. For homogeneous bounary computation, to demonstrate the accuracy of this approach, we solve the fractional diffusion equation and fractional Helmholtz equation on a 2D square, a 3D cubic/cylindrical domain and compare the results with the analytic solutions. Then we present the simulation results for solving the fractional diffusion equation on a hand-shaped domain discretized with hexahedrons and prisms in 3D. Finally, we apply the algorithm to solve the surface quasi-geostrophic (SQG) equation on a cubic and a cubic with a circle inside in 3D with the implementation of fractional spectral-viscosity vanishing (SVV) technique to enhance the stability. Simulation results demonstrate that our algorithm can compute the fractional Laplacian on an arbitrary-shaped 2D/3D domain with great precision with various element types with nonhomogeneous boundary, i.e., triangles, hexahedrons, prisms, tetrahedrons and etc. Moreover, our algorithm can capture the subtle dynamics of systems of anomalous diffusion modeled by the fractional Laplacian.

Xiaoning Zheng
Division of Applied Mathematics
Brown University
xiaoning_zheng@brown.edu

CP22

Comparison of Global, Stochastic Optimization Algorithms with Toy Problems and Fitting Multiparameter Models to Dynamic Systems

The evaluation of multiple parameters involved in nonlinear dynamic simulation models based on a minimization of the sum of the squares of the differences between the predictions and experimental data is often a non-trivial step. Classical least squares minimization methods are all local methods that only converge to a local minimum that is not necessarily the global one, the answer depending crucially of the initial guess. The evaluation of the sensitivity of the local minimization solution to the initial guess can be quite time-consuming, especially when the model predictions involve the solution of a set of ODEs the time-integration of which requires by itself a non-negligible computational time. In this work we present a parallel tempering, stochastic method to evaluate that dependence effectively with an application to the evaluations of parameters in dynamic systems. We then compare the parallel tempering algorithm to several other global, stochastic algorithms: generic algorithm (GA), particle swarm algorithm (PSO), simultaneous perturbation stochastic approximation (SPSA) and simulated annealing (SA) using the toy problems, and finally demonstrate and compare the algo-

rithms at fitting several dynamic, multi-parameter models to transient rheology and kinetic fermentation data. With respect to the comparison we use relative accuracy of fitting, time to get to known solution, and number of iterations to arrive at the know solutions.

Matthew J. Armstrong, Corey James, April Miller
United States Military Academy
matthew.armstrong@usma.edu, corey.james@usma.edu, april.miller@usma.edu

CP22

Simulation-based Optimal Placement of Slow Release Oxidant Cylinders

Slow-release oxidant cylinders (SROCs) are an effective and passive way to remediate some contaminated groundwater sites. The fate and transport of the oxidant, contaminant, and Natural Oxidant Demand (NOD) species is modeled with a system of coupled non-linear PDEs. A Fortran simulator is used, solving the system of PDEs with Radial Basis Functions (RBFs). The number, placement, and replacement of these cylinders is optimized using the Implicit Filtering Enhanced Genetic Algorithm (IFEGA) which treats the simulator as a black box. The end result is an optimization tool that groundwater remediators can use to determine the appropriate placement of these cylinders, in the field.

Jesse Clark-Stone
Clarkson University
Department of Mathematics
clarksjl@clarkson.edu

Kathleen Kavanagh, Guangming Yao
Clarkson University
kkavanagh@clarkson.edu, gyao@clarkson.edu

Crimi Michelle
Clarkson Univeristy
mcrimi@clarkson.edu

CP22

ExceLab: Transforming Excel Spreadsheet into a Powerhouse for Calculus and Dynamical Optimization

We present an innovative tool for computational calculus founded on a natural extension of Excel spreadsheet functions. The tool introduces a new breed of spreadsheet calculus functions which accept formulas as a new type of argument, yet can be utilized in formulas just like built-in math functions. For example, a calculus integration function accepts a formula and limits as inputs, and outputs an integral value - much like an intrinsic function accepts a number and computes its square root. The merits of our new calculus functions which overcome inherent spreadsheet restrictions are significant. First, the design permits complete encapsulation of numerical algorithms for solving virtually any computational problem modeled by equivalent formulas using simple input/output pure function evaluation. Several calculus functions are demonstrated for computing integrals, derivatives, and solving differential equations. Second, the calculus functions can be combined naturally with Excel NLP Solver for solving dynamical optimization problems with just a few formulas, and without any programming skills. We demonstrate a simple direct solution method for optimal control problems which combines the NLP Solver with two calculus functions: an ODE solver and an integrator, with remarkable performance in terms of reliability, and computing time. The calculus functions are assembled in an Add-In which integrates seamlessly with MS Excel available at excel-works.com.

Chahid K. Ghaddar
ExcelWorks LLC
cghaddar@excel-works.com

CP22

Optimal Airline De-ice Scheduling

We present a decision support framework for optimal flight re-scheduling on an airline's day of operations when de-icing suddenly becomes necessary due to snow and ice events. Winter weather, especially in areas where such weather is not commonplace, can cause cascading delays and cancellations throughout the system due to the unforeseen need to add de-ice time to each aircraft's turnaround time. Our model optimally re-schedules remaining flights of the day to minimize system delays and cancellations. The model is formulated as a mixed integer linear program (MILP). Structural properties of the model allow it to be decomposed into a finite set of linear programs (LP) and a computationally tractable algorithm for its solution is described. Finally, numerical simulations are presented for a case study of Horizon Air, a regional airline based in the Pacific Northwest of the United States.

Jakob J. Kotas
University of Portland
University of Hawaii at Manoa
kotas@up.edu

Andrew Bracken
Horizon Air
andrewbracken@gmail.com

CP22

The P-center Refueling Facility Location Problem

The p-center refueling facility location problem locates p refueling facilities to minimize the maximum percentage deviation of all drivers. It is a social equity resource allocation model as opposed to a social efficiency p-maximum coverage model. We propose an integer program based on link formulation and analyze its relationship with p-maximum coverage and set covering problems. We develop a link-based implicit enumeration algorithm with an embedded vehicle range-constrained shortest path subproblem to optimally solve the problem. The computational results show that multiple optimal solutions may exist but that they are associated with different total trip distances. In addition, the maximum deviation may not necessarily decrease as the vehicle range or the number of refueling facilities marginally increases.

Cheng-Chang Lin, Chuan-Chih Lin
National Cheng Kung University
cclin@mail.ncku.edu.tw, lindaniel1976@gmail.com

CP22

Geometry of Integer Hulls of Strictly Convex Sets

We study various interesting geometric properties of integer hulls of a class of strictly convex sets. We discuss sufficient conditions under which minimal faces of inte-

ger hulls of costrictly convex sets (a strictly convex set is called a costrictly convex set if either it is a relatively open set or its closure is a strictly convex set) are integral affine sets. We show that under mild assumptions integer hulls of costrictly convex sets are locally polyhedral sets (a convex set is called a locally polyhedral set if its intersection with each polytope is a polytope). Narayanan (2013) studied facial properties of the convex hull of the extreme points of the integer hull of a pointed closed convex set, and we notice that these facial properties also hold for the associated object of a pointed costrictly convex set under mild assumptions. We present alternative proofs of a couple of well established results by studying geometry of integer hulls of costrictly convex sets. Dey and Morán R. (2013) showed that the convex hull of the integer points of a full-dimensional closed strictly convex set is a closed set, and we provide another proof of this result. Moreover, we show that the convex hull of the integer points of an **A**-polyhedral set (a pointed polyhedral set satisfying certain additional assumptions) is a locally polyhedral set (Moussafir established this result in 2003, and we give an alternative proof of this result).

Umakanta Pattanayak
IIT BOMBAY
umakanta@iitb.ac.in

Vishnu Narayanan
Assistant professor, Industrial Engineering and Operations
Research, Indian Institute of Technology Bombay
vishnu@iitb.ac.in

CP22

Gradswaps: A New Heuristic for Large Scale Quadratic Assignment Problems

Gradswaps is a new matrix-based technique for Quadratic Assignment Problems (QAP's) that is particularly appropriate for large-scale QAP's. This is a technique that is generally applicable for optimization problems over permutations where the objective function can be conveniently represented as a smooth nonlinear function of the permutation matrix. It has been used on a visualization problem called ELM-VIS+ and is competitive with other methods. Some of these problems involve optimization over permutations on over 70,000 items.

David E. Stewart
University of Iowa
Department of Mathematics
dstewart@math.uiowa.edu

Cole Stiegler
Department of Mathematics
University of Iowa
cole-stiegler@uiowa.edu

CP23

Numerical Solution of Singular Control Problems Arising in Epidemiology

In this presentation the numerical solution of a class of singular optimal control problems is considered. The approach involves determining the switching times for bang-bang controls as well as determining the points where the solution enters or leaves a singular region. Numerical examples of epidemiology models and cancer models are solved to illustrate the proposed approach.

Mahya Aghaee
Department of Mathematics
University of Florida
mahyaaghaee@ufl.edu

William Hager
University of Florida
Department of Mathematics
hager@ufl.edu

CP23

Analytic Center for the Passivity LMI

Passivity is a desired property of a dynamical system, since physical systems without any external input do not produce energy, i.e., are passive. Thus, for robustness reasons it is interesting to analyze the distance to non-passivity of a passive system w.r.t. to disturbances of the system matrices. In this talk we will consider a new approach for the computation of the passivity radius of linear time-invariant systems with the help of the so-called analytic center. The analytic center is the minimizer of a certain convex functional related to the passivity linear matrix inequality (LMI) and can be characterized by a cubic matrix equation. It has certain nice properties, and, thus, the hope is that being at this point will provide a 'good' method for computing the passivity radius. We will show how one can compute the analytic center effectively and consider a simple example for the computation of the passivity radius. We will also see that the equations defining the analytic center are not preserved under the Cayley transform.

Daniel S. Bankmann, Volker Mehrmann
Technische Universität Berlin
bankmann@math.tu-berlin.de,
mehrmann@math.tu-berlin.de

Paul Van Dooren
Université Catholique de Louvain
paul.vandooren@uclouvain.be

Yurii Nesterov
CORE
Universite catholique de Louvain
yurii.nesterov@uclouvain.be

CP23

Geometric Nonlinear Controllability and Flight Mechanics

Linear controllability conditions for linearized systems are not necessary. That is, there exists a class of nonlinear systems that are linearly uncontrollable but nonlinearly controllable. Geometric control theory provides useful tools for analyzing nonlinear controllability of dynamical systems. In particular, it allows for identification of the ability to generate motions along unactuated (non-intuitive) directions through specific interactions between the system dynamics and control inputs. In this work, we will summarize the most useful tools in the literature of Geometric Control Theory. Then, we will provide some of our recent results, in which we applied successfully some the most general, but hard to apply theorem on nonlinear controllability, to flight mechanics.

Sameh Eisa
New Mexico Tech

seisa@uci.edu

Haithem Taha
University of California, Irvine
hetaha@uci.edu

CP23

Decay Estimates for Semilinear Timoshenko Systems with Local Memory

We investigate decaying behaviors of the solutions to a semilinear Timoshenko system, with equal wave speeds and subject to just a local memory damping mechanism. With the help of the multiplier method, energy estimation, and some specially designed analysis approaches for the problem, we establish uniform decay rates for the solutions to this Timoshenko system, which are optimal in some sense, under only basic conditions on the memory kernels. Also, we obtain polynomial/exponential decay rates, when the memory kernel decays polynomially/exponentially. These results indicate that a local memory effect is enough to produce an entire dissipation mechanism, and the same decay rates, as those for the case of the entire memory effect, can be obtained. Moreover, assuming much weaker conditions on the memory kernels, the theorems here gives stronger conclusions than the previously given ones (when with local memory effect). This is joint work with Kun-Peng Jin and Ti-Jun Xiao.

Jin Liang
Shanghai Jiao Tong University
jinliang@sjtu.edu.cn

CP24

Coupling of Material Point Method with Finite Element Method based on a Shared Background Grid

I will present an new strategy for the coupling of the material point method (MPM) with the finite element method (FEM). In [1], the coupling requires the finite element grid and the material point background grid to have a comparable size. As shown in [2] however, when the two sizes are not comparable, the solution accuracy may suffer, and the MPM particles may penetrate the FEM body, producing unphysical results. This issue has been solved in [2], using a particle-to-surface contact algorithm. However, the algorithm is computationally demanding since a global search is necessary. Moreover, in [2], only quadrilateral (or hexahedral) finite elements are considered. We propose a new monolithic coupling strategy where the MPM background grid is a finite element grid attached to the body discretized with the FEM. To locate the material point particles within the MPM background grid, the point locating algorithm described in [3] is used. In this way, we completely eliminate the need of a global search since at every time step the finite element hosting a given MPM particle is known. Moreover, thanks to the monolithic coupling, the MPM particles cannot penetrate the FEM elements so no contact search algorithm is necessary. [1] YP Lian, X Zhang, and Y Liu, COMPUT METHOD APPL M, 2011. [2] ZP Chen, XM Qiu, X Zhang, and YP Lian, COMPUT METHOD APPL M, 2015. [3] G Capodaglio and E Aulisa, COMPUT FLUIDS, 2017.

Giacomo Capodaglio
Texas Tech University
giacomo.capodaglio@ttu.edu

Eugenio Aulisa
Department of Mathematics and Statistics.
Texas Tech University
eugenio.aulisa@ttu.edu

CP24

A Finite-volume, Semi-implicit Multifluid Algorithm for the Simulation of Counterstreaming Plasma Dynamics

The simulation of counterstreaming plasmas requires a multifluid model to accurately represent phenomena such as species interpenetration. The use of a single velocity field in multispecies fluid codes often results in unphysical solutions; on the other hand, kinetic approaches are too expensive for practical simulations. This talk will present EUCLID, a high-order finite-volume semi-implicit multifluid code. The Euler equations are solved for each ion species and the electrons, and the species interact through electrostatic forces, friction, and thermal equilibration. A high-order Poisson solver is used to compute the electrostatic potential at each time step. The equations are discretized in space using the 5th order WENO scheme. Adaptive mesh refinement is used around regions of strong interactions through Chombo, a block-structured AMR library. The semi-implicit additive Runge-Kutta methods are used for time integration, where the stiff modes are integrated implicitly in time, while the remaining terms are integrated explicitly. We present the verification of EUCLID for several benchmark test cases, as well as the simulation of counterstreaming plasmas. We show that this approach is able to accurately capture plasma interpenetration. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344 and funded by the LDRD Program at LLNL under project tracking code 17-ERD-081.

Debojyoti Ghosh
Lawrence Livermore National Laboratory
Center for Applied Scientific Computing
ghosh5@llnl.gov

Christos Kavouklis, Thomas Chapman
Lawrence Livermore National Laboratory
kavouklis1@llnl.gov, chapman29@llnl.gov

Richard Berger
AX DIVISION
Lawrence Livermore National Laboratory
berger5@llnl.gov

CP24

Nonlinear Electrophoresis of a Charged Dielectric Droplet: A Numerical Study

The study of electrophoresis of a charged spherical droplet is important for its wide applications in atmospheric physics, inkjet printers, pharmaceutical, lab-on-a-chip, and electrospray applications. The dielectric polarization of the droplet under an external electric field creates a nonlinear dependence of the electrophoretic velocity on the applied electric field. The surface of the droplet is not stationary and a lower droplet viscosity increases the fluid convection in the Debye layer, which in turn enhances the double layer polarization and surface conduction. The polarization effect of the double layer due to fluid convection is analyzed extensively in the present work. Fluid inside and outside the droplet is governed by the Navier-Stokes equations, ion transport in the electrolyte is described by

Nernst-Planck equation, the electric potential within and outside the droplet is governed by the Laplace and Poisson equations, respectively. These nonlinear governing equations along with proper boundary conditions are solved numerically through a pressure correction based iterative SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm. Electrophoretic velocity diminishes with the increase of droplet-to-electrolyte viscosity ratio and it also decreases with the rise of droplet-to-electrolyte permittivity ratio. The impact of double layer polarization and surface conduction effect is illustrated extensively.

Partha Sarathi Majee
Indian Institute of Technology Kharagpur
psmajee5@gmail.com

Somnath Bhattacharyya
I.I.T. Kharagpur
somnath@maths.iitkgp.ernet.in

CP24

A New Approach for Designing Moving-water Equilibria Preserving Schemes for the Shallow Water Equations

Shallow water models are widely used to describe and study free-surface water flow. They are hyperbolic systems of balance law and usually solved by finite volume methods, which are appropriate numerical tools for computing nonsmooth solutions. One requirement when designing numerical schemes for shallow water models is to preserve a delicate balance between the flux and source terms since many physical related solutions are small perturbations of some steady state solutions. In this presentation, we construct a new general approach of designing well-balanced central-upwind schemes for shallow water models, which can capture and preserve the "lake at rest" steady states and also the moving steady states, even with complicated bottom frictions, and illustrate their performance on a number of numerical examples.

Tong Wu
Tulane University
twu18@ncsu.edu

Yuanzhen Cheng
Tulane Univeristy
ycheng@tulane.edu

Alina Chertock
North Carolina State University
Department of Mathematics
chertock@math.ncsu.edu

Michael Herty
RWTH Aachen University
herty@mathc.rwth-aachen.de

Alexander Kurganov
Tulane University
kurganov@math.tulane.edu

CP24

A New Implementation of the Vortex Method

We present a new implementation of the vortex method for the incompressible Euler equations. This work focuses on smooth vorticity distributions as opposed to vortex sheets. As usual the vorticity is carried by Lagrangian particles and the velocity is recovered by the Biot-Savart law. The new implementation combines remeshing, adaptive refinement, and treecode acceleration to resolve complex features of the flow. Applications are given to tracer transport and vortex dynamics on a rotating sphere, and to vortex dynamics in two-dimensional free-space.

Robert Krasny
University of Michigan
Department of Mathematics
krasny@umich.edu

Peter A. Bosler
Sandia National Laboratories
Center for Computing Research
pabosle@sandia.gov

Ling Xu
University of Michigan, Ann Arbor
lingxu@umich.edu

CP25

Investigating the Role of Non-covalent Interactions in Conformation and Assembly of Triazine-based Sequence-defined Polymers

Grate and co-workers at Pacific Northwest National Laboratory recently developed high information content triazine-based sequence-defined polymers that are robust by not having hydrolyzable bonds and can encode information by having various side chains. Through molecular dynamics (MD) simulations, the triazine polymers have been shown to form particular sequential stacks, have stable backbone-backbone interactions through hydrogen bonding and pi-pi interactions, and conserve their cis/trans conformations throughout the simulation. However, we do not know the effects of having different side chains and backbone structures on the entire conformation and whether the cis or trans conformation is more stable for the triazine polymers. For this reason, we investigate the role of non-covalent interactions for different side chains and backbone structures on the conformation and assembly of triazine polymers in MD simulations. Since there is a high energy barrier associated to the cis-trans isomerization, we use replica exchange molecular dynamics to sample various conformations of triazine hexamers. To obtain rates and intermediate conformations, we use the recently developed concurrent adaptive sampling algorithm for dimer of triazine trimers. We found that the hydrogen bonding ability of the backbone structure is critical for the triazine polymers to self-assemble into nanorods, rather than that of the side chains, which can help researchers design more robust materials.

Surl-Hee Ahn
Stanford University
sahn1@stanford.edu

Jay Grate
Pacific Northwest National Laboratory
jwgrate@pnnl.gov

Eric F. Darve
Stanford University
Mechanical Engineering Department

darve@stanford.edu

CP25

Approaching Solidification Fronts in the Extended Stefan Problem for Binary Alloys in Finite Domains

The manner in which an alloy solidifies has an impact on its microstructure, and thus on the quality of the final product. In order to gain an understanding of this process, we consider a model for the solidification of a binary alloy which accounts for constitutional supercooling. Although a similarity solution exists when the problem domain is semi-infinite, in practice solidification problems related to many real-world applications are posed on finite domains. We consider the solidification of a binary alloy on a symmetric one-dimensional planar domain, finding that two identical solidification fronts start from each boundary and move inward toward one another. We perform an asymptotic analysis to better understand the solidification front dynamics. The two fronts are initially far from one another and move in a self-similar manner toward the interior of the domain for small time. However, when the two fronts are sufficiently close, there is a build-up of impurities in the liquid phase between the fronts, which increases the supercooling and thereby slows the fronts. Eventually, the system evolves to its minimum temperature, with the liquid phase following in thermodynamic equilibrium. The asymptotic solutions show excellent agreement with numerical simulations of the full problem, as well as with experimental data involving the solidification of silicon in a cast. Our analysis highlights the important role of supercooling in the solidification of binary alloys.

Ferran Brosa Planella, Colin Please, Robert Van Gorder
Mathematical Institute
University of Oxford
brosa@maths.ox.ac.uk, please@maths.ox.ac.uk, vangorder@maths.ox.ac.uk

CP25

Higher Order Methods for Simulating Crack Propagation

High order finite element solutions of crack and re-entrant corner problems in elasticity are notoriously challenging to attain. The slow convergence rates for these classes of problems are tied to the low degree of regularity possessed by the solution. The need for high order solutions is motivated by long running simulations of crack propagation. To this extent, we develop higher order finite element methods for crack and re-entrant corner problems in elasticity. The method exploits a priori knowledge of the singular behavior of the fields to construct an alternate regular solution. Solving for the alternate problem yields optimal rates of convergence. Namely, standard finite element error estimates in the L^2 and H^1 norm are proved to hold. The salient feature of the method is the lack of additional degrees of freedom in comparison with standard Galerkin finite element formulation. Effectively, for the same computational cost we obtain a higher order of accuracy. Furthermore, unlike other state of the art tools, the method preserves the well conditioned nature of the linear system and does not require the knowledge of the exact asymptotic behavior, hence the method can be readily applied to singular problems for which we are not endowed with an explicit asymptotic solution(eg. as cracks in graded materials). The method is verified with respect several analytical.

Maurizio M. Chiaramonte
Princeton University
chiaramonte@princeton.edu

CP25

Effect of Nonlocality on Guided Waves in an Elastic Plate with Voids

In this paper, the propagation of guided waves in an infinite plate of finite thickness constituted of nonlocal elastic material with voids has been studied. The theory of nonlocal elastic solid with voids recently developed by Singh et al. [Singh, D., Kaur, G., Tomar, S.K., Waves in nonlocal elastic solid with voids, *J*ournal of Elasticity, 2017] has been used for the purpose. Dispersion relations for symmetric and anti-symmetric vibrations have been derived using appropriate boundary conditions at the faces of plate. It is found that both symmetrical and anti-symmetrical vibrations are dispersive in nature and found to be affected by the presence of nonlocality as well as voids in the plate. Due to the presence of nonlocality, both the families face critical frequencies above which they cease to propagate. For a particular model, the variations of phase speeds and attenuation coefficients of both the families with frequency, nonlocality and void parameters are depicted graphically. Some earlier derived results have been deduced from present formulation [Chandrasekharaiah, D.S., Rayleigh-Lamb waves in an elastic plate with voids, *J*ournal of Applied Mechanics, 1987].

Gurwinderpal Kaur
Panjab University Chandigarh
grewalgk1991@gmail.com

Dilbag Singh
Department of Mathematics,
Panjab University, Chandigarh, India
kahlondilbag80@gmail.com

Sushil Kumar Tomar
P.U. CHANDIGARH
sktomar66@gmail.com

CP25

Defining Crystals Locally via Voronoi Topology

In a perfect world, fewer objects are easier to define than a crystal: all integral combinations of a set of basis vectors. The real world, though, is certainly not perfect, and a more robust definition of crystallinity is desirable. We introduce and develop one such an approach in which crystals are defined locally, instead of globally, using Voronoi topology. In addition to providing a natural setting in which to define finite-temperature crystals, this approach also facilitates the precise characterization and identification of traditional defects. Jumping from the native continuous to the more natural discrete setting enables the application of combinatorial techniques to the study of real physical systems.

Emanuel A. Lazar
University of Pennsylvania
mlazar@seas.upenn.edu

CP26

Multi-scale Asymptotics for Atmospheric Waves

and Precipitation

The lack of understanding of the tropical atmosphere is a major hinderance to improve the predictability of the global climate. In tropics, the Madden-Julian Oscillation (MJO) is the dominant component of intraseasonal (30-60 days) variability. The MJO is an equatorial wave envelope of complex convective processes, coupled with planetary-scale circulation anomalies. In this talk, I will present a new model that captures the mechanisms of the interactions between MJO and other tropical and extratropical waves. By using the method of multis-cale asymptotics with different time scales, simplified asymptotic equations are derived for the resonant interaction of tropical and extratropical waves, such as Rossby waves. The reduced equations is an ODE system for wave amplitudes. The ODE system are shown to illustrate the initiation/termination of MJO.

Shengqian Chen
Nanjing University of Information and Science Technology
shengqianchen11@163.com

CP26

A Linearized Stability Analysis of Acoustic-Gravity Waves in a Volcanic Conduit with a Spatially Variable Background State

Explosive volcanic eruptions involve the ascent of multiphase magma through crustal conduits towards Earth's surface at sufficiently high rates that the mixture fragments from a suspension of bubbles and crystals in a melt to a mixture of liquid and solid fragments in a gas. Eruptions are largely driven by the growth and expansion of bubbles during ascent which may accelerate the flow to high speeds, up to or perhaps even exceeding the fluid sound speed. Here we consider short-time, unsteady behavior during explosive volcanic eruptions by considering perturbations to a steady state, fragmenting flow of bubbles and liquid through an axisymmetric conduit. We study flow stability in the presence ofsmall amplitude mechanical disturbances. The linearized governing equations describe wave motion in an accelerating flow with strongly variable material properties, within a conduit of non-constant cross sectional area. The equations are solved numerically by applying a finite difference discretization with weak enforcement of boundary conditions (that leads to a provably stable method) and an eigenmode analysis determines the stability of perturbations to various background states.

Brittany Erickson
Portland State University
berickson@pdx.edu

Leif Karlstrom
University of Oregon
leif@uoregon.edu

CP26

Mathematical Modelling of Rayleigh Wave Propagation in Non-homogeneous Media

A finite difference technique has been applied to study the numerical stability of phase velocity and group velocity of the Rayleigh wave propagation in non-homogeneous layered media. The study will be compared the numerical solution with analytic solution. It has been observed that with the small changes of non-homogeneity parameters presented in the layered media phase and group velocity make large changes in their propagation due to the ill-condition of the problem.

Santanu Manna
Indian Institute of Technology Indore
smanna@iiti.ac.in

CP26

A New Scheme for Water Flow-driven Stratigraphic Forward Modeling with Multiple Lithologies

Stratigraphic forward models are essential tools to understand the nature of subsoil rocks and the architecture of sedimentary basins. In these models, sediment transport is governed by a linear diffusion law at the continuous level while water flow is described through an ad hoc algorithm at the discrete level, such as MFD (Multiple Flow Direction). In this work, we propose a new model that enables us to couple sediment transport with water flow at the continuous level, taking into account multiple lithologies. The resulting water and lithology fluxes are nonlinear and involve p-Laplacians in order to get more realistic landscape evolutions, ensuring finite speed of propagation for knickpoints. Our model also considers several diffusion coefficients in order to distinguish between marine and continental domains. Furthermore, dealing with several lithologies leads to a better understanding of the structure of the subsoil. In particular, it allows us to observe the formation of the sediment layers over time and to record their concentration in each lithology. To approximate the associated system of equations, our numerical scheme is based on the Finite Volume method. Due to the p-Laplacians, it requires an approximation of the gradient norms to be built at each interface between cells. The resolution is then made using a Newton method. To illustrate the model and to show the capabilities of the numerical scheme, various configurations in several test cases are presented.

Nicolas Peton, Quang Huy Tran
IFP Energies nouvelles
nicolas.peton@ifpen.fr, quang-huy.tran@ifpen.fr

Clément Cancès
Inria
clement.cances@inria.fr

Sylvie Wolf
IFP Energies Nouvelles
sylvie.wolf@ifpen.fr

Didier Granjeon
IFP Energies nouvelles
didier.granjeon@ifpen.fr

CP26

Polluting is Easy, Cleaning is Hard: The Challenge of Flow Heterogeneity for Direct Air Capture of Co_2

Extracting large quantities of CO_2 from the atmosphere is necessary to meet the goals set in the Paris Agreement on climate change. Direct air capture (DAC) of CO_2 by chemical processing plants could play a pivotal role in meeting these negative emissions targets. The question is: Where should CO_2 capturing units be placed? More generally, we consider the problem of positioning intake units in a heterogeneous flow environment to capture something moved by the flow through the environment. For example, dis-

tributed sensor networks, and colonies of mussels – congregated on the concrete pilings of offshore wind farms – feeding on plankton in the ocean. We consider a simple model of a heterogeneous flow environment: a two-dimensional mixing flow with both chaotic and regular regions. This model reduction reveals the most salient and noteworthy features of the capture problem, such as that the more ambitious the capture target is, the more dominant becomes consideration of unit location, and that intake unit efficiency varies with the required capture rate. Most importantly, placing capturing units in random locations without accounting for flow heterogeneity carries a remarkably high risk of failure.

Lachlan Smith
Dept. of Chemical & Biological Engineering
Northwestern University
lachlan.smith@northwestern.edu

Julio Ottino
Northwestern University
Evanston, IL 60208-3109
jm-ottino@northwestern.edu

Guy Metcalfe
School of Mathematical Sciences
Monash University
guy.metcalfe@monash.edu

CP27

Joule Heating Effect of Electroosmotic Flow through Soft Nanochannel

The present study deals with thermal transport characteristics of an electrolyte solution flowing through a slit nanochannel with polyelectrolyte (PEL) walls, known as soft nanochannel. The sources of the fluid flow are the electrokinetic effects that trigger an electroosmotic flow (EOF) under the impact of a uniformly applied electric field. The direction and flow rate of EOF is governed by strength of the electric field, concentration of electrolytes, temperature, pressure, viscosity etc. The thermal transport characteristics is mainly dependent on Joule heating which is generated when an electric field is applied across conductive liquids. The present study includes the coupling Poisson- Boltzmann equation, the modified Darcy-Brinkman extended Navier-Stokes equations, the modified Nernst-Planck equation and the modified energy equation. Governing equations along with proper boundary conditions are solved numerically through a control volume approach over a staggered grid arrangement. Discretized equations are solved through the pressure correction based iterative SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm. The results are expressed in form of average velocity (u_{avg}), average entropy generation (S_{avg}) for both step-like PEL and diffuse PEL.

Sirsendu Sekhar Barman
IIT Kharagpur
sirsendu012@maths.iitkgp.ernet.in

Somnath Bhattacharyya
I.I.T. Kharagpur
somnath@maths.iitkgp.ernet.in

CP27

Heat Transfer through a Viscous Droplet at Moderate Re: A Numerical Study

A numerical study on heat transfer across the interface of a viscous deformable heated droplet falling under gravity in another fluid medium is analyzed. The Navier-Stokes equations together with the energy equation is solved through a pressure correction based iterative algorithm SIMPLE, along with a suitable boundary condition at the interface separating two immiscible fluids. The droplet surface evolution is captured by the level set method, in which the interface is represented by the embedded set of zero level of a scalar distance function defined in the whole computational domain. The form of the wake due to the viscous droplet and its influence on heat transfer and drag coefficient are analyzed for a wide range of physical parameters. For viscous droplets, results show a region of high temperature in the wake region behind the droplets and a temperature distribution along the droplet surface. It is evident that increasing the Reynolds number, the rate of heat transfer is significantly increased due to enhancement in the internal circulation. Also the increment in viscosity decelerate fluid circulation inside the droplet which reduces the rate of heat transfer. It is shown that, as the droplet become more distorted, the interfacial area increases, resulting total interfacial transfer is higher than the case of spherical particles. The droplet becomes more elongate in the direction of its major axis when lower surface tension force is considered at the droplet surface.

Dipankar Kundu
IIT KHARAGPUR
dip06kundu@gmail.com

Somnath Bhattacharyya
I.I.T. Kharagpur
somnath@maths.iitkgp.ernet.in

CP27

On a Navier-Stokes-Fourier-like System Capturing Transitions Between Viscous and Inviscid Fluid Regimes and Between No-slip and Perfect-slip Boundary Conditions

We study a model with implicit constitutive relations that captures non-Newtonian fluids with temperature-dependent coefficients, in particular those which are able to describe the threshold slip phenomenon with the temperature-dependent activation criteria. Such a model is able to describe all states of the fluid from the yield stress, through the Newtonian fluid up to the inviscid case only by the temperature change. Also, concerning the boundary conditions, we are able to capture the standard Navier's slip, but also the threshold slip case, i.e. the stick-slip or the perfect slip-slip condition. These models always include the activation, however, the standard constitutive relations (yield stress, inviscid fluid, no slip or perfect slip boundary conditions) are the limit cases when certain activating coefficient tends to infinity for some temperature. Finally, also the large-data and the long-time existence analysis is provided.

Erika Maringova
Charles University
maringova@karlin.mff.cuni.cz

Josef Zabensky
University of Wuerzburg

josef.zabensky@gmail.com

CP28

Python Tools for Linking EFDC with Openfoam in Support of Pier Design and Placement in a Tidal System

We present a set of Python tools for linking the EFDC (Environmental Fluid Dynamics Code) modeling program, which was developed by the US EPA (United States Environmental Protection Agency), with OpenFOAM (Open source Field Operation And Manipulation), a highly scalable and open-source CFD (Computational Fluid Dynamics) software. The new tools provide a feed-forward linkage between EFDC and OpenFOAM for the purpose of simulating the performance of alternative pier designs and placements in a tidal system. The EFDC code is used to simulate sediment scour and deposition that occurs as a result of tidal flows around two pier structures emplaced in a bay. The OpenFOAM code is used to develop and visualize high-fidelity tracks of fluid flow around the piers and associated areas of scour and deposition in the bay. The Python linkage tools automatically generate the required OpenFOAM mesh and boundary files based on the bottom elevation contours provided with the EFDC output. A sixth-order inverse distance weighting scheme for interpolating the bottom elevation data was found to provide adequate smoothing for mesh generation, allowing the icoFoam solver to be applied at a 25 cm by 25 cm by 25 cm grid cell resolution. Increasing the resolution to 10 cm by 10 cm by 10 cm required switching to the more robust (and computationally expensive) pimpleFoam solver.

Shawn L. Matott
University at Buffalo
Center for Computational Research
lsmatott@buffalo.edu

Michael Silver
University at Buffalo
Architecture and Urban Planning
mike.s.silver@gmail.com

CP28

The Suitability of the Effective Wavefield as a Tool to Predict Wave Attenuation over Long Distances

For an incident wave train propagating into a rough (randomly disordered) medium, wave localisation refers to exponential attenuation (on average) of the wave train in the rough medium. A key quantity of interest is the attenuation rate as a function of the incident wave properties (frequency) and the properties of the given medium, including the statistical properties of the disorder in media. Effective media theory is an appealing way to approach the problem, as it provides analytical insight, circumventing the need to compute individual wave fields repeatedly for different realisations of the disorder, as well providing the opportunity for elegant mathematical analysis. I will present the theory alongside corresponding results and discuss the applicability of effective media theory for making predictions of attenuation of (linear) waves over long distances in media with continuously varying properties.

Malte A. Peter
University of Augsburg
malte.peter@math.uni-augsburg.de

Luke Bennetts
University of Adelaide
luke.bennetts@adelaide.edu.au

Sebastian Rupprecht
University of Augsburg
sebastian.rupprecht@math.uni-augsburg.de

CP28

Mathematical Model of Lead vs Lag on Left-turn Phasing at Traffic Lights

Left-Turn arrows at intersection across the United States are primarily leading left-turn. Meaning that the left turn happens before the traffic light turns green. Similarly, lagging left-turn use a green left arrow after the green light. We are going to present a mathematical model to compare how these two choices impact traffic safety. We will use data from Phoenix, AZ metropolitan area where different townships have different left-turn policies. We will present the model, its results, and its limitations and how it could drive public policy.

Filippo Posta
Grand Canyon University
filippo.posta@gcu.edu

CP28

Adaptive Regulation of Nitrate Transceptor Protein NRT1.1 in Fluctuating Soil Nitrate Conditions

Plant adaptation to changes in soil nitrate concentrations involves sophisticated nitrate signaling and transport systems that modulate a variety of physiological and developmental responses. Many of these responses are regulated by a transceptor NRT1.1—a transporter cum a receptor of nitrate signaling. However, we know very little about their molecular mechanisms. Here we report an adaptive mechanism by which NRT1.1 mediated dual nitrate uptake and biphasic primary nitrate responses are regulated in a wide range of nitrate variations. High and low affinity modes of nitrate binding differentially enhance intrinsic asymmetries between the two protomers of NRT1.1. This generates strong/weak form of intramolecular allosteric communications between the nitrate binding and the phosphorylation site, Thr-101. The resulting NRT1.1 dimerization generates two distinct signals that are integrated by a Gate Function forming an incoherent feedforward circuit. This circuit controls a phosphorylation switch that eventually establishes biphasic stable states of NRT1.1. It therefore reveals that adaptive role of NRT1.1 is achieved through proportional activation/inhibition of upstream components of nitrate signaling not primarily through feedback mechanisms.

Mubasher R. Rather
CENTRAL UNIVERSITY OF RAJASTHAN, AJMER, INDIA
2014phdmt04@curaj.ac.in

Amit Chakraborty
School of Mathematics, Statistics and Computational Sciences
Central University of Rajasthan, Ajmer, India
amitc.maths@curaj.ac.in

Bai-Lian Li
University of California, Riverside

bai-lian.li@ucr.edu

CP28

Numerical Simulation of Solid Phase Adsorption Models using Time-integrated, Upwinded Finite Element Strategies

The emergence of biopharmaceuticals as a way to manage chronic disease has created a need for technologies that deliver purified products efficiently and quickly. This has led to increased research on the development of high-capacity ion-exchange membranes to improve adsorption-based bioseparations processes. In this work, a numerical scheme for approximating solutions to mathematical models associated with advection-dominated solid phase adsorption processes is developed and analyzed. The scheme utilizes continuous Galerkin finite elements for discretization of the transport equation, stabilized via streamline upwinding. The work is motivated by previous research which uses temporal integration and mixed finite element methods to discretize similar model equations. The analysis verifies solvability of the upwinded discrete scheme, and numerical convergence rates that follow the expected estimates are also provided. The results of the algorithm are compared with experimental data and the effects of various velocity profiles on the model results are examined.

Anastasia B. Wilson
Augusta University
Department of Mathematics
anawilson@augusta.edu

Eleanor Jenkins
Clemson University
lea@clemson.edu

Juan Wang
Bristol-Myers Squibb
juanw@g.clemson.edu

Scott Husson
Clemson University
Department of Chemical and Biomolecular Engineering
shusson@clemson.edu

MS1

Quantifying the Effects of Intraluminal Thrombi and their Poroelastic Properties on Abdominal Aortic Aneurysms

An abdominal aortic aneurysm (AAA) occurs when weakened aortic walls bulge or dilate. Because the aorta is the primary conduit of blood to the body, a ruptured AAA can cause life-threatening bleeding. Intraluminal thrombi (ILT) are found in most of AAAs of clinically relevant size, and their influence on the wall stress and risk of rupture remains highly controversial. We will present a novel, poroelastic model for intraluminal thrombus (ILT), which captures both the flow within ILT and its deformation. The model for ILT is coupled with pulsatile blood flow and arterial wall deformation. The fully coupled model is used to study the biomechanics in a patient-specific abdominal aortic aneurysm (AAA). Using finite element analysis, numerical simulations were performed to investigate the role of ILT on the risk of AAA rupture as assessed by Peak Wall Stress (PWS). We will present a numerical study of the effects of ILT permeability on the vascular wall stress, as well as the risk of ILT embolization.

Martina Bukac
University of Notre Dame
mbukac@nd.edu

Miguel Rodriguez
University of California Berkeley
miguelr@berkeley.edu

Shawn Shadden
University of California, Berkeley
shadden@berkeley.edu

MS1

Cardiac Fluid-Structure Interaction by a Hyperelastic Immersed Boundary-finite Element Method

The immersed boundary (IB) method is a mathematical framework for fluid-structure interaction (FSI) that models systems in which an incompressible structure is immersed in a viscous incompressible fluid. Modern versions of the IB method allow the immersed structures to be described using nonlinear constitutive laws that can account for the structure of biological materials, and that can be fit to experimental data. This talk will describe progress towards developing a new IB FSI model of the heart with a realistic anatomical geometry based on magnetic resonance image data along with invariant-based hyperelastic constitutive models that account for the fiber architecture of the atria and the ventricles of the heart as well as the cardiac valves. Large-scale simulations of cardiac FSI using this model will also be presented.

Boyce E. Griffith
Departments of Mathematics and Biomedical Engineering
University of North Carolina at Chapel Hill
boyceg@email.unc.edu

Charles Puelz, Simone Rossi
Department of Mathematics
University of North Carolina at Chapel Hill
cpuelz@unc.edu, srossi@email.unc.edu

MS1

A Mathematical Framework for Analysis of Vascular Stents

Abstract not available at time of publication.

Josip Josip Tambaca
University of Zagreb, Croatia
tambaca@math.hr

MS1

A Multiscale/Multiphysics Coupling Framework for Bioprosthetic Heart Valves (BHVs)

Bioprosthetic heart valves (BHVs) are the most popular replacements for diseased valves. However, the mechanisms that underlie BHVs failure remain poorly understood. Therefore, developing a mathematical framework which captures material damage phenomena in the fluid-structure interaction environment would be very valuable for studying BHVs failure. We introduce two coupling problems and the corresponding numerical methods for this framework. In the first problem the coupling strategy for fluid and thin structure is investigated. This problem

presents unique challenge due to the large deformation of BHV leaflets which causes dramatic changes in the fluid subdomain geometry. To overcome the challenge we developed the immersogemetric method where the fluid and structure are discretized separately and coupled through penalty forces. To ensure the capability of the developed method in modeling BHVs, we verified and validated this method. In the second problem we developed a coupling strategy for peridynamics and classical elastic theory. Here the peridynamic model and the elastic model are solved with a partitioned approach, and the two solvers communicate by exchanging proper boundary conditions. We analyzed different coupling scenarios on a simplified problem to obtain explicit expressions for the optimal convergence rate index. Both analysis and numerical experiments suggest that the Robin boundary condition with optimal coefficient is the most robust choice.

Yue Yu
Department of Mathematics, Lehigh University
yuy214@lehigh.edu

MS2

Sensitivity and Bifurcation Analysis of a Differential Algebraic Equation Model for a Microbial Electrolysis Cell

Microbial electrolysis cells (MECs) are a promising new technology for producing hydrogen cheaply, efficiently, and sustainably. The technology is based on microbial fuel cells in which bacteria oxidize an organic substrate to generate current, providing decreased electricity costs when compared to direct electrolysis. MECs are also more efficient than fermentation methods and can be fed fermentation effluent or cheap and readily available wastewater. However, to scale up this technology, we need a better understanding of the processes in the devices. In this effort, we present an semi-explicit index one differential-algebraic equation (DAE) model of a microbial electrolysis cell with an algebraic constraint on current. We then perform sensitivity and bifurcation analysis for this DAE system. The sensitivity analysis yields temporal regions wherein reactor adjustments will have the largest impact on productivity. For the bifurcation analysis, we present results concerning the classification of transcritical bifurcations in the input flow rate. Overall, our conclusions provide guidance on optimizing performance of batch-fed and continuous-flow reactors.

Harry Dudley
Applied Mathematics
University of Colorado - Boulder
harry.dudley@colorado.edu

David M. Bortz
University of Colorado
Department of Applied Mathematics
dmbortz@colorado.edu

MS2

Transport and Feedback in Models of Self-organizing Vegetation Patterns

Bands of vegetation alternating periodically with bare soil have been observed in many dryland environments since their discovery in the Horn of Africa in the 1950s. Mathematical modeling efforts over the past two decades have sought to account for these bands via a selforganizing interaction between vegetation and water resources. Various modeling frameworks have been proposed that are capable of generating similar patterns through self organizing mechanisms which stem from key assumptions regarding plant feedbacks on surface/subsurface water transport. We discuss a hierarchy of hydrology/vegetation models for the coupled dynamics of surface water, soil moisture, and vegetation biomass on a hillslope. We identify distinguishing features and trends for the periodic traveling wave solutions when there is an imposed idealized topography.

Mary Silber
University of Chicago
msilber@uchicago.edu

Sara Bonetti
Duke University
sara.bonetti@duke.edu

Punit Gandhi
Mathematical Biosciences Institute, Ohio State University
gandhi.138@mbi.osu.edu

Sarah Iams
Harvard University
Cambridge, MA
siams@seas.harvard.edu

Amilcare Porporato
Duke University
amilcare.porporato@duke.edu

MS2

Topological Data Analysis of Biological Aggregation Dynamics

This talk assumes no prior knowledge of topology. Collective motion is seen in biological aggregations such as bird flocks, fish schools, and insect swarms. We use computational persistent homology, the workhorse of topological data analysis, to analyze a seminal model of collective motion due to Vicsek et al. (1995). The model describes an ensemble of self-driven particles. At each time step, each particle's heading is determined by interactions with neighbors, subject to noise. Using time series of the particles' positions and headings, we assign a topological signature to the evolving ensemble. This signature identifies dynamical events that traditional methods do not. Time permitting, we pose open questions related to topological signatures averaged over many simulations of the noisy model, and discuss how topological signatures may be used to select between models of experimental aggregation data.

Chad M. Topaz
Department of Mathematics and Statistics
Williams College
chad.topaz@gmail.com

Lori Ziegelmeier, Tom Halverson
Dept. of Mathematics, Statistics, and Computer Science
Macalester College
lziegel1@macalester.edu, halverson@macalester.edu

MS2

Solitary Waves in an FPU Lattice with Second-neighbor Interactions

The interplay between dispersion and nonlinearity in many physical systems leads to the formation of solitary waves,

localized coherent structures that carry energy through the system. For example, such waves were experimentally observed in granular materials and are believed to be responsible for energy transport in muscle proteins. We consider solitary waves in a one-dimensional lattice with nonlinear first-neighbor and harmonic second-neighbor interactions. We show that when the interactions are strongly competitive, such waves must be strictly supersonic, in the sense that solitary wave solutions do not exist in a velocity gap above the sonic limit and below a certain minimal velocity threshold. Solutions with velocities above the threshold bifurcate from a short-length linear wave and have damped oscillatory tails, thus representing a discrete analog of capillary-gravity waves. We derive modulation equations allowing us to construct these solutions to the leading order near the bifurcation point and use this approximation to obtain the solitary waves numerically at larger velocities. If time permits, quasicontinuum descriptions and construction of exact solutions of this type for a lattice with piecewise linear nearest-neighbor interactions will also be discussed.

Anna Vainchtein
Department of Mathematics
University of Pittsburgh
aav4@pitt.edu

Lev Truskinovsky
ESPCI ParisTech
lev.truskinovsky@espci.fr

MS3

Uniform Matrix Product States are not Closed

We give a general (geometric) framework for computing the image of a polynomial map and, in particular, testing whether the image is closed. We apply this framework to prove that the set of tensors that admit a uniform matrix product state representation with fixed rank is not closed. This answers a question posed by W. Hackbusch.

Corey Harris
MPI MiS
Corey.Harris@mis.mpg.de

Mateusz Michalek
Max Planck Institute
mateusz.michalek@mis.mpg.de

Emre Sertöz
MPI MiS
emresertoz@gmail.com

MS3

Ranks and Symmetric Ranks of Cubic Surfaces

We study cubic surfaces as symmetric tensors of format $4 \times 4 \times 4$. We consider the non-symmetric tensor rank and the symmetric Waring rank of cubic surfaces, and show that the two notions coincide over the complex numbers. The corresponding algebraic problem concerns border ranks. We show that the non-symmetric border rank coincides with the symmetric border rank for cubic surfaces. As part of our analysis, we obtain minimal ideal generators for the symmetric analogue to the secant variety from the salmon conjecture. We also give a test for symmetric rank given by the non-vanishing of certain discriminants. The results extend to order three tensors of all sizes, implying the equality of rank and symmetric rank when the symmetric rank is at most seven, and the equality of border rank and symmetric border rank when the symmetric border rank is at most five.

Anna Seigal
University of California, Berkeley
seigal@berkeley.edu

MS3

Representation Theory and Fast Matrix Multiplication

Determining the algorithmic complexity of matrix multiplication is one of the central open problems in computer science. This problem can be shown to be equivalent to determining the Waring rank of the *symmetrized matrix multiplication tensor* $SM_n \in S^3(sl_n^*)$. Motivated by this, we study the plethysm $S^k(sl_n)$ of the adjoint representation sl_n of the Lie group SL_n. This talk is based on a current work in progress with Mateusz Michałek.

Tim Seynnaeve
Max Planck Institute for Mathematics in the Sciences in Leip
tim.seynnaeve@mis.mpg.de

MS3

Decomposition of Symmetric Tensors on Varieties

The decomposition of symmetric tensors into the sum of powers of linear forms has been widely studied. This problem is related to the study of the secant variety of Veronese varieties. In this talk, we will discuss a generalization of the decomposition of symmetric tensors. Namely, we want to decompose a symmetric tensor as the sum of powers of linear forms where each linear form is a point of a given algebraic variety X. Such a decomposition problem can be studied via the geometry of the secant variety of Veronese re-embeddings of X. We will present both theoretical and algorithmic results about this problem. If time permits, we will exhibit some numerical examples of our algorithm. This talk is a joint work with Jiawang Nie and Lihong Zhi.

Jiawang Nie
University of California, San Diego
njw@math.ucsd.edu

Ke Ye
Chinese Academy of Sciences
kennyyeke@gmail.com

MS4

Parametric Model Reduction for Distributed Parameter Systems

We consider the problem of designing reduced-order models for distributed parameter systems that are accurate under parametric changes. We limit our discussion to a special class of partial differential equation models that are dissipative and may include bilinear or quadratic nonlinearities. The parametric changes include those to initial conditions or model coefficients. By extending the interpolatory model reduction framework, we are able to build models such that measured outputs of the reduced model remain accurate under arbitrary control inputs.

Jeff Borggaard
Virginia Tech

Department of Mathematics
jborggaard@vt.edu

Andrea Carracedo Rodriguez
Virginia Tech
crandrea@vt.edu

Serkan Gugercin
Virginia Tech
Department of Mathematics
gugercin@vt.edu

MS4

High Order Approximations for Control of PDE Systems

In this paper we consider higher order methods for approximating PDE control systems defined by coupled hyperbolic and parabolic differential equations. This work is motivated by applications to modeling, control and optimization of heat exchangers. We discuss and compare two numerical schemes and their convergence properties. A numerical example is provided to illustrate the advantages of higher order methods in optimization and control.

John A. Burns
Virginia Tech
Interdisciplinary Center for Applied Mathematics
jaburns@vt.edu

MS4

Mixed Guidance Policies for Mobile Agents in the Cooperative Estimation of Spatially Distributed Processes in Hazardous Environments

The guidance of mobile sensor-agents used in the estimation of spatially distributed processes often neglects the effects of the process on the health and reliability of the sensor. When the spatially distributed process negatively impacts the health status and functionality of the sensing devices then the standard gradient-based sensor guidance will accelerate the demise of the sensor and negatively impact the performance of the estimator. A mixed policy that takes into account the cumulative effects of the environment on the health status of the sensing devices will provide a compromise between sensor functionality and estimator performance. This work considers a mixed policy where initially an information-sensitive guidance policy is implemented. Using performance-based criteria, the sensor guidance switches to an information-neutral policy and when certain thresholds pertaining to the life expectancy of the sensing devices are exceeded, then the guidance policy switches to an information-averse policy.

Michael A. Demetriou
Worcester Polytechnic Institute
mdemetri@wpi.edu

MS4

Observability Analysis for Non-cooperative Swarms

For large swarms of autonomous agents, the quality of control decisions is largely relied on the accuracy of available information and knowledge about the system, including the mathematical model, coordination strategy, network topology and communication protocol, state and parameter estimation, etc. For cooperative swarms, the controller design and real-time operation have the advantage of acquiring essential information as needed. However, the problem of estimation and detection becomes much more challenging from an outsiders perspective, i.e. the swarm is non-cooperative or even adversarial. The observability tends to be weak or practically unobservable for large swarms whose models have very high dimensions. In this paper, we address the problem of detecting the internal cooperating strategies of non-cooperative swarms through the estimation of parameters. This is a nonstandard estimation problem. With limited information about the mathematical model, the goal is to detect how individual agents cooperate to achieve the swarm behavior that is observed by outsiders. For stable swarms, it is unobservable. We show that this problem can be solved by introducing an intruder penetrating the swarm in a way so that the observability is adequately improved. The problem is not solvable analytically. Numerical methods are introduced and illustrated using several examples.

Wei Kang
Naval Postgraduate School
Department of Applied Mathematics
wkang@nps.edu

Hyeongjun Park
New Mexico State University
hjpark@nmsu.edu

Qi Gong, Claire Walton
University of California, Santa Cruz
qigong@soe.ucsc.edu, cwalton@soe.ucsc.edu

Isaac Kaminer
Naval Postgraduate School
kaminer@nps.edu

MS5

Low Algebraic Dimension Matrix Completion

Low rank matrix completion (LRMC) has received tremendous attention in recent years. The low rank assumption means that the columns (or rows) of the matrix to be completed are points on a low-dimensional linear variety. Our work extends this thinking to cases where the columns are points on low-dimensional nonlinear algebraic varieties. While others have recently studied matrix completion in such settings, existing results focus mainly on algorithms and experiments, without supporting theory. Our work proposes a new approach to what we call Low Algebraic-Dimension Matrix Completion (LADMC). We propose a new LADMC algorithm that leverages existing LRMC methods on a tensorized representation of the data. We also provide a formal mathematical justification for the success of our method. In particular, the new algorithm can succeed in many cases where traditional LRMC is guaranteed to fail. We also provide experimental results showing that the new approach significantly outperforms existing state-of-the-art methods for matrix completion in many situations.

Greg Ongie
University of Michigan
gongie@umich.edu

MS5

Sampling Lattice Points in Polytopes

The ability to sample lattice points of a polytope is an

important tool. For example, sampling lattice points is related to the problem counting lattice points and in a statistical setting, sampling from contingency polytopes can be used for independence testing. To sample the lattice points of a polytope P using the hit and run and round algorithm, first move to a larger polytope $\tilde{P}$ such that $P \subseteq \tilde{P}$. Then generate a point $X \in \tilde{P}$ using the hit and run sampler and round to the nearest lattice point $rd(X)$. If $rd(X) \in P$ then accept the point. If $rd(X) \notin P$ then reject and repeat. In this talk we discuss a strategy for carefully choosing $\tilde{P}$ so that the algorithm samples near-uniformly while minimizing the expected number of rejections.

Caprice Stanley
North Carolina State University
crstanl2@ncsu.edu

MS5

Generalized Linear Models for Binary-valued Tensor Response

Recently, tensors of order 3 or greater, known as higher-order tensors, have attracted increased attention in many fields. Methods built on tensors provide powerful tools to capture complex structures in data that lower-order methods may fail to exploit. Unfortunately, extending familiar matrix concepts to higher-order tensors is not straightforward, and indeed it has been shown that most computational problems for tensors are NP-hard. In this talk, I will present some results on exponential family tensor decompositions that have statistical applications, including logistic tensor PCA and tensor response regression.

Miaoyan Wang
University of Wisconsin–Madison
miaoyan@berkeley.edu

MS5

Tropical Principal Component Analysis

Principal component analysis is a widely-used method for the dimensionality reduction of a given data set in a high-dimensional Euclidean space. Here we define and analyze two analogues of principal component analysis in the setting of tropical geometry. In one approach, we study the Stiefel tropical linear space of fixed dimension closest to the data points in the tropical projective torus; in the other approach, we consider the tropical polytope with a fixed number of vertices closest to the data points. We then give approximative algorithms for both approaches and apply them to phylogenetics, testing the methods on simulated phylogenetic data and on an empirical dataset of Apicomplexa genomes.

Ruriko Yoshida
Operations Research
Naval Postgraduate School
ryoshida@nps.edu

Leon Zhang
University of California, Berkeley
leonyz@berkeley.edu

Xu Zhang
University of Kentucky
xzh323@g.uky.edu

MS6

On the Numerical Solution of Elliptic PDEs on Polygonal Domains

Abstract not available at time of publication.

Jeremy Hoskins
Yale University
jeremy.hoskins@yale.edu

MS6

Integral Equation Methods for Viscoelastic Flows

The simulation of viscoelastic flows presents fundamental difficulties for all numerical methods in experimentally relevant parameter regimes. Steep boundary layers and fine structures near extensional points impose high resolution requirements and typically lead to the apparent divergence of solutions. We present an algorithm that couples fast integral equation methods for the solution of the Stokes equations with a semi-Lagrangian scheme for the evolution of the polymeric stress tensor. We present preliminary results for benchmark problems and demonstrate the capability of the algorithm to handle geometries with large numbers of complex boundaries.

David Stein
Flatiron Institute
Simons Foundation
dstein@flatironinstitute.org

MS6

Fast BEM Solver for Transient Stokes Flow

Since the fundamental solution for transient Stokes flow in three dimensions is complicated it is difficult to implement discretization schemes and fast methods for boundary integral formulations. We derive a representation of the Stokeslet and stresslet in terms of incomplete gamma functions. Here, multipole translation operators can be expressed in tensor product form which reduces the computational cost of their evaluation. Further, we develop a Galerkin discretization scheme and show how to handle moving geometries.

Johannes Tausch
Southern Methodist University
Department of Mathematics
tausch@mail.smu.edu

MS6

Integral Equation Method for the Heat Equation in Moving Geometry

Many problems in physics and engineering require the solution of the heat equation in moving geometry. Integral representations are particularly appropriate in this setting since they satisfy the governing equation automatically and, in the homogeneous case, require the discretization of the space-time boundary alone. In this talk, we present a new method for solving the 2D heat equation in moving geometry that makes use of a spatially adaptive mesh, a new version of the fast Gauss transform that allows for volume and boundary sources, and a new hybrid asymp-

totic/numerical method for local-in-time quadrature.

Jun Wang
Flatiron Institute
Simons Foundation
jwang@flatironinstitute.org

Leslie Greengard
Simons Foundation and Courant Institute
New York University
greengar@cims.nyu.edu

MS7

A Trefftz-Nystrom Finite Element Method

We consider families of finite elements on (curvilinear) polygonal meshes, that are defined implicitly on each mesh cell as solutions of local Poisson problems with polynomial data, in the spirit of Trefftz methods. Functions in these local spaces are computed via Nyström discretizations of associated second-kind integral equations, and we describe how such an approach can be used to efficiently and accurately evaluate such functions as well as their interior and boundary derivatives, which are used in the formation of finite element stiffness matrices. Several experiments demonstrate the approximation quality of these function spaces on meshes that may include non-convex and curvilinear mesh cells.

Jeffrey S. Ovall
Portland State University
jovall@pdx.edu

Steffen Weisser
Saarland University
weisser@num.uni-sb.de

Akash Anand
IIT, Kanpur
akasha@iitk.ac.in

Samuel Reynolds
Portland State University
ser6@pdx.edu

MS7

Virtual Element Method in the Presence of Curved Edges

In this talk we introduce the analysis of Virtual Elements in the presence of curved faces. We consider in particular the case of a fixed curved boundary in two dimensions, as it happens in the approximation of problems posed on a curved domain. We show (both theoretically and numerically) that the proposed curved VEM lead to an optimal rate of convergence, without any approximation of the boundary.

Alessandro Russo
Milan University
alessandro.russo@unimib.it

Lourenco Beirao da Veiga, Giuseppe Vacca
University of Milano-Bicocca
Italy
lourenco.beirao@unimib.it, giuseppe.vacca@unimib.it

MS7

Recent and New Developments of Primal-dual Weak Galerkin Finite Element Methods

Weak Galerkin (WG) is a newly developed finite element technique for PDEs where the differential operators (e.g., gradient, divergence, curl, Laplacian) in the variational forms are reconstructed by using a framework based on the theory of distributions. The framework yields discrete weak differential operators such as weak gradients etc. The computation of the discrete differential operators involves the solution of inexpensive problems defined locally on each element. Stabilizers that are PDE-specific are employed to provide weak continuities/smoothness necessary for the original formulations. Due to its structural flexibility, WG-FEM is well suited to most PDEs by providing the needed stability and accuracy. In this talk, the speaker will discuss a primal-dual weak Galerkin (PD-WG) approach. The essential idea of PD-WG is to interpret the numerical solutions as constrained minimization of functionals with constraints that mimic the weak formulation of the PDEs. The resulting Euler-Lagrange formulation offers a symmetric numerical scheme involving both the primal and the dual variable. The PD-WG method will be applied to several challenging problems for which existing methods have difficulty in applying, including the second order elliptic equation in nondivergence form, Fokker-Planck equation, convection dominated convection-diffusion equations, and elliptic Cauchy problems.

Junping Wang
National Science Foundation
jwang@nsf.gov

MS7

A Non-conforming Element on Polygonal Meshes

We present a nonconforming lowest order Crouzeix-Raviart type finite element on general polygonal meshes, constructed using the generalized barycentric coordinates. There is a fundamental difference in the Crouzeix-Raviart type degrees of freedom between polygons with odd and even number of vertices, which results in slightly different local constructions of finite elements on these two types of polygons. Because of this, the topological structure of connected regions consisting of polygons with even number of vertices plays an essential role in understanding the global finite element space. To analyze such topological structure, a new technical tool using the concept of cochain complex and cohomology is developed. Despite the seemingly complicated theoretical analysis, implementation of the element is straight-forward. The nonconforming finite element method has optimal a priori error estimates.

Yanqiu Wang
Oklahoma State University
yqwang@njnu.edu.cn

MS8

Parallel Algorithms for Time-space Fractional Reaction Diffusion Equations

In this work, we develop a novel numerical scheme for time-space fractional reaction-diffusion equations. The schemes are similar to the Crank-Nicholson scheme (for integer order PDEs) and are shown to be convergent and un-

conditionally stable. The schemes consist of two parts: the local and history term; and are implemented in a predictor-corrector manner. Both the predictor and corrector schemes make use of same history term. The predicted value is computed as a sum of a local term and the history term, and the corrected value is computed as a sum of the predicted local term and same history term. The computation of the history term can be time consuming for problems having long time interval. To avoid this, we developed parallel algorithms using the shared (OpenMP) and distributed (MPI or POSIX threads) memory systems. We showed the advantages of the parallel algorithms over the sequential algorithms by implementing on problems with long time intervals.

Toheeb A. Biala, Abdul Khaliq
Middle Tennessee State University
tab7v@mtmail.mtsu.edu, abdul.khaliq@mtsu.edu

MS8

Asymptotic Stability of a Multiscaled Compact Scheme for Self-focusing Optical Beam Propagation Problems

Focusing laser beams have been difficult to simulate effectively due to the long term instabilities in many existing numerical methods. In computations, linear or nonlinear Helmholtz partial differential equations are used together with significantly large wave numbers. In this preliminary report, we introduce a new multiscaled finite difference methods. Regional decomposition and compact algorithmic design are utilized. A self-focusing optical beam propagation problem modeled by a linear Helmholtz equation is considered on a radially symmetric transverse field. We will show rigorously that, though the multiscaled compact scheme shies away from conventional stability in the von Neumann sense, it is unconditionally stable with index one in an asymptotical sense. Computational experiments and beam propagation simulations further verify our results.

Tiffany N. Jones
Baylor University
Tiffany_Jones1@baylor.edu

Qin Sheng
Department of Mathematics
Baylor University
Qin_Sheng@baylor.edu

MS8

Flux Based Finite Element Methods

In this talk, we present a new finite element method based on flux variables. In many applications, the flux variables are often the quantity of interest. To approximate the flux variable accurately and efficiently, one transforms the second-order equations into a system of first-order and approximates both the primary and flux variables simultaneously. While this indeed produces accurate approximations for the flux variables, the resulting algebraic system is large and expensive to solve. We present a new method approximating the flux variables only without approximations of the primary variable. If necessary, the primary variable can be recovered from the flux approximation with the same order of accuracy.

Jaeun Ku
Oklahoma State University
jku@math.okstate.edu

MS8

Computational Aspects of New Hybrid Schemes for the Approximation of Darcy's Flow

In this talk we first review on the new hybrid schemes to approximate the Darcy flow variable without calculating the pressure variable. We will compare our schemes with the standard mixed finite element approach. Several efficient numerical methods will be considered to implement our new hybrid schemes. Numerical comparisons between these methods and mixed finite element methods will be shown.

Imbumn Kim
Seoul National University
ibkim11@gmail.com

JaEun Ku
Oklahoma State University
jku@math.okstate.edu

Dongwoo Sheen
Seoul National University
Department of Mathematics
sheen@snu.ac.kr

MS9

Identifying Unknown Chemical Inputs and Context Dependence in Synthetic Circuits

We discuss the two applications of Bayesian inference and model selection to studying synthetic biological circuits. In the first application, we assess the dependence of biological parameters in a cell growth control circuit on the unmodeled external environment. We collect experimental data from the growth control circuit in You et al. 2004 under different environmental conditions such as multiple pH and induction levels. We develop mathematical models of the circuit across different experimental contexts. For each type of context relationship, we use Bayesian inference to assess its plausibility and to estimate the circuit parameters. We find that the there is significant experimental context-dependence and that the parameter estimates are sensitive to our assumption of a context relationship. In the second application, we detect and infer the properties of chemical inputs to a temporal logic gate circuit that acts as a memory device. This synthetic circuit uses integrase enzymes to flip DNA segments inside an E. coli cell in response to these chemical inputs. Hence, the presence and the properties of chemical inputs are captured in the DNA states across an E. coli population. First, we develop a stochastic model of the cell population response with and without chemical inputs. Then we use data measurements of the E. coli cell population response to infer whether any chemical pulse event has occurred, and if it has, to infer its properties of timing and amplitude.

Ania-Ariadna Baetica
Controls and Dynamical Systems
California Institute of Technology
abaetica@caltech.edu

Reed McCardell
California Institute of Technology
mccardellr@caltech.edu

Victoria Hsiao
Amyris
vhsiao@caltech.edu

Richard Murray
Control and Dynamical Systems
California Institute of Technology
murrayrm@cds.caltech.edu

MS9

Sequential Tempered Markov Chain Monte Carlo for Model Selection of Synthetic Biological Circuits

System identification questions in systems and synthetic biology can be answered using the framework of Bayesian inference. Our uncertainty about a biological system's model stems from not capturing all the underlying dynamics of the system and its interactions with the environment. Selecting between different candidate models to describe the system can be challenging, but Bayesian methods can be used to solve this problem. While Bayesian inference is used to estimate uncertain parameters, it can also be used to estimate the relative probability of candidate mathematical models of a system given data measurements. This is a mathematically rigorous approach, which requires computing the model likelihood that naturally trades off the model complexity and the data fit. Computing the model likelihoods is often difficult for complex systems; however, it can be done efficiently using population-based Markov Chain Monte Carlo (MCMC) methods. The advantage of this approach is that the same process for identifying parameters in the model is used to compute its likelihood. In this talk, we present a population-based MCMC method called Sequential Tempered MCMC (ST-MCMC) and illustrate how it can be used for model selection and parameter estimation. This algorithm combines annealing, importance sampling, and MCMC to develop an efficient and parallel method for Bayesian inference. Ultimately, we accurately identify the models and parameters in two synthetic biocircuit applications.

Thomas A. Catanach
Sandia National Laboratories
tacatan@sandia.gov

Ania-Ariadna Baetica
Controls and Dynamical Systems
California Institute of Technology
abaetica@caltech.edu

Reed McCardell
California Institute of Technology
mccardellr@caltech.edu

Victoria Hsiao
Amyris
vhsiao@caltech.edu

Richard Murray
Control and Dynamical Systems
California Institute of Technology
murrayrm@cds.caltech.edu

MS9

Noise Makes Gene Regulation Mechanisms Harder to Analyze But Easier to Identify and Predict

Crucial biological responses are regulated by discrete and stochastic single-molecule events that result in spatiotemporal mRNA fluctuations characterized by discrete, positive, and non-symmetric distributions. These are far from the Gaussian shape underlying many modern statistical tools. In addition, the limited amount of data available from single-cell measurements means that we cannot invoke the Central Limit Theorem for accurate moment estimations of the underlying distributions. We will present an alternative approach based on the finite state projection (FSP) that fits the empirical distributions directly to the solution of the chemical master equation. Unlike methods that infer from summary statistics, the FSP-based approach seeks to fully capture discrete, non-normal effects within finite datasets. We present examples where this discrete, non-Gaussian approach allows the identification and prediction of single-cell dynamics from realistically small datasets whereas inference from means and variances leads to inaccurate results. While our model-data integration approach extends to any discrete dynamic process with rare events and realistically limited data, the computational complexity of solving the underlying master equation remains a challenge for high-dimensional systems. We discuss how reduced order modeling may provide efficient approximate analyses while maintaining acceptable accuracy.

Huy Vo
Department of Chemical & Biological Engineering
Colorado State University
huy.vo@colostate.edu

Zachary Fox
School of Biomedical Engineering
Colorado State University, Fort Collins
zrfox@rams.colostate.edu

Brian Munsky
Department of Chemical and Biological Engineering
Colorado State University, Fort Collins
munsky@colostate.edu

MS9

Deep Stochastic Koopman Learning for Synthetic Gene Networks

Synthetic gene networks are engineered to execute a specific purpose, e.g. storing events as memory, catalysis of a substrate, over-expression of a protein. A challenge in engineering functional synthetic gene networks is that the operational envelope of the system is unknown. We introduce a novel Koopman operator approach for learning stochastic-moment models directly from time-series flow cytometry data. We show how deep learning efficiently discovers a lifted set of Koopman observable functions that enable accurate approximation of a Koopman operator, even when the underlying configuration space of the probability distribution is very large. These observable functions include covariate moments that capture critical interactions between physical states. Most importantly, we show how deep stochastic Koopman operators can be used to predict the behavior of a synthetic gene network over a range of initial conditions, resulting in a model-based description of the system's operational envelope. Specifically, we learn deep stochastic-moment Koopman operator models of a genetic toggle switch from time-series experiments varying multiple inducer concentrations to explore the underlying phase space of the system. We use this computational framework to characterize the operational envelope of the toggle switch, in 2 distinct host-chassis and across a range

of growth conditions.

Enoch Yeung
Pacific Northwest National Laboratory
enoch.yeung@pnnl.gov

MS10

A Posteriori Error Estimates and Adaptivity for Fully Mixed Finite Element Discretizations for Biot's Consolidation Model

This paper is concerned with the analysis of fully mixed finite element method applied to the Biot's consolidation model. We consider two mixed formulations that use the stress tensor and Darcy velocity as primary variables as well as the displacement and pressure. The first formulation is with a symmetric stress tensor while the other enforces the symmetry of the stress weakly through the introduction of a Lagrange multiplier. The two formulations are then discretized with the backward Euler scheme in time and with two mixed finite elements in space. We present next a unified a posteriori error analysis for the two formulations. Our estimates are based on $H^1(\Omega)$-conforming reconstruction of the pressure and a suitable $\left[H^1(\Omega)\right]^2$-conforming reconstruction of the displacement; both are continuous and piecewise affine in time. These reconstructions are used to infer a guaranteed and fully computable upper bound on the energy-type error measuring the differences between the exact and the approximate pressure and displacement. The error components resulting from the spatial and the temporal discretization are distinguished. They are then used to design an adaptive space–time algorithm. Numerical experiments illustrate the efficiency of our estimates and the performance of the adaptive algorithm.

ELyes Ahmed
Department of Mathematics
University of Bergen
elyes.ahmed@uib.no

Florin A. Radu
Institute of Mathematics
University of Bergen
florin.radu@math.uib.no

Jan M. Nordbotten
Department of Mathematics
University of Bergen
jan.nordbotten@math.uib.no

MS10

Two Phase Compaction of a Sedimentary Basin

Porosity of a visco-elastic medium satisfies a pseudo-parabolic partial differential equation consisting of porous medium equation added to a semi-linear degenerate elliptic operator acting on the time-derivative. The latter third order term distinguishes this equation from the classical porous medium equation. The porous medium term can be the sum of monotone and Lipschitz functions. We establish existence for the initial-boundary-value problem, establish bounds on the solution that prevent degeneracy of the semilinear elliptic operator, and prove regularity properties of the solution. These results are obtained by methods of monotonicity and compactness.

Ralph Showalter, Dwight Holland
Department of Mathematics
Oregon State University
show@math.oregonstate.edu, holladwi@oregonstate.edu

MS10

Deformation of Porous Media at Multiple Scales

Here we discuss models for modeling deformation of saturated porous materials at the microscale (scale at which we can distinguish between the fluid and solid phase) and the macroscale (scale at which we cannot distinguish between the fluid and solid phase). In geomechanics, the most pervasive deformation model is based on a principle called the Terzaghi stress principle, which generally assumes the behavior of rocks/soils is linear elastic at the macroscale and is practically feasible. However data indicates unexplained deviations from this principle. Here we discuss potential explanations: microscale modeling demonstrates that the macroscale model cannot predict consequences of localized stresses, and for swelling porous materials, the Terzaghi stress principle needs to be re-interpreted.

Lynn Schreyer
Washington State University
lynn.schreyer@wsu.edu

Howard Schreyer
University of New Mexico
Mechanical Engineering
schreyer@unm.edu

MS11

Theoretical Mahjong Discard Piles Algorithm Simulator

Description of code base to generate mahjong discard piles according to a 100% offence efficiency focused tile discards algorithm based on the mentsu completion probability function. Faculty Advisor: Burge, Janet, Professor of Computer Science at Colorado College, k_aoki@coloradocollege.edu

Kon Aoki, Kochi Nakajima
Colorado College, USA
k_aoki@coloradocollege.edu,
k_nakajima@coloradocollege.edu

MS11

Currency Risk Management

This project focuses on developing a simple model to predict the exchange rate between the Euro (EUR) and the US Dollar (USD). The prediction results are used to help investors hedge against short term exchange rate risk, and tested empirically. Based on the theories behind some common investment strategies, a linear regression model to predict the EUR/USD exchange rate was built by choosing the Purchasing Power Parity (PPP), which represents valuation, Basis SWAP Libor rates, which represents carry, and historical volatility, as the risk measure, to be the predictor variables. We then incorporated a momentum signal consisting of the crossover of two EWMAs to improve the accuracy of our predictions by using another linear regression model to fit the error obtained in our previous model. To confirm the effectiveness of our predictions we generated a trading strategy which consisted on comparing the predictions to the corresponding forward rates to decide whether we should wait until next month to make the transaction or enter a forward contract. We obtained the payoff given

by always entering the forward contract, choosing to enter according to our first model, and choosing to enter according to our improved model. We find that in both latter cases we generate a positive profit, confirming the worthiness of this approach to predict the EUR/USD exchange rates. Faculty Advisor: Wang, Gu, WPI, gwang2@wpi.edu

Andrea Bayas
Worcester Polytechnic Institute, USA
acbayas@wpi.edu

MS11

A Stochastic Model for the West Nile Virus

In this presentation, I will discuss a deterministic model and a stochastic model for the West Nile Virus (WNV). Using these models, we can analyze the mosquito, bird, and human populations. For the human population, we consider the multiple symptoms of human infection (i.e. asymptomatic, feverish, and neurological disease traits). Using the stochastic model, we approximate the probability of disease extinction of WNV, as well as the probability of an outbreak. Faculty Advisor: Lahodny, Glenn, Texas A&M University, glahodny@math.tamu.edu

Timothy Cheng
Texas A&M University, USA
timothycheng29@gmail.com

MS11

Mathematical Analysis of Photoreceptor Degeneration in Retinal Detachment

The retina is the lining in the back of the eye responsible for vision. When light photons hits the retina, the photoreceptors within the retina respond by sending impulses to the optic nerve, which connects to the brain. If there is injury to the eye or heredity retinal problems, this part can become detached. Detachment leads to loss of nutrients, such as oxygen and glucose, to the cells in the eye and causes cell death. Sometimes the retina is able to be surgically reattached. If the photoreceptor cells have not died and the reattachment is successful, then these cells are able to regenerate their outer segments (OS) which are essential for their functionality and vitality. In this work we will explore how the regrowth of the photoreceptor cells in a healthy eye after retinal detachment can lead to a deeper understanding of how eye cells take up nutrients and regenerate. This work uses a mathematical model for a healthy eye in conjunction with data for photoreceptors' regrowth and decay. Using parameter estimation and sensitivity analysis we can better understand how certain processes represented by these parameters, change within the model as a result of retinal detachment. Faculty Advisor: Camacho, Erika, ASU, Erika.camacho@asu.edu

Miriam Goldman
Arizona State University, USA
miriamagoldman@gmail.com

MS12

Deformation and Rigidity

Deformation of a triangle mesh is an important theme in many applied areas such as computer graphics, computer vision and scientific shape analysis. Rigidity, the absence of deformation, has been studied mainly in mathematics, but it seems natural to consider what light the study of rigidity can shed on deformation. Heres a classical rigidity result. Given an embedded triangle mesh homeomorphic to the sphere, we consider the vector formed by its edge lengths. Provocatively, the length of this vector matches the number of degrees of freedom of the embedding up to rotation and translation. And indeed for an edge length vector in general position, the mesh is rigid. In other words, if you constructed the Stanford bunny out of toothpicks, it would not fall down, even if the joints at the vertices were totally flexible. While this classic idea does not seem to be directly helpful for computing with shape deformations (edge lengths are just too intrinsic, and embeddings are not unique), there are other ways we could assign a number to each edge. Each of these leads to a different model of rigidity, some of which might be more useful. We will discuss two: the dihedral angles, and the discrete mean curvature.

Nina Amenta
UC Davis
California 95616
amenta@cs.ucdavis.edu

MS12

Medial Fragments for Segmentation of Articulating Objects in Images

We propose a method for extracting objects from natural images by combining fragments of the Blum medial axis, generated from the Voronoi diagram of an edge map of a natural image, into a coherent whole. Using techniques from persistent homology and graph theory, we combine image cues with geometric cues from the medial fragments in order to aggregate parts of the same object. We demonstrate our method on images containing articulating objects, with an eye to future work applying articulation invariant measures on the medial axis for shape matching between images. This is joint work with Erin Chambers and Kathryn Leonard.

Ellen Gasparovic
Union College
gasparoe@union.edu

MS12

Skeletal Models and Shape Representation

This talk will consider skeletal models for shapes in two and three dimensions from the perspective of complexity, compression, parts decomposition and recognition, including similarity and articulation. We will discuss mathematical skeletal constructions such as the Blum medial axis, and functions on those skeletons that provide important information about a shape. We will also present results from a massive user study on shape part perception that provides insight into human cognition about shape parts.

Kathryn E. Leonard
Dept of Computer Science
Occidental College
kleonardci@gmail.com

MS12

Computational Design and Fabrication

The recent emergence of additive manufacturing - otherwise known as 3D printing - has expanded the accessibility for rapid prototyping objects of interest. However, the applicability of additive manufacturing is often limited by

the quality of available models, and by the ability of the designer to produce good representations of the objects. My work has been to alleviate these limitations by developing geometric modeling and processing tools that are premeditative of the mechanical and aesthetic properties of physical objects. I have advanced the quality assurance of additive manufacturing, especially for desktop 3D printers, which is core to customized manufacturing. For instance, I have built support generation systems that optimize aesthetics, material usage and mechanical properties of 3D printed objects. I have also developed computational geometric technologies for additive manufacturing that bring new insights into product complexity and opportunities over traditional manufacturing methods, such as shell models with varying thickness and medical instruments.

Xiaoting Zhang
Boston University
xiaoting@bu.edu

MS13

Stable Computation of Generalized Matrix Functions via Polynomial Interpolation

Generalized matrix functions (GMFs) extend the concept of a matrix function to rectangular matrices via the SVD. Several applications require the action of a GMF of a large, sparse matrix on a vector. We present a new method for applying GMFs to vectors based on Chebyshev interpolation that is matrix-free and requires no orthogonalization. We prove that our method is stable and compare it with existing approaches based on Lanczos bidiagonalization.

Anthony P. Austin
Argonne National Laboratory
austina@anl.gov

Jared Aurentz
Instituto de Ciencias Matemáticas
jaredaurentz@gmail.com

Michele Benzi
Department of Mathematics and Computer Science
Emory University
benzi@mathcs.emory.edu

Vassilis Kalantzis
University of Minnesota
kalan019@umn.edu

MS13

The FEAST Algorithm as a Generator of Polynomial Eigenvalue Filters

The FEAST eigenvalue algorithm uses a rational filter function in order to selectively calculate the eigenvectors of a matrix whose eigenvalues lie in a specific, user-defined region in the complex plane. The action of the rational filter function is implemented by solving linear systems of equations, which are (ideally) solved exactly by using matrix factorization methods. In practice, however, there are many applications of interest in which matrix factorization is inefficient or even impossible. In these cases the FEAST linear systems of equations are instead solved approximately, using algorithms that rely on only matrix-vector multiplication for performing computations. By implementing eigenvalue filters using only matrix-vector multiplication (through solving linear systems), FEAST implicitly uses polynomial filter functions rather than rational filter functions for selecting eigenvalues. In this presentation we show explicitly what these polynomial filter functions are, and how they can explain the ways in which the behavior FEAST with approximate linear system solves is similar to, or different from, the behavior of FEAST with exact linear system solves.

Brendan Gavin
ECE Department
University of Massachusetts, Amherst
bgavin@ecs.umass.edu

Eric Polizzi
University of Massachusetts, Amherst, USA
polizzi@ecs.umass.edu

MS13

Consistent Symmetric Greedy Coordinate Descent Method

We propose a consistent symmetric greedy coordinate descent method for solving leading eigenvalue problem from an optimization viewpoint. Since different coordinates converge to the optimal value at different speeds, coordinate-wise method has been shown to outperform the full gradient method. Our proposed algorithm is able to select and update the most important coordinates in O(kn) time at each iteration, where k is the number of coordinates and n is the matrix size. Although the objective function in the optimization problem is non-convex, we prove that any local minimum is the global minimum and a stochastic version of the algorithm helps the iteration escaping from every single saddle point. Experimental results show that our methods achieve a great speedup over the basic power method. Meanwhile, due to their coordinate-wise nature, our methods can be implemented in an synchronized manner and is very suitable for the cases when data cannot fit into memory.

Yingzhou Li
Duke University
yingzhouli0417@gmail.com

Jianfeng Lu
Mathematics Department
Duke University
jianfeng@math.duke.edu

Zhe Wang
Duke University
zhe.wang3@duke.edu

MS13

Polynomial Preconditioned Arnoldi for Eigenvalues

Polynomial preconditioning of large eigenvalue problems has been discussed for many years but has not become standard. Here we give a simple choice for a polynomial to use with the Arnoldi method. Results demonstrate significant reduction in orthogonalization costs, which can reduce communication in parallel settings. For difficult problems, the preconditioner can also reduce the number of matrix-vector products required. Furthermore, we discuss ways to keep the method stable even for high-degree polynomials.

Jennifer A. Loe, Ron Morgan
Baylor University
jennifer_loe@baylor.edu, Ronald_Morgan@baylor.edu

Mark Embree
Department of Mathematics
Virginia Tech
embree@vt.edu

MS14

A Guaranteed Locally Adaptive Algorithm for Univariate Function Approximation and its Computational Cost

Establishing an algorithm to approximate a function within prescribed tolerance often requires computing the error bounds of some interpolation methods. Most existing error bounds depend on semi-norms of the function being interpolated. However, such semi-norms are often not known a priori. Many existing adaptive algorithms choose the data sites based on heuristic error estimates and lack theoretical guarantees of accuracy. This talk describes a new locally adaptive algorithm for univariate function approximation based on function values instead of semi-norms. The algorithm is capable of automatically sampling the function where it fluctuates more. More than that, if the function is in some cone, our algorithm is guaranteed to provide a linear interpolant that satisfies a user-specified absolute error tolerance. In addition to that, the computational cost of our algorithm is proven to be of the same order as that of the best function approximation algorithm for all the functions in this cone. This is to say that our algorithm is an optimal algorithm. We also provide numerical experiments to compare our algorithm with Chebfun.

Yuhan Ding
Misericordia University, US
yding@misericordia.edu

MS14

Guaranteed Adaptive Monte Carlo Methods for Estimating Means of Random Variables with a Hybrid Error Tolerance

Monte Carlo is a versatile computational method that may be used to approximate the mean, μ, of a random variable, Y, whose distribution is not known explicitly. This talk illustrates how to reliably construct a fixed width confidence interval for μ with some prescribed absolute error tolerance, relative error tolerance, or generalized error criterion. Our algorithm assumes that the kurtosis of the random variable Y does not exceed some given upper bound. The variance of Y is confidently estimated in the first stage and the mean is calculated in an iteration process until the stopping criterion is met. The algorithm is implemented in the Guaranteed Automatic Integration Library (GAIL).

Lan Jiang
Hyatt Hotels Corporation
lan.jiang@hyatt.com

MS14

Automatic Bayesian Cubature

Automatic cubatures provide approximations to multidimensional integrals that satisfy user-specified error tolerances. For multidimensional problems, the sampling density is fixed, but the sample size, n, is determined automatically. Bayesian cubature postulates that the integrand is an instance of a stochastic process. Prior information about mean and covariance of this process is used to form data-driven error bounds. However, the process of inferring the mean and covariance governing the stochastic process from n integrand values involve computing matrix inverses and determinants, which are in general time-consuming $O(n^3)$ operations. Our work employs low discrepancy data sites and matching kernels that lower the computational cost to $O(n \log n)$. The confidence interval for the Bayesian posterior error is used to choose n automatically to satisfy the user-defined error tolerance. This approach is demonstrated using rank-1 lattice sequences and shift-invariant kernels. This is joint work with Fred J. Hickernell.

Jagadeeswaran Rathinavel
Illinois Institute of Technology
jrathin1@hawk.iit.edu

MS14

A Locally Adaptive Algorithm for Global Minimization of Univariate Functions

In this talk, I will introduce a locally adaptive algorithm for global minimization of univariate functions on a bounded interval. These functions are smooth and not too highly oscillatory, but are not necessarily convex, in the Sobolev space $W^{2,\infty}([a,b])$. This algorithm samples more function values where the function is small in value and more spiky. It provides an estimated minimum that satisfies a user-specified absolute error tolerance. An upper bound of computational cost will be presented briefly. This algorithm, called **funmin_g**, is implemented in the Guaranteed Automatic Integrate Library (GAIL). We will show numerical examples that illustrate its superior performance in comparison to other more established solvers including MATLAB's **fminbnd** and Chebfun's **min**.

Xin Tong
University of Illinois at Chicago
xtong20@uic.edu

MS15

Derivative-free Optimization Leveraging Square-root Uncertainty Measures

Delaunay-based derivative-free optimization via global surrogates (Δ-DOGS), introduced in [Beyhaghi & Bewley, *Journal of Global Optimization* **66** (3)], is a family of surrogate-based derivative-free optimization schemes designed for the global optimization of nonconvex (possibly, nonsmooth) functions. Schemes in this family are remarkably efficient at minimizing complex functions with a minumum number of function evaluations, while remaining (under the appropriate assumptions) provably globally convergent. Various schemes in this family address different subproblems, including (a) optimization within nonconvex (even, disconnected) feasible domains, (b) accelerating convergence via dimension reduction during intermediate iterations, and (c) accelerating local refinement by leveraging local derivative information while still assuring global convergence. A key computational challenge with the Δ-DOGS family of schemes is their inherent dependence on Delaunay triangulations over the datapoints, which quickly become expensive to compute as the dimension of the problem increases. This talk will discuss recent efforts to remove this dependence, by introducing an uncertainty function based on a new square-root measure to characterize the uncertainty of the interpolant based on the distance to the nearest function evaluation. Preliminary numerical tests will be presented to compare the speed of

convergence to the original Δ-DOGS formulation.

Thomas R. Bewley
Dept of Mechanical and Aerospace Engineering
University of California, San Diego
bewley@eng.ucsd.edu

Muhan Zhao
Dept of MAE, UC San Diego
muz021@ucsd.edu

MS15

Applications of SNOPT to Engineering Design Optimization

We will show examples of the application of SNOPT—a software package for solving large-scale nonlinear optimization problems—to various engineering design problems that we have solved over the last few years in the Multidisciplinary Design Optimization Laboratory. Most of the problems involve functions that require computational fluid dynamic simulations, structural finite-element simulations, or both. The combination of an effective gradient-based optimizer such as SNOPT, and the efficient computation of derivatives via adjoint methods is the key to making the solution of these problems tractable. The applications include the design optimization of aircraft wings, wind turbine blades, car shapes, hydrofoils, and satellites. Some of these applications involve multiphysics simulations, making them multidisciplinary. We end with a perspective on what it will take to solve even larger-scale multidisciplinary design optimization problems in the future.

Joaquim R. R. A Martins
University of Michigan
jrram@umich.edu

MS15

Evolution of a Mathematical Model: Optimization, Matching, and More

A New York City government agency offers regular opportunities for employees to request changes in their work location. Deciding how to make this transfer process efficient and correct has led to an interesting application of applied mathematics and computer science. Although standard continuous optimization initially appeared to be the appropriate solution method, subsequent analysis revealed that the transfer problem can be formulated as a structured matching problem. Collaborations between university faculty and agency employees have thus far been successful in producing both a reasonable mathematical formulation and associated software.

Margaret H. Wright
Courant Institute of Mathematical Sciences
New York University
mhw@cs.nyu.edu

MS16

Defining Equations of Bayesian Networks via Colored Probability Trees

One of the fundamental insights in Algebraic Statistics is that exponential families 'are' toric varieties. A full characterisation of the algebraic geometry surrounding a special class of these, called decomposable graphical models, was given by Geiger et al. [2006]. We now investigate a more recent statistical model represented by a coloured probability tree and called a staged tree [Smith et al., 2017]. Staged tree models include decomposable graphical models as a special case but in their algebro-geometric description sum-to-1 conditions on the probability simplex cannot be ignored. These hence constitute a wider class of models—and of varieties—which are toric only under very special conditions. In this talk we will explain what are the implications of ignoring sum to one conditions on the parameters and characterise the case in which staged tree models are toric.

Eliana Duarte
Otto von Guericke Universität Magdeburg
eliana.duarte@mis.mpg.de

Christiane Görgen
Max Planck Institute for Mathematics in the Sciences
christiane.goergen@mis.mpg.de

MS16

Geometry of Exponential Random Graph Models

When given network data, we can either compute descriptive statistics (degree distribution, diameter, clustering coefficient, etc.) or we can find a model that explains the data. Modeling allow us to test hypotheses about edge formation, understand the uncertainty associated with the observed outcomes, and conduct inferences about whether the network substructures are more commonly observed than by chance. Modeling is also used for simulation and assessment of local effects. Exponential random graph models (ERGMs) are families of distributions defined by a set of network statistics and, thus, give rise to interesting graph theoretic questions. Our research focuses on the ERGMs where the edge, 2-path, and triangle counts are the sufficient statistics. These models are useful for modeling networks with a transitivity effect such as social networks. One of the most popular research questions for statisticians is the goodness-of-fit testing, how well does the model "fit" the data? This is a difficult question for ERGMs. And one way to answer this question is to understand the reference set. Given an observed network G, the reference set of G is the set of simple graphs with the same edge, 2-path, and triangle counts as G. In algebraic geometry, it is called the fiber of G and are the 0-1 points on an algebraic variety, which we refer to as the reference variety. The goal of this paper is to understand reference variety through the lens of algebraic geometry.

Ha Khanh Nguyen
The Ohio State University
nguyen.1833@osu.edu

Elizabeth Gross
San Jose State University
elizabeth.gross@sjsu.edu

Chris O'Neill
UC Davis
musicman3320@gmail.com

Rodolfo Garcia
San Jose State University

rodolfo.garcia@sjsu.edu

MS16

Exact Tests for Stochastic Block Models

We develop a finite-sample goodness-of-fit test for latent-variable block models for networks and test it on simulated and real data sets. The main building block for the latent block assignment model test is the exact test for the model with observed blocks assignment. The latter is implemented using algebraic statistics. While we focus on three variants of the stochastic block model, the methodology extends to any mixture of log-linear models on discrete data. This is joint work with Vishesh Karwa, Debdeep Pati, Sonja Petrović, Liam Solus, Nikita Alexeev, Mateja Raič, Robert Williams, and Bowei Yan

Dane Wilburne
Illinois Institute of Technology
dwilburn@hawk.iit.edu

MS17

Effect of use Dependent Plasticity on Information Transfer at Hippocampal Synapses

Simple models of short term synaptic plasticity that incorporate facilitation and/or depression have been created in abundance for different synapse types and circumstances. The analysis of these models has included computing mutual information between a stochastic input spike train to the presynaptic synapse, and some sort of representation of the postsynaptic response. While this approach has proven useful in many contexts, for the purpose of determining the type of process underlying a stochastic output train, it ignores the ordering of the responses, leaving an important characterizing feature on the table. In this work we use a broader class of information measures on output only, and specifically construct hidden Markov models (known as epsilon machines or causal state models) to differentiate between synapse type, and classify the complexity of the process. We find that the machines allow us to differentiate between processes that otherwise have similar output distributions. We are also able to understand these differences in terms of the dynamics of the model used to create the output response, bringing the analysis full circle. Hence this technique provides a complimentary description of the synaptic filtering process, and potentially expands the interpretation of future experimental results.

Emily F. Stone
The University of Montana
Department of Mathematical Sciences
stone@mso.umt.edu

Elham Bayat-Mokhtari
University of Montana - Missoula
elham.bayatmokhtari@umconnect.umt.edu

MS17

Electronic Gene Networks as True Random Number Generators

An important tool of modern cybersecurity is the true random number generator, a device that generates random numbers from a physical process, such as thermal noise in an electronic circuit. To avoid possibilities of hacking such devices, Rambus Inc. (California) has proposed a novel design that is inherently chaotic in addition to having the random thermal fluctuations of any electronic circuit. The equations that describe this analog circuit are closely related to a class of piecewise-linear equations used in modeling the behavior of gene-regulatory networks. Tools from the study of such systems are used here to demonstrate that the Rambus circuit is chaotic, producing entropy at a positive rate even without considering thermal noise.

Roderick Edwards
University of Victoria
Dept. Math and Statistics
edwards@uvic.ca

MS17

A New Frame for Phase Plane Analysis: Using Differential Geometry to Reveal Local Dynamics

In this talk, we introduce a new change of coordinates, which we term *local orthogonal rectification* or LOR, that can be applied at any selected manifold in the phase space of a dynamical system. LOR yields a coordinate system, the *LOR frame*, which allows us to rigorously study dynamics near the selected manifold. We have used the LOR approach to derive a novel definition for rivers, long-recognized but poorly understood trajectories that locally attract other orbits yet need not be related to invariant manifolds or other familiar phase space structures, and to identify rivers within several example systems. We also demonstrate that canard dynamics in fast-slow systems can be more easily identified and analyzed using the LOR frame.

Benjamin G. Letson
University of Pittsburgh
bgl14@pitt.edu

MS17

Modeling and Control of Nonlinear Oscillations in Neuroscience and Energy Systems

The ability to organize and finely manipulate the hierarchy and timing of dynamic processes is important for understanding and influencing phenomena in natural and engineered systems. Establishing spatiotemporal structures in oscillator ensembles is a challenging task that requires controlling large collections of complex nonlinear dynamical units. I will present a method to design entrainment signals that create stable phase-selective patterns in ensembles of heterogeneous nonlinear oscillators without using state feedback information, and demonstrate the approach using experiments with electrochemical reactions on multi-electrode arrays. I will then present a control policy for modulating the power consumption of aggregated thermostatically-controlled loads for use in demand response to balance supply and demand on the power grid while maintaining power quality and grid stability, and demonstrate tracking of a regulation signal that has been filtered in different bandwidths.

Anatoly Zlotnik
Los Alamos National Laboratory
azlotnik@lanl.gov

MS18

Improving Path Trackers for Homotopy Continuation Methods

Path trackers are numerical algorithms designed to "walk along" implicitly defined curves. They are the key compo-

nent of any efficient homotopy continuation method which, in turn, form the basis of Numerical Algebraic Geometry. Though path trackers usually work inside the affine or projective spaces, recently a wide range of ideas for tracking paths through their lifting into curved spaces have been explored. In this talk, we outline a general framework for designing simple yet efficient path trackers through the use of nonlinear lifting. We also explore the algebraic connection of this framework to moment maps and tropical geometry. Finally, we present an open source library implementing this framework that can take advantage of massively parallel GPU devices and many-core processors such as Intel Xeon Phi.

Tianran Chen
Auburn University Montgomery
ti@nranchen.org

MS18

Using NAG to Advance Our Capabilities of Computing Matrix Manifold Means

For a given data set, a natural task is to find the mean of the set. We introduce two algorithms that generate mean representatives: the projection mean of a set of orthonormal matrices and the max-length-vector line of best fit for a set of vector subspaces. In both cases, the associated optimization problems require solving complicated equations that evade clean, closed form solutions. We have found that solving these equations is best accomplished with sophisticated computational machinery, such as numerical algebraic geometry software Bertini.

Justin D. Marks
Gonzaga University
marksj@gonzaga.edu

MS18

Statistical Estimation of the Number of Solutions to Motion Generation Problems

Large structured polynomial systems, such as those arising in motion generation of linkages in kinematics, tend to have far fewer solutions than traditional upper bounds would suggest. In this talk, we will describe a statistical method for estimating the total number of solutions. The new approach extends previous work on success ratios of parameter homotopies to monodromy loops and adds a trace test stopping criteria for validating that all solutions have been found. Several examples will be presented demonstrating the method including solving Watt I six-bar motion generation problems.

Samantha Sherman
Notre Dame
Notre Dame, IN USA
samantha.n.sherman.47@nd.edu

Jon Hauenstein
University of Notre Dame
hauenstein@nd.edu

MS18

3D Printing Herwig Hauser's Gallery of Algebraic Surfaces with Bertini_real

Herwig Hauser's Gallery of Algebraic Surfaces is a beautiful set of images and equations of three-dimensional algebraic surfaces, many with singularities. Bertini_real is a numerical software for decomposing real algebraic curves and surfaces in any number of variables. It exploits homotopy continuation, path tracking, and random real linear projections to parameterize algebraic surfaces implicitly. Bertini_real is able to compute full models from the Hauser gallery by solving singularities and embedded curves. In order to tangibly visualize the Hauser gallery using Bertini_real, we print the decomposed surfaces in 3D.

Foong Min Wong, David Bachmeier
University of Wisconsin - Eau Claire
wongf3284@uwec.edu, bachmedj1415@uwec.edu

MS19

Parallel-in-Time Symplectic Integrators for Isospectral Flows

Parallel-in-time symplectic integators based on the Magnus expansion and Munthe-Kaas Runge-Kutta (MK-RK) scheme are described and analyzed. These integrators are able to preserve the important physical characteristics of a va- riety of systems over long time scales unlike traditional differential equation solvers such as Euler or Runge-Kutta methods. We present an efficient paral- lel formulation of fourth- and sixth-order Magnus methods that is counter to the conventional approach of minimizing the number of commutators required for higher-order accuracy. In comparison to our Magnus method results, the MK-RK approach is dramatically simpler to construct, and can be made to be arbitrary order simply by increasing the number of nodes used in the chosen quadrature scheme. Performance and convergence behavior for the two classes of methods is highlighted through numerical examples of isospectral flow prob- lems such as the periodic Toda lattice and electron dynamics simulations.

Brandon Krull
LBL
bkrull@lbl.gov

Michael Minion
Lawrence Berkeley National Lab
Stanford University
mlminion@lbl.gov

MS19

An Algebraic Multigrid Approach to Parallel-in-Time Integration

Many parallel-in-time (PiT) methods can be seen as a geometric multigrid method applied to the temporal domain of a space-time problem. Here, we present a new perspective on PiT through algebraic multigrid (AMG). Given a spatial and temporal discretization to PDE, the discrete space-time solution can be obtained through solving a single large sparse linear system. However, such matrices take on highly nonsymmetric structures, a far cry from the spd matrices that AMG is typically designed for. Recently, a reduction-based AMG method was developed for upwind discretizations of hyperbolic PDEs, based on an approximate ideal restriction (AIR). AIR is able to solve high-order discretizations of advection-dominated problems, which are intractable for other AMG methods. Here, we recognize that time-stepping schemes are simply upwind discretizations of advection in one dimension. The algebraic approach is particularly promising to overcome difficulties, which can be associated to geometric time grids. For hyperbolic PDEs, PiT methods often struggle with coarse-grid

instabilities due to CFL-like conditions, which must hold for all levels. Similarly, PiT methods based on a geometric time grid are often not well-suited to handle unstructured or adaptive meshes in a full space-time discretization. We discuss AIR as a linear solver for space-time discretizations. Two different parallel realizations of AIR will be introduced, followed by results for full space-time discretizations.

Ben Southworth
Department of Applied Mathematics
University of Colorado, Boulder
ben.southworth@colorado.edu

Tom Manteuffel
University of Colorado, Boulder
tmanteuf@colorado.edu

MS19

Hybrid Parareal Methods in Electrophysiology

The propagation of cardiac excitation is described by the bidomain model or its monodomain simplification. Due to very different time and length scales, their simulation is extremely expensive, such that spatial parallelization is used widely. Parallelization in time has been investigated much less. In this talk we will discuss the application of hybrid SDC parareal schemes to the excitation propagation. In particular we will design an eikonal fast propagator and compare it to traditional low order fast propagators in terms of convergence rate and parallel efficiency.

Martin Weiser
Zuse Institute (ZIB)
Berlin, Germany
weiser@zib.de

MS19

Micro-macro Acceleration Method with Relative Entropy Moment Matching for Scale-separated SDEs

Many systems exhibit behavior on a wide range of time scales, which cannot be simulated directly on macroscopic time intervals. In such a setting, efficient time-parallel methods can be constructed that iteratively approximate a coarse-grained model by time-parallel fine-scale corrections. The method couples the microscopic model, of which we have full knowledge, to a macroscopic level, of which we assume only limited information. The macroscopic model is described by a finite set of state variables—averages over the microscopic distribution. A crucial part is the appropriate inference of a fine-scale state that is consistent with an imposed macroscopic state. We call this step matching. We will present and discuss this matching step to efficiently simulate the macroscopic observables of SDEs having strong separation between time-scales. To bypass the prohibitive cost of the full Monte Carlo simulation, the method combines short bursts of path simulation with extrapolation of macroscopic states. To address the inference problem, we introduce a matching operator based on the minimization of distances between probability distributions logarithmic relative entropy. We discuss the relation of the method to coarse-graining and its basic properties. We study the convergence in the numerically weak sense, inquire about the stability for test models, and provide a convenient numerical approach. We discuss the relevance of this work for time-parallel integration.

Giovanni Samaey, Przemyslaw Zielinski
Department of Computer Science, K. U. Leuven
giovanni.samaey@cs.kuleuven.be, przemyslaw.zielinski@cs.kuleuven.be

MS20

An Introduction to Consistent Bayesian Inversion

A significant challenge facing the computational science and engineering community is the development of reliable and efficient methods to enable data-informed computational models. In this presentation, we introduce the recently developed "consistent Bayesian" approach for solving a stochastic inverse problem based on measure-theoretic principles. This approach produces a posterior distribution that is consistent in the sense that the push-forward of the posterior distribution through the model is guaranteed to match the distribution on the observable data. While understanding the details of this approach requires some background in measure theory, we focus on a conceptual understanding of the problem and demonstrate that constructing an approximation to the posterior is as easy as solving a forward UQ problem with simple Monte Carlo sampling techniques. We provide Python scripts in the form of interactive Jupyter notebooks to help the attendees get started using this approach while building valuable intuition on solving this type of stochastic inverse problem. We also discuss the utilization of approximate models, e.g., surrogates, in the context of stochastic inverse problems. Attendees are encouraged to bring their own data sets from forward UQ studies as we will show that this data can be easily post-processed to solve a stochastic inverse problem.

Troy Butler
University of Colorado Denver
troy.butler@ucdenver.edu

Timothy Wildey
Sandia National Laboratories
tmwilde@sandia.gov

MS20

Sensitivity Analysis in 4D-Var Data Assimilation: Theoretical Aspects and Applications

Data assimilation systems (DAS) combine information from a numerical model, observational data, and error statistics to analyze and predict the state of a dynamical system. Four-dimensional variational data assimilation (4D-Var) provides an estimate (analysis) to the true state by solving a large scale model-constrained optimization problem. The weight assigned to the information provided by a prior (background) state estimate and time-distributed measurements is determined by the representation of the statistical properties of the errors in the model and observations. Valuable insight on the relative importance and contribution of various DAS components to reduce the forecast errors may be obtained by performing sensitivity studies to assess the analysis and forecast impact induced by variations in the input parameters. This tutorial introduces theoretical and practical aspects of the sensitivity analysis in a 4D-Var DAS including observations, prior state estimate, and parametrized error covariance models. Illustrative examples from atmospheric data assimilation and applications to numerical weather predic-

tion are also presented.

Dacian N. Daescu
Portland State University
Department of Mathematics and Statistics
daescu@pdx.edu

MS21

Discretization of Hypersingular Kernels on Surfaces

In this talk, we present a procedure for the design of moderately high order quadrature rules for discretizing hypersingular kernels on smooth surfaces. The resulting quadratures are compatible with collocation based discretization schemes and can be viewed as a convenient tool for applying Dirichlet-Neumann maps and evaluating derivatives of double layer potentials.

Zydrunas Gimbutas
National Institute of Standards and Technology
zydrunas.gimbutas@nist.gov

James Bremer
UC Davis
bremer@math.ucdavis.edu

MS21

On the Solution of the Biharmonic Equation on Regions with Corners

In this talk, I will discuss the numerical solution of the biharmonic equation on regions with corners. Historically, this has been a somewhat refractory class of problems, in part due to the complicated behavior of the corresponding Green's functions. We show that, when the biharmonic equation is reformulated as a pair of coupled integral equations on the boundary, the solutions are representable by rapidly convergent series of elementary functions which oscillate with frequency proportional to the logarithm of the distance from the corner. Such representations are constructed explicitly and are used to create highly accurate and efficient Nyström discretizations, significantly reducing the number of degrees of freedom required to solve the corresponding integral equations. We illustrate the performance of the method with several numerical examples.

Kirill Serkh
Courant Institute
New York University
kserkh@cims.nyu.edu

MS21

Integral Equation Methods for Electrohydrodynamics of Biological Cells

Abstract not available at time of publication.

Shravan Veerapaneni
Department of Mathematics
University of Michigan
shravan@umich.edu

MS21

Resolving Collisions in Stokes Suspensions with an Efficient and Stable Potential-free Constrained Optimization Algorithm

Abstract not available at time of publication.

Wen Yan
Flatiron Institute
Simons Foundation
wyan@flatironinstitute.org

MS22

Finite-Deformation Cohesive Polygonal Finite Elements for Pervasive Fracture Simulations

We present dynamic fracture simulations using cohesive surfaces inserted on inter-element surfaces on polytopal meshes. Cohesive finite elements provide a natural means for modeling nucleating and extending cracks in solids. However, a sufficient network of possible internal crack surfaces is required to insert cohesive elements. An optimal network would both have no preferential direction and be able to accurately follow arbitrary paths. To meet these criteria, we use polytopal elements generated from a maximal Poisson-disk sampled domain. Maximal Poisson-disk sampling provides a means to robustly and rapidly generate a geometry conforming mesh with an optimal fracture network. Elements are convex and can be modified to have good element quality for finite element analysis, while still maintaining an optimal fracture network. Wachspress and maximum entropy basis functions are used to form a finite element basis over the polytopes. Cohesive zone elements are dynamically inserted at facets between the polytopes in the mesh. As the analysis progresses, we track and update the evolving mesh topology using a graph-based approach, which allows mesh operations to be completed robustly and rapidly. Contact is enforced through a penalty method which is applied to both closed cohesive surfaces and general interpenetration of two polytopal elements. Several numerical examples are presented which illustrate the capabilities of the method and demonstrate convergence of solutions.

Eric Chin
University of California, Davis
ebchin@ucdavis.edu

Joseph Bishop
Sandia National Laboratory
jebisho@sandia.gov

Rao V. Garimella
Los Alamos National Laboratory
rao@lanl.gov

N. Sukumar
University of California, Davis
nsukumar@ucdavis.edu

MS22

Robust Polyhedral Meshing of Non-convex Domains with Sharp Features and Narrow Regions

We present VoroCrust: a novel approach to polyhedral meshing that simultaneously generates a quality mesh of the surface of a Piecewise Linear Complex (PLC) model and decomposes the enclosed volume by unweighted Voronoi cells with good aspect ratios conforming to the surface mesh, without clipping or bad normals. Up to our knowledge, our method is the first to solve this problem. VoroCrust also outputs an approximation of the medial

axis of the input model and provides a fast technique for in/out point classification. To design our solution, we introduce new definitions of the medial axis and the local feature size that cater to PLC models. To further ensure enough protection around sharp features of the input model, we also present the concept of Maximal-Poisson disk Sampling (MPS) with extended coverage, and provide a solution method. We experimentally illustrate the robustness and output quality of VoroCrust through a collection of models of varying complexity, successfully preserving sharp features if any. In this talk we will also discuss the recently released VoroCrust Software.

Mohamed S. Ebeida
Sandia National Laboratories
msebeid@sandia.gov

MS22

Computational Finite Element Differential Forms on Quadrilateral Meshes

The Periodic Table of the Finite Elements (see https://femtable.org/) classifies many families of conforming families of finite elements suited to simplicial and cubical meshes. In recent work, we have described a new family of methods called "trimmed serendipity elements' that fit within the same framework described by the table. The computational effort required to employ a trimmed serendipity element method is significantly less that what is required for comparable alternatives from the table, thereby presenting a host of potential benefits to the speed and accuracy of finite element methods in practice. Producing suitable computational bases for these spaces, especially for use on generic quadrilateral or hexahedral meshes, is not immediate. I will discuss our recent progress in this direction and explain how our approach relates to contemporary research in polytopal element methods.

Andrew Gillette, Tyler Kloefkorn
University of Arizona
Department of Mathematics
agillette@math.arizona.edu, tkloefkorn@math.arizona.edu

MS22

Construction of C^1 Vertex Splines over Quadrilateral Partitions: Part I

Polygonal splines were first developed by Floater and Lai in 2016, and were implemented to solve Poisson equations. However, the splines developed at this time were only able to maintain continuity, without any global differentiability. This talk will detail a construction of Wachspress polygonal splines which are globally C^1 over partitions of quadrilaterals, along with some applications, including function interpolation and surface design.

James Lanterman
Department of Mathematics
University of Georgia
jay.lanterman@gmail.com

MS23

Efficiently Solving PDEs with a New Software-PHOEBE Solver V2.0

I will introduce a new software named PHOEBE Solver V2.0 we have recently performed development for numerical solution to partial differential equations (PDEs). Functions and characteristics of this software will be introduced. Some examples will be given to show how to use this software to conveniently and efficiently to solve various kinds of PDEs with various finite difference schemes.

Yongbin Ge, Tianlong Ma
Ningxia University
gyb@nxu.edu.cn, matianlong315@126.com

MS23

Numerical Schemes for Jump Discontinuity, Corner Singularity to Compressible Stokes Flows

I will talk about numerical schemes based on jump discontinuity and regularity result for compressible Stokes equations on polygonal domains. Solutions are decomposed into singular and regular parts. Numerical simulations will be given to demonstrate the regularity of each decomposition.

Jae Ryong Kweon
POSTECH(Pohang University of Science and Technology)
Korea
kweon@postech.ac.kr

MS23

Analysis of Exponential-type Integration Method for Non-local Diffusion Problems

In recent years numerous physically relevant phenomena have been shown to demonstrate a non-standard diffusive process known as anomalous diffusion. Such models are mathematically interesting due to the non-local nature of the involved operators, such as the fractional Laplacian. Despite the growing interest in such problems, the existing numerical methods are still plagued by reduced convergence rates and inefficient implementations. This talk will focus on approximating an abstract Bessel-type equation which is an extension of the non-local problem of interest. From this extension problem, an efficient method with desirable convergence properties will be developed and analyzed. Numerical examples will be provided to demonstrate the results.

Joshua L. Padgett
Texas Tech University
joshua.padgett@ttu.edu

MS23

New Adaptive Alternating Direction Eikonal Methods for the Numerical Solution of Optical Beam Systems

This research report concerns the latest adaptive eikonal splitting methods for solving paraxial Helmholtz systems on high wave numbers. New alternating direction implicit based decomposition procedures are proposed. Mesh adaptations are implemented in the transverse and beam propagation directions. Asymptotic stability of the computational procedures is introduced and studied. It is found that the fully discretized oscillation-free numerical procedures on nonuniform grids are fast, effective and stable in the asymptotic sense with a stability index one. Simulation experiments are carried out to illustrate our accomplishments and conclusions.

Qin Sheng
Department of Mathematics
Baylor University

Qin_Sheng@baylor.edu

MS24

Mean Field Limit of Interacting Filaments for 3D Fluids

Abstract not available at time of publication.

Hakima Bessaih
University of Wyoming
Bessaih@uwyo.edu

MS24

Stochastic Reaction-diffusion Equations on Metric Graphs

Abstract not available at time of publication.

Wai-Tong Fan
University of Wisconsin-Madison
ariesfanhk@gmail.com

MS24

Scaling Limits of Diffusion on a Comb

Abstract not available at time of publication.

Gautam Iyer
Carnegie Mellon University
gautam@math.cmu.edu

MS24

Averaged vs. Quenched Large Deviations and Entropy for Random Walk in a Dynamic Random Environment

We consider random walk with bounded jumps on a hypercubic lattice of arbitrary dimension in a dynamic random environment. The environment is temporally independent and spatially translation invariant. We study the rate functions of the level-3 (i.e., process level) averaged and quenched large deviation principles from the point of view of the particle. In the averaged case the rate function is a specific relative entropy, while in the quenched case it is a Donsker-Varadhan type relative entropy for Markov processes. We relate these entropies to each other and seek to identify the minimizers of the level-3 to level-1 contractions in both settings. These minimizers describe how the walk and the environment (from the point of view of the particle) behave when the former is conditioned to have an atypical velocity.

Atilla Yilmaz
New York University
atilla@gmail.com

Firas Rassoul-Agha
University of Utah
firas@math.utah.edu

Timo Seppalainen
University of Wisconsin - Madison
seppalai@math.wisc.edu

MS25

Numerical Simulations of Strongly Coupled Geoscientific Applications using the Open-source Simulator DuMu^{x}

Coupled processes occur in engineering applications in the geosciences in many variations. We present a software concept to handle strongly coupled systems with grids of different dimension, multiple domains, and multi-physics. The concept is applied to real engineering application and cutting edge research problems in fractured porous media systems, in porous media with embedded network systems, applications including free-flow porous media interfaces, and coupled geomechanics and multi-phase flow processes. In contrast to approaches where different software frameworks are non-intrusively and weakly coupled to solve PDE systems arising from such coupled problems, we choose an intrusive design to achieve a strong and efficient coupling. The design is such that non-coupled applications can be reused as building blocks for coupled applications. The mathematical models may give rise to strongly coupled PDE systems. To solve such systems, we choose a monolithic solver strategy (single system matrix), which we found to be more efficient and accurate than iterative / sequential solver strategies in many cases.

Timo Koch
IWS, University of Stuttgart
timo.koch@iws.uni-stuttgart.de

Dennis Glaeser, Kilian Weishaupt
IWS, University of Stuttgart, Germany
dennis.glaeser@iws.uni-stuttgart.de,
kilian.weishaupt@iws.uni-stuttgart.de

Bernd Flemisch
University of Stuttgart, Germany
bernd.flemisch@iws.uni-stuttgart.de

Rainer Helmig
IWS, University of Stuttgart, Germany
Dept. of Hydromechanics
rainer.helmig@iws.uni-stuttgart.de

MS25

Hydrate Modeling Across the Scales

We discuss a collection of issues and results on the analysis and numerical convergence of transport of methane in the sub-ocean sediments. The model comprises diffusive and advective transport, and equilibrium and kinetic phase transitions, as well as multiple components which influence phase behavior. Of interest are time scales spanning kiloyears for basin modeling and hours or days for interface evolution at the porescale. This is joint work with many students and other collaborators to be named in the talk.

Malgorzata Peszynska
Department of Mathematics
Oregon State University
mpesz@science.oregonstate.edu

MS25

Non-standard Mathematical Models for Flow in Porous Media: From Mathematical Analysis to Experimental Results

Standard models for flows in porous media assume that quantities like saturation, phase pressure differences, or relative permeability are related by monotone, algebraic relationships. These relationships are determined experimentally, assuming that the involved quantities have reached a

local equilibrium. Under such assumptions, the solutions of the resulting mathematical models have properties like stability in various norms, and satisfy the maximum principle. In particular, standard models rule out effects like saturation overshoot or the formation of finger profiles, which have been evidenced experimentally. This contradiction is the main motivation when considering non-equilibrium models, where dynamic effects and hysteresis are included in the above mentioned relationships. The resulting models are nonlinear evolution systems of (pseudo-)parabolic and possibly degenerate equations, and may involve differential inclusions. In this contribution we discuss the behaviour of the solutions to such models based on the travelling wave anakysis, and analyze different numerical schemes (multipoint flux approximation, discontinuous Galerkin) for approximating the solutions. In particular, we present the rigorous convergence analysis of the numerical solution to the weak solution of the model. Also, we analyze different linear iterative methods for approximating the numerical solution to the nonlinear, fully discrete problems encountered at each time step.

Iuliu Sorin Pop
Hasselt University
sorin.pop@uhasselt.be

Hans van Duijn
TU Eindhoven
C.J.v.Duijn@tue.nl

Xiulei Cao
Department of Mathematics and Statistics, York University
xiuleicao@gmail.com

Koondanibha Mitra
Eindhoven University of Technology
k.mitra@tue.nl

Stefan Karpinski
Esprit Engineering GmbH
stefan.karpinski@esprit-engineering.de

Florin A. Radu
Institute of Mathematics
University of Bergen
florin.radu@math.uib.no

Rainer Helmig
IWS, University of Stuttgart, Germany
Dept. of Hydromechanics
rainer.helmig@iws.uni-stuttgart.de

MS25

Seismic Velocity Inversion using Two-stage Markov Chain Monte Carlo and Operator Upscaling for the Acoustic Wave Equation

Abstract not available at time of publication.

Georgia Stuart
University of Texas at Dallas
georgia.stuart@utdallas.edu

MS26

Analysis and Design of Time-modulated Metamaterials

In this talk, we discuss our recent efforts in modeling and designing time-modulated metamaterials to enable broadband magnet-less non-reciprocal devices and delay lines exhibiting no group velocity dispersion. We rigorously compute the dispersion of infinite cascades of such networks to show that we can largely overcome the limitations of time-invariant systems, and apply these findings to realistic devices. We will also show experimental verification of our analytical predictions.

Andrea Alu
The University of Texas at Austin
aalu@gc.cuny.edu

Mykhailo Tymchenko
University of Texas at Austin
mih.timchenko@gmail.com

Dimitrios Sounas
The University of Texas at Austin
dsounas@gmail.com

MS26

Optimization-centric Approach for Electromagnetic Scattering from Metamaterials

Metamaterials, metasurfaces, and photonic crystals are manipulating light in ways previously thought impossible. These complex structures present new opportunities for imaging and optical computing but are substantially more difficult to design optimally than their traditional counterparts. In this talk, we discuss a fast method to solve the electromagnetic scattering problem presented by some of these complex photonic structures based on a multiple-scattering formulation. Specifically, we solve the Helmholtz equation in two dimensions and accelerate by reducing redundant computations and utilizing FMM. Incorporating gradient-based optimization algorithms into this method allows us to automate design of metamaterials, and obtain better-performing devices than those realized by imprecise analytical simplifications or manual tweaking. We demonstrate the validity of our approach with a few devices improved by optimization to local extrema.

Boaz Blankrot, Clemens Heitzinger
Vienna University of Technology
boaz.blankrot@tuwien.ac.at,
clemens.heitzinger@tuwien.ac.at

MS26

Electromagnetic Field Enhancement in Subwavelength Metallic Structures: Asymptotic Analysis and Numerical Approach

Since the discovery of the extraordinary optical transmission through nanohole arrays in metallic films by Ebbesen, a wealth of research has been sparked in the experimental and theoretical investigation of localized electromagnetic field enhancement in subwavelength nanostructures. This remarkable phenomenon can lead to potentially significant applications in near-field imaging, bio-sensing, etc. However, there has been a long debate on the interpretation of the enhancement effect since Ebbesens work. In addition, quantitative and rigorous analysis of the field enhancement in subwavelength structures is still widely open. In this talk, using two-dimensional slits as a prototype, I will present mathematical studies of the electromagnetic

field enhancement in the subwavlength structures. Both the theoretical and computational issues will be addressed.

Junshan Lin
Auburn University
jzl0097@auburn.edu

MS26

Optimal Wavefront Control: From Metasurfaces to Optically Induced Force and Torque

Wavefront manipulation represents a new frontier in nanophotonics. We formulate wavefront design for problems ranging from optical force and torque generation to superresolution as quadratic programming problems, with easily computable global optima. Then, we use inverse design to discover complex nanophotonic structures that can generate the desired fields at state-of-the-art performance levels.

Owen D. Miller
Yale Applied Physics
owen.miller@yale.edu

MS27

On Runge-Kutta Methods for the Water Wave Equation and Its Simplified Nonlocal Hyperbolic Model

There is a growing interest in investigating numerical approximations of the water wave equation in recent years, whereas the lack of rigorous analysis of its time discretization inhibits the design of more efficient algorithms. In this work, we focus on a nonlocal hyperbolic model, which essentially inherits the features of the water wave equation, and is simplified from the latter. For the constant coefficient case, we carry out systematic stability studies of the fully discrete approximation of such systems with the Fourier spectral approximation in space and general Runge-Kutta methods in time. In particular, we discover the optimal time step constraints, in the form of a modified CFL condition, when certain explicit Runge-Kutta methods are applied. Besides, the convergence of the semi-discrete approximation of variable coefficient case is shown, which naturally connects to the water wave equation. Extensive numerical tests have been performed to verify the stability conditions and simulations of the simplified hyperbolic model in the high frequency regime and the water wave equation are also provided. Faculty Advisors: Liu, Jian-Guo, Duke University, jliu@phy.duke.edu; Li, Lei, Duke University, leili@math.duke.edu; Zhou, Zhennan, Peking University BICMR, zhennan@bicmr.pku.edu.cn; Yang, Yi, Tsinghua University, yiyang16@mail.tsinghua.edu.cn

Zibu Liu
Peking University, China
nibio21@pku.edu.cn

MS27

Computing Interior and Boundary Derivatives of Harmonic Functions in Planar Domains with Harmonic Conjugates

We provide a derivation of a high-order numerical method capable of evaluating arbitrary interior derivatives of a harmonic function in a planar domain, as well as its boundary derivatives, given its Dirichlet trace. Consideration of the harmonic conjugate, whose normal derivative is proportional to the tangential derivative of the function we seek, leads to a complementary Neumann problem. The latter is equivalent to a second-kind integral equation that is solved numerically via a Nystrm method. The trace of the harmonic conjugate may be differentiated with an FFT to recover the normal derivative of the original function. The interior derivatives are found by observing that the original function and its harmonic conjugate are the real and imaginary parts of a holomorphic function, and Cauchys integral formulas allow us to evaluate the interior derivatives by doing calculations entirely on the boundary. We tackle domains with piecewise smooth boundaries by employing Kress quadrature. We provide several numerical examples that demonstrate convergence trends, and suggest how the method can be incorporated into FEM solvers. Faculty Advisor: Ovall, Jeffrey, Portland State University, jovall@pdx.edu

Samuel Reynolds
Portland State University
ser6@pdx.edu

MS27

The Gravitational Two Body Problem Under Different Laws of Gravity

In physics, the gravitational two body problem studies the time evolution of a system of 2 masses due to the gravitational interaction between them. This is described by Newtons Law of Universal Gravitation, which models gravity as a radial vector field inversely proportional to the cube of the distance between the masses. Functions with the same form, but different powers are analyzed. The approach for this is to begin with a differential equation describing the motion of two massive bodies interacting via gravity. Typically, this is done with the power of negative three, and it is shown that this differential equation implies Keplers first and third laws. In this research, the implications of the differential equation under different powers are analyzed. One focus of this is to discover whether or not different powers imply analogues to Keplers laws. Faculty Advisor: De Leenheer, Patrick, Oregon State University Mathematics Department, deleenhp@science.oregonstate.edu

Tyler Schimleck
Oregon State University, USA
schimlet@oregonstate.edu

MS27

Harmonic Mappings from Generalizations of Hypocycloids: Rosette Mappings

A family of generalized hypocycloids known as rosettes display unique mathematical properties. The rosette is a harmonic mapping with canonical decomposition identical to the simple polynomials that generate the harmonic hypocycloid, but with additional factors that are hypergeometric 2F1 series. While the hypocycloid is well-known in the mathematical realm, the rosette was only discovered in 2016. This project explores the intricacies of rosettes and their relationship with hypocycloids, through an analysis of the relationships between relevant formulae and the use of the computer algebra system Mathematica. The graphics of hypocycloids and rosettes that this system generates are of particular significance to this research endeavor. Important findings include the following properties of the rosette: its nested behavior, the mirror image property on the boundary of its mappings, the equal and opposite

tangent vectors that produce this property, and the distinct shapes that are generated based on the relative angle rotation of the functions of the canonical decomposition. Faculty Advisor: McDougall, Jane, Colorado College, jmcdougall@coloradocollege.edu

Lauren Stierman
Colorado College, USA
l_stierman@coloradocollege.edu

MS28

Generative Representations of the World

Generative approaches enable creating numerous scenarios coherent with the reality, as long as the representations are good approximations of the real world. In this talk, we will discuss extracting such generative representations from 2D and 3D data for mapping, modeling, and reconstruction of spatial data and urban models. We will introduce shape processing algorithms to exploit similarities, grammar discovery approaches to extract procedural rules, and machine learning methods to understand spatial information. The talk will conclude by proposed applications and experimental results on various types of geometric data.

Ilke Demir
Facebook
idemir@fb.com

MS28

Finding Communities and Roles in Networks

Community detection and role detection in networks are broad problems with many applications. Existing methods for community discovery frequently make use of edge density and node attributes; however, the methods ultimately have different definitions of community and build strong assumptions about community features into their models. Furthermore, users in online social networks often have very different structural positions which may be attributed to a latent factor: roles. In this talk, I will present recent advances in community and role discovery in networks, and discuss how their interplay can lead to a new definition of community viewed as interactions of roles.

Carlotta Domeniconi
George Mason University
cdomenic@gmu.edu

MS28

Consistent Shape Matching via Coupled Optimization

In this talk, I will present a new method for computing accurate point-to-point mappings between pairs of triangle meshes, given imperfect initial correspondences. Unlike the majority of existing techniques, our approach optimizes for a map while leveraging information from the inverse map, yielding results which are highly consistent with respect to map composition. Furthermore, for each point on the source mesh, our method considers only a linear number of candidate points on the target mesh, allowing us to work directly with high resolution meshes. Key to this dimensionality reduction is a novel iterative candidate selection process, combined with an efficient optimization method for intrinsic distortion minimization. Qantitative and qualitative comparison of our method with state-of-the-art techniques show that it provides a powerful matching tool when accurate and consistent correspondences are required.

Anastasia Dubrovina
Stanford University
anastasiad@cs.stanford.edu

MS28

Stratifying High-dimensional Data Based on Proximity to the Convex Hull Boundary

The convex hull of a set of points, C, serves to expose extremal properties of C and can help identify elements in C of high interest. For many problems, particularly in the presence of noise, the true vertex set (and facets) may be difficult to determine. One solution is to expand the list of high interest candidates to points lying near the boundary of the convex hull. We propose a quadratic program for the purpose of stratifying points in a data cloud based on proximity to the boundary of the convex hull. For each data point, a quadratic program is solved to determine an associated weight vector. We show that the weight vector encodes geometric information concerning the point's relationship to the boundary of the convex hull. The computation of the weight vectors can be carried out in parallel, and for a fixed number of points and fixed neighborhood size, the overall computational complexity of the algorithm grows linearly with dimension. As a consequence, meaningful computations can be completed on reasonably large, high-dimensional data sets.

Lori Ziegelmeier
Dept. of Mathematics, Statistics, and Computer Science
Macalester College
lziegel1@macalester.edu

MS29

A Golub-Kahan Davidson Method for Accurately Computing Singular Triplets of Large Sparse Matrices

Obtaining high accuracy singular triplets for large sparse matrices is a significant challenge, especially when searching for the smallest triplets. Due to the difficulty and size of these problems, efficient methods must function iteratively, with preconditioners, and under strict memory constraints. In this research, we present a Golub-Kahan-Davidson method (GKD), which satisfies these requirements and includes features such as soft-locking with orthogonality guarantees, an inner correction equation similar to Jacobi-Davidson, GD+k restarting, and the ability to find real zero singular values in both square and rectangular matrices. Additionally, our method achieves full accuracy while avoiding the augmented matrix, which often converges slowly due to the difficulty of interior eigenvalue problems. We describe our method in detail, including implementation issues that may arise. Our experimental results confirm the efficiency and stability of our method over the current implementation of PHSVDS in the PRIMME software package.

Steven Goldenberg
College of William & Mary

sgoldenberg@email.wm.edu

MS29

The Nonlinear Feast Algorithm

Abstract not available at time of publication.

Agnieszka Miedlar
University of Kansas
amiedlar@ku.edu

MS29

Nonlinear Eigenvalue Problems with Square Roots: Theory and Applications

Abstract not available at time of publication.

Roel Van Beeumen
Lawrence Berkeley National Laboratory
rvanbeeumen@lbl.gov

MS29

A Block Preconditioned Harmonic Projection Method for Nonlinear Eigenproblems

Abstract not available at time of publication.

Fei Xue
Clemson University
fxue@clemson.edu

MS31

On Performance Portability for Unstructured High-order Finite Element Computations

High order discretizations such as spectral element and discontinuous Galerkin offer great potential for memory locality and vectorization, leading to high utilization of modern computational resources. Indeed, such methods underlie leading applications in broad range of scientific and engineering disciplines including many Gordon Bell Prizes. Unfortunately, many optimizations are architecture- and parameter-specific, requiring substantial effort to optimize. Existing applications are often difficult to re-purpose for solving different problems, especially in different software environments, leading to a lot of overlapping optimization effort and a high barrier to entry for a new application to deliver high performance across a range of modern architectures. The code for efficient extensible discretization (libCEED) is a portable, lightweight library providing high performance operations with minimal assumptions. It includes support for just-in-time compilation and supports plugins providing backend optimizations. Application and library developers can use the libCEED interface to obtain high performance using a portable, high-level interface. Meanwhile, vendors and computer scientists can work on optimization techniques using only simple algebraic concepts, and those optimizations will benefit all applications.

Jed Brown
University of Colorado Boulder
jed.brown@colorado.edu

Jean-Sylvain Camier
CEA, DAM, DIF
Jean-Sylvain.Camier@cea.fr

Veselin Dobrev, Tzanio Kolev
Lawrence Livermore National Laboratory
dobrev1@llnl.gov, kolev1@llnl.gov

David Medina
Rice University
dmed256@gmail.com

Thilina Rathnayake
University of Illinois
thilinarmtb@gmail.com

Jeremy Thompson
University of Colorado Boulder
jeremy.thompson@colorado.edu

MS31

MFEM Efficient Partial Assembly Algorithms

Computing with high-order finite element methods often results in a large number of sparse matrix-vector products in an iterative linear solver. For high orders it is more efficient to construct the products using a series of relatively small repeated tensor contractions for each finite element, instead of first computing and storing the large sparse matrix. This talk explores efficient algorithms for fusing tensor contractions resulting from the action of finite element operators for both continuous and discontinuous spaces. These algorithms are used in a mini-app called Laghos, which is designed to help test such ideas.

Johann Dahm
IBM
Johann.Dahm@ibm.com

Steve Rennich
NVIDIA Corporation
srennich@nvidia.com

Yohann Dudouit
LLNL
dudouit1@llnl.gov

MS31

A Distributed Mesh Infrastructure for Particle-in-Cell Simulations

Particle-in-cell (PIC) methods are becoming more commonly applied to resolve fine scale physics in problems in which PDE based methods alone are not sufficient. In these simulation methods the motion of the particles is influenced by fields that are solved for on a mesh and the mesh fields are influenced by the field values associated with the particles in their current positions. Thus there is a strong coupling between the particle motion and mesh-based solution processes as the solution steps from an initial state to a final state. In many applications areas, in particular ones with complex geometries and highly varying and/or anisotropic fields, there is a desire to employ unstructured meshes for the field solutions. Since the operations on the particles, which typically number in the billions, dominate, both in terms of computation and total memory, the particles are always distributed. However, it is common to maintain a copy of the mesh, which currently may reach a million elements, and its fields, in each memory space across the parallel computer. However, the combination of more complex systems being analyzed, higher accuracy needed for the field solve, and finite memory per process,

is driving a need to distribute the mesh. The focus of this presentation is to outline an approach being developed to support massively parallel PIC calculations on distributed meshes and to indicate the status of the implementation of the approach to support fusion plasma simulations.

Mark S. Shephard
Rensselaer Polytechnic Institute
Scientific Computation Research Center
shephard@rpi.edu

Eisung Yoon
Rensselaer Polytechnic Institute
yoone@rpi.edu

E. Seegyoung Seol
Rensselaer Polytechnic Institute
Scientific Computation Research Center
seols@rpi.edu

MS31

Towards Large-scale Fusion Energy Science with MFEM

The Department of Energy's (DOE's) Scientific Discovery through Advanced Computing (SciDAC) projects are designed to bring together research scientists from various fields with computational scientists at the DOE's high performance computing laboratories. In particular the RF SciDAC project is intended to improve modeling capabilities related to radio frequency (RF) interactions within Tokamac devices. A Tokamak is a torus shaped device which uses powerful magnetic fields to confine a plasma and RF waves to heat that plasma with the goal of achieving nuclear fusion. Such devices have been studied for decades and numerous physical models exist to help understand the complex interactions taking place in different regions of the device. The goal of this project is to improve the physics fidelity of existing applications and to develop new applications as a step towards whole device modeling of Tokamak reactors. RF SciDAC efforts will focus on the physics outside the core of the reactor in a region called the Scrape Off Layer (SOL) where plasma turbulence, formation of a plasma sheath, impurity generation and transport, and heat transfer all impact the propagation of the RF waves as they make their way towards the core. These efforts will involve finding ways to modernize and accelerate existing computational tools as well as creating new tools to more fully exploit the available computing resources while more accurately approximating the relevant geometry and physics.

Mark L. Stowell, Tzanio Kolev
Lawrence Livermore National Laboratory
stowell1@llnl.gov, kolev1@llnl.gov

Syun'ichi Shiraiwa
Massachusetts Institute of Technology
shiraiwa@psfc.mit.edu

MS32

Innovative Projects and Funding Opportunities in Applied Mathematics Education Supported by the National Science Foundation

The National Science Foundation (NSF) has many funding opportunities to support the development and implementation of innovative pedagogical practices, curricular reforms and teaching resources in mathematics education. In this presentation we will provide examples of several innovative projects which have been funded by programs in the Division of Undergraduate Education (DUE) or the Division of Mathematical Sciences (DMS) that are intended to improve teaching and learning in the applied mathematics classroom. In particular, we will discuss projects supported by the Improving Undergraduate STEM Education (IUSE) program in DUE and the Infrastructure program in DMS as well as other related programs. An explanation of the NSF merit review criteria and suggestions for crafting competitive education-related proposals will be provided.

Ron Buckmire, Talitha Washnigton
Division of Undergraduate Education
National Science Foundation
rbuckmir@nsf.gov, twashing@nsf.gov

MS32

Math Modeling and Sustainability: Using Service Learning Projects to Deepen Student Engagement with Modeling

We will describe a course on Math Modeling and Sustainability in which students learn how to apply mathematics (Calculus 1 and 2 and below) to study problems of sustainability and then apply their knowledge to carry out a service learning project with a community partner. We start with the seemingly innocuous question: Is it worth it to change from incandescent to CFL or LED light bulbs? What does worth it mean and how does one quantify it? Then we look at other sustainability issues from a mathematical modeling perspective such as CO2 levels, Arctic ice sheet melting, solar panel energy generation and storm water management. The students work in teams to carry out service learning project in which they model a sustainability project of relevance to a community partner and provide recommendations to the partner. We will provide examples of the wide range of projects on which students have worked and share resources we developed as Chair of the organizing committee for Mathematics Awareness Month 2013 the Mathematics of Sustainability.

Victor Donnay
Bryn Mawr College
vdonnay@brynmawr.edu

MS32

Preparation for Industrial Careers in Mathematical Sciences (PIC Math)

PIC Math is a program to prepare undergraduate students in the mathematics and statistics to succeed in careers in business, industry, and government (BIG). Funded by NSF, this program strives to (a) increase awareness among faculty and students about non-academic career options, (b) provide undergraduate research experience using problems from industry, and (c) prepare students for industrial careers. The program includes a 3-day faculty summer training workshop, a spring semester course in which students learn skills and work on research problems from industry, and an end-of-program research conference at which the students present. For the semester course, we have developed a set of educational and informative videos and prepared materials for the course such as sample syllabi, set of sample research problems from industry, sample student solutions to industrial research problems, and sample videos of student presenting their research. During the first three years of PIC Math, over 100 universities, 100 faculty members, 1400 undergraduate students, and 100 industrial

partners have participated.

Michael Dorff
Brigham Young University
mdorff@math.byu.edu

Darren Narayan
Rochester Institute of Technology
darren.narayan@rit.edu

Suzanne L. Weekes
Worcester Polytechnic Institute (WPI)
sweekes@wpi.edu

MS32

Enhancing Undergraduate Education in Applied Mathematics through Multidisciplinary and Global Problem Solving

In this talk, we will describe how faculty, teachers and students at all levels can be engaged and challenged collaboratively to solve multidisciplinary global challenges using applied mathematics. The session will present successful pedagogical practices including inquiry-based learning environments, active-learning and experiential learning strategies and a design thinking framework that can help enhance undergraduate education in applied mathematics. Integral to this is the development of an integrated curriculum that incorporates rich applied mathematical tasks that require the use of higher-level critical thinking strategies and self-monitoring problem solving skills. Benchmark examples will include the use of applied mathematics to understand the spread of an infectious disease such as Zika in Latin America, development of strategies to stop poaching in Africa as well as predicting movement of gangs in Puerto Rico. These examples will demonstrate how educators can provide transformational experiences in applied mathematics education to address the growing national need to improve the performance of the American undergraduate workforce in mathematics and science.

Padmanabhan Seshaiyer
George Mason University
pseshaiy@gmu.edu

MS33

Geolocation of RF Emitters via Polynomial Systems

Radio signals from an emitter are picked up by receivers. When multiple receivers pick up the same signal, it is simple to compute TDOA (time delay on arrival) and FDOA (frequency delay on arrival) measurements for each pair of receivers. The location of the emitter can then be pinpointed by solving a system of polynomial equations that include the TDOA and/or FDOA measurements, assuming enough measurements are available. In this talk, we develop these polynomial systems and discuss some recent results that make use of this relatively new formulation of the geolocation problem.

Dan Bates
Colorado State University
bates@math.colostate.edu,

Karleigh Cameron
Colorado State University
Fort Collins, CO 80523
cameron@math.colostate.edu

MS33

Randomized Aspects of Polynomial System Solving

Generating "random" monodromy loops is a basic subroutine in numerical algebraic geometry. For certain applications, it is vital that the loops generated be correspond to permutations of the fiber set sampled from a nearly-uniform distribution. In practice, loops generated by various heuristic schemes may induce a distinctly non-uniform distribution. Nevertheless, any loop generating scheme induces a random walk on the monodromy group which (under mild technical conditions) converges to a uniform stationary distribution. We consider a broad class random walks on the monodromy group which evolve by composing some random number of elementary loops (eg. transpositions) at each stage. We give conditions for rapid convergence towards stationarity and, under suitable hypotheses, the cutoff phenomenon for this Markov chain. We also assess the predictions of this model experimentally, with varying loop-generating schemes and statistical tests. Additionally, we consider the robustness of monodromy techniques in the presence of path-tracking failures—this leads to some interesting questions in probabilistic combinatorics.

Tim Duff
Georgia Tech
Atlanta, GA USA
tduff3@gatech.edu

MS33

Using Machine Learning to Control a Path Tracker

Machine learning is one of the fastest growing fields in computing. Through the use of Google's free and open source API, "Tensorflow," it is becoming easier for amateurs to use machine learning for personal projects. One area of study to which this can be applied is Numerical Algebraic Geometry (NAG). An integral part of NAG is the concept of path tracking. Path tracking includes many variables and parameters, which can affect the efficiency and the accuracy of the algorithm. Our talk will consist of how we have utilized Tensorflow to control the parameters of the path tracking algorithm used in Bertini 2.

Dan Hessler, Sarah Ericson
University of Wisconsin - Eau Claire
hessledd3607@uwec.edu, ericsosm5070@uwec.edu

MS33

Computing Fundamental Groups of Smooth Real Surfaces

Computing topological information such as Euler characteristic, genus, Betti numbers, and the generators of the fundamental group can be computationally challenging for smooth, compact, orientable real algebraic surfaces. In this talk, I will discuss a new approach which uses a cell decomposition computed by numerical algebraic via the software package `Bertini_Real` to create a simplicial complex modeling the real algebraic surface. From this complex, we are able to use the software package `Javaplex` to compute topological information. The talk will conclude with several examples demonstrating the new approach and software.

Margaret Regan

University of Notre Dame
Notre Dame IN USA
mregan9@nd.edu

Jon Hauenstein
University of Notre Dame
hauenstein@nd.edu

MS34

PDE-Net: Learning PDEs from Data

Partial differential equations (PDEs) are commonly derived based on physical laws or empirical observations. With the rapid development of sensors, computational power, and data storage in the past decade, it offers new opportunities for data-driven discovery of hidden physical laws. Inspired by the latest development of neural network designs in deep learning, we propose a new feed-forward deep network, called PDE-Net, to fulfill two objectives at the same time: to accurately predict dynamics of complex systems and to uncover the underlying hidden PDE models. The basic idea of the proposed PDE-Net is to learn differential operators by learning convolution kernels (filters), and apply neural networks or other machine learning methods to approximate the unknown nonlinear responses. Comparing with existing approaches, our approach has the most flexibility by learning both differential operators and the nonlinear responses at the same time. Numerical experiments show that the PDE-Net has the potential to uncover the hidden PDE of the observed dynamics, and stably predict the dynamical behavior for a relatively long time, even in a noisy environment.

Zichao Long, Yiping Lu, Xianzhong Mao, Bin Dong
Peking University
zlong@pku.edu.cn, luyiping9712@pku.edu.cn, xianzhongma@pku.edu.cn, dongbin@math.pku.edu.cn

MS34

Data-driven Methods for Modeling and Control of Nonlinear Dynamical Systems

In this talk, I will discuss recent advances in data-driven, equation-free architectures for nonlinear dynamical systems leveraging advances in sparsity-promoting techniques and machine learning. One direction is related to Koopman operator theory, which has emerged as a principled framework to obtain linear embeddings of nonlinear dynamics, enabling the estimation, prediction and control of strongly nonlinear systems using standard linear techniques. In addition, I will discuss work related to statistical modeling in fluids and how to exploit sparsity in dynamical systems for modeling and sensing. The presented work is demonstrated on Hamiltonian systems and different high-dimensional nonlinear systems from fluids.

Eurika Kaiser
University of Washington
eurika@uw.edu

MS34

A Game Theoretic Approach to Numerical Approximation and Algorithm Design

This talk will cover interplays between Game Theory, Numerical Approximation and Gaussian Process Regression. We will illustrate this interface between statistical inference and numerical analysis through problems related to numerical homogenization, operator adapted wavelets, fast solvers, and computation with dense kernel matrices.

Houman Owhadi
Applied Mathematics
Caltech
owhadi@caltech.edu

Florian Schaefer
California Institute of Technology
florian.schaefer@caltech.edu

Clint Scovel
Caltech
clintscovel@gmail.com

Tim Sullivan
Free University of Berlin / Zuse Institute Berlin
sullivan@zib.de

Lei Zhang
Shanghai Jiao Tong University
lzhang2012@sjtu.edu.cn

MS34

An Artificial Neural Network as a Troubled-cell Indicator

High-resolution schemes for conservation laws need to suitably limit the numerical solution near discontinuities, in order to avoid Gibbs oscillations. In the context of DG schemes, this issue can be resolved by i) identifying the *troubled-cells* in the mesh which contain discontinuities, and ii) suitably limiting the numerical solution in these cells to suppress spurious oscillations. The solution quality and the computational cost of such schemes strongly depend on their ability to correctly identify troubled-cells. Most classical indicators, such as the minmod-type TVB limiter, require the specification of problem-dependent parameters. In general, however, it is difficult to estimate these parameters a priori. With the objective of constructing a universal troubled-cell indicator that can be used for general conservation laws, we propose a new approach to detect discontinuities using *artificial neural networks* (ANNs). In particular, a multilayer perceptron (MLP) is constructed, which is trained offline using a supervised learning strategy, and thereafter used as a black-box to identify troubled-cells. The advantage of the proposed ANN method is that it is parameter-free, non-intrusive and can easily be integrated into existing code frameworks. Several numerical results are presented to demonstrate the robustness of the MLP indicator in the framework of Runge-Kutta DG schemes.

Deep Ray
EPFL-SB-MATH-MCSS
deep.ray@epfl.ch

Jan S. Hesthaven
EPFL
jan.hesthaven@epfl.ch

MS35

An Introduction to Parameter Space Dimension Reduction

Scientists and engineers use computer simulations to study relationships between a physical model's input parame-

ters and its output predictions. However, thorough parameter studies—e.g., constructing response surfaces, optimizing, or averaging—are challenging, if not impossible, when the simulation is expensive and the model has several inputs. To enable studies in these instances, the engineer may attempt to reduce the dimension of the model's input parameter space using techniques such as sensitivity analysis or variable screening to identify unimportant variables that can be fixed for model analysis. Generalizing classical coordinate-based reduction, there are several emerging subspace-based dimension reduction tools that identify important directions in the input parameter space with respect to a particular model output. I will motivate and provide an overview of subspace-based dimension reduction techniques and discuss strategies for exploiting such low-dimensional structures—including analysis and computation—to enable otherwise infeasible parameter studies. For more information, see activesubspaces.org

Paul Constantine
University of Colorado Boulder
pconstan@mines.edu

MS35

Pattern Formation in Spatially Extended Systems - An Overview

I will give an overview of the phenomenology, theoretical approaches, and applications of pattern formation in spatially extended systems. The talk will cover localized spots, traveling waves, and spiral waves, as well as domain-filling patterns such as stripes and hexagons. The review of theoretical techniques will focus on spatial-dynamics approaches.

Bjorn Sandstede
Division of Applied Mathematics
Brown University
bjorn_sandstede@brown.edu

MS36

New Anisotropic Mesh Algorithms for 3D Singular Solutions

We discuss a new construction of 3D anisotropic meshes to improve the finite element approximation of elliptic boundary value problems with singular solutions from the non-smoothness of the domain. These algorithms are based on simple and explicit principles that lead to significant fewer geometric constraints in the mesh. We derive optimal error estimates for the proposed method.

Hengguang Li
Wanye State University
li@wayne.edu

MS36

Intrinsic Finite Element Methods over Manifolds

Abstract not available at time of publication.

Martin Licht
UC San Diego
mlicht@ucsd.edu

MS36

Discrete Comparison Principles for Finite Element Solutions of Quasiinear PDE

We will discuss discrete comparison principles for a class of quasilinear elliptic partial differential equations. As in the continuous setting, the comparison principle can be used in the finite element setting to establish uniqueness of the solution. We find for piecewise linear finite elements that without the presence of lower-order terms, it is sufficient for the meshsize to be locally controlled based on the variance of the solution over each element. Essentially, the mesh is required to be fine where the gradient is steep. We will consider the role of angle conditions in establishing the result.

Sara Pollock
Wright State University
sara.pollock@wright.edu

Yunrong Zhu
Department of Mathematics
Idaho State University
zhuyunr@isu.edu

MS36

Regularization of a Nonlinear Transport Model of Methane Gas with Space-dependent Flux Function, and Numerical Approximation

Methane is a greenhouse gas, and extraction of methane from subsea sediment has been of interest for energy sources. Under low temperature and high pressure, methane and water form methane hydrate, an ice-like substance present in subsea sediments. We study a transport model of methane gas with space-dependent flux functional. The first challenge is that the model has a multi-valued graph, and we used a change of variable to rewrite the model. Another challenge is that the obtained flux function is not smooth and depends on two variables. We use regularization to obtain a smooth concave flux function and discuss the seemingly unphysical, and at first glance, unexpected blow-up behavior of this problem. We also discuss the convergence of the numerical solution to this problem using the Godunovs scheme with local phase behavior solver.

Choah Shin
Oregon State University
Department of Mathematics
shinc@oregonstate.edu

Malgorzata Peszynska
Department of Mathematics
Oregon State University
mpesz@science.oregonstate.edu

MS37

Optimal Bayesian Experimental Design of Borehole Locations for Inferring Past Ice Sheet Surface Temperature

Borehole data are essential for calibrating ice sheet models, but field expeditions for acquiring data are often time-consuming, expensive, and dangerous. It is thus essential to identify drilling locations that maximize the value of data while minimizing costs and risks. We employ optimal experimental design (OED) to select locations that yield the highest expected information gain, a quantity that is computed using nested Monte Carlo. We model the glacier using a computationally intensive and nonlinear physical

model that quickly makes this approach intractable. We propose estimating an upper bound of the expected utility, and accelerating its computation via a polynomial surrogate function for approximating the Bayesian evidence. This surrogate is locally adaptive, where additional simulations are performed in inaccurate neighborhoods as assessed by an error indicator. The borehole data measurements are subsequently used for Bayesian inference of past surface temperatures via efficient Markov chain Monte Carlo. Through this work, we demonstrate the value of practical OED in combining data and models for environmental and climate research.

Andrew D. Davis
MIT
davisad@mit.edu

Xun Huan
Sandia National Laboratories
xhuan@sandia.gov

Patrick Heimbach
EAPS, Massachusetts Institute of Technology, and
ICES, University of Texas at Austin
heimbach@mit.edu

Youssef M. Marzouk
Massachusetts Institute of Technology
ymarz@mit.edu

MS37

Multifidelity Model Management using Latent Variable Bayesian Networks

Abstract not available at time of publication.

Alex Gorodetsky
University of Michigan
goroda@umich.edu

MS37

Polynomial Chaos Expansions for Dependent Random Variables

Polynomial chaos methods have been repeatedly used to efficiently build surrogates of models with independent uncertainties. Very little attention however, has been given to building approximations for dependent variables. The approaches that have been developed are computationally expensive, often suffer from ill-conditioning and are rarely used in practice. In this talk I will present sampling methods for regression, interpolation and compressive sensing in the presence of dependent variables, which maintain stability whilst focusing sampling in high-probability regions. The approaches build upon recent advances, based upon change of measure, for tensor product variables. The efficacy of the proposed approaches will be demonstrated on a number of numerical examples. Comparisons to approaches that use the Nataf and Rosenblatt transformation to map dependent variables to a set of independent variables will also be given.

John D. Jakeman
Sandia National Labs
jdjakem@sandia.gov

Akil Narayan
University of Utah
akil@sci.utah.edu

MS37

A Consistent Bayesian Inference Problem with Time Series Data

To quantify uncertainties of inputs to models of dynamical systems, a fixed spatial configuration of sensors is often designed and deployed to collect time-series data for solving stochastic inverse problems. A general goal is to configure the sensors so that they provide useful information for the stochastic inverse problem over the full duration of the experiment and provide us with minimally redundant data. We use a recently developed Consistent Bayesian framework for formulating and solving stochastic inverse problems to investigate the effects of measurement frequency, duration, and quality on posterior distributions and predictions.

Michael Pilosov
University of Colorado: Denver
michael.pilosov@ucdenver.edu

Troy Butler
University of Colorado Denver
troy.butler@ucdenver.edu

MS38

Exposure Time and Mass Balance

Mass balance expressions are the foundation of quantitative analyses of transport and transformation of multiphase multicomponent mixtures in many fields. In a number of cases the processes governing such mixtures may depend on the time-of-exposure of one mixture component to another. Some examples include groundwater age (groundwater exposure time to aquifer), heterogeneous-phase reaction (solute exposure time to reactive surfaces), dose-dependent illness progression (susceptible population exposure time to chemical stressor), and multidomain mass transfer (immoble-zone solute exposure time to immobile zone). These systems call for a method to keep track of the exposure time of one mixture to another, and this is achieved by including an additional dimension of exposure time and an advection operation in that direction, within systems of mass balance equations. The exposure time advection operator serves as a clock that allows accounting of memory within the transport and transformation constitutive expressions in a general manner. After presentation of the basic formulation approach, two geoscience examples are detailed: 1. development and analysis of the governing equation for groundwater age, and 2. a phase exposure-dependent exchange (PhEDEx) mass transfer model that captures non-Fickian transport processes including multirate mass-transfer, continuous time random walks, and time-fractional advection-dispersion.

Tim Ginn
Civil and Environmental Engineering
Washington State University
tim.ginn@wsu.edu

MS38

Linking Scales in the Sea Ice System

Polar sea ice is a key component of the Earths climate system. It exhibits complex composite structure on length scales ranging from microns to tens of kilometers. I will

give an overview of how we are using theories of composite materials and statistical physics to link behavior on various scales in the sea ice system. In particular, we address fundamental questions in sea ice homogenization, where information on smaller scales is incorporated into rigorous representations of effective large scale behavior. We also consider the inverse problem where small scale structure is inferred from larger scale effective properties. Examples include fluid flow through the porous brine microstructure, wave propagation in the marginal ice zone, convection enhanced thermal conduction, remote sensing, and the evolution of melt ponds on Arctic sea ice. This work is helping to advance how sea ice is represented in climate models, and to improve projections of climate change and the response of polar ecosystems.

Kenneth M. Golden, Elena Cherkaev
University of Utah
Department of Mathematics
golden@math.utah.edu, elena@math.utah.edu

N. Benjamin Murphy, Noa Kraitzman
University of Utah
murphy@math.utah.edu, noa@math.utah.edu

Christian Sampson
SAMSI
University of Northcarolina, Chapel Hill
christian.sampson@gmail.com

Jingyi Zhu
Department of Mathematics
University of Utah
zhu@math.utah.edu

Ivan Sudakov
University of Dayton
Department of Physics
isudakov1@udayton.edu

Yiping Ma
Department of Applied Mathematics
University of Colorado, Boulder
yiping.m@gmail.com

Court Strong
Department of Atmospheric Sciences
University of Utah
court.strong@utah.edu

MS38

Multiscale Methods for Non Linear Multiphase Flow Problems

It is well-known that numerically solving flow and transport problems in porous media require a very fine computational mesh, and some model reduction techniques are therefore necessary. A number of model order reduction approaches are available in the existing literature for approximating the solution at a coarse scale. We will present a model reduction technique based on the generalized multiscale finite element method (GMsFEM). An expanded mixed finite element formulation is used to separate the spatial scales between non-linear, flow and transport problems. An adaptive approach is used for local enrichment to improve the accuracy of the numerical solution.

Wing Tat Leung
University of Texas at Austin
wleungo@ices.utexas.edu

MS38

Influence of Changing Pore Scale Geometries on Upscaled Flow and Transport Models

Pore scale simulations can help to predict many important properties of the flow and transport at higher scales, and have become ubiquitous in the applications to geosciences, from fundamental geologic processes to energy resource storage and production. When pore scale geometry changes the crucial macro scale parameters such as porosity and permeability change as well. We extend our previous studies on the impact of pore scale geometry changes due to reactive transport or phase transitions, to include dissolution, as well as generation of plausible stochastically generated geometries for both precipitation and dissolution, and crystal formation at pore scale. In this presentation we show the impact of changes in the pore scale geometry on upscaled results.

Joe Umhoefer
Oregon State University
joseph.umhoefer@math.oregonstate.edu

Malgorzata Peszynska
Department of Mathematics
Oregon State University
mpesz@science.oregonstate.edu

Timothy Costa
Numerical Solutions, Inc.
timothy.costa@numericalsolutions.org

MS39

AMReX: An Overview

AMReX is a new software framework that supports the development of block-structured AMR algorithms for solving systems of partial differential equations with complex boundary conditions on exascale architectures. AMR reduces the computational cost and memory footprint compared to a uniform mesh while preserving the essentially local descriptions of different physical processes in complex multiphysics algorithms. AMReX supports solution strategies ranging from level-by-level approaches with multilevel synchronization to full-hierarchy approaches, and any combination thereof. In addition to the conventional representation of field variables on a mesh, AMReX supports particle data as well as embedded boundary (cut cell) representations of complex geometries. Both particles and embedded boundary representations introduce additional irregularity and complexity to the way data is stored and operated on, requiring special attention in the presence of the dynamically changing hierarchical mesh structure and AMR timestepping approaches. Block-structured AMR provides the basis for the temporal and spatial discretization strategy for a large number of applications. Current AMReX applications include accelerator design, astrophysics, combustion, cosmology, microfluidics, materials science and multiphase flow. In this talk I will give an overview of the software components provided by AMReX and how those components are used to support different applications that use the framework.

John B. Bell
CCSE
Lawrence Berkeley Laboratory

jbbell@lbl.gov

MS39

An Overview of FASTMath: Frameworks, Algorithms and Scalable Technologies for Mathematics

In this talk I provide an overview of the newly-established SciDAC-4 mathematics institute, FASTMath, and our eight core technologies: structured grids, unstructured grids, time integration, linear solvers, eigensolvers, numerical optimization, uncertainty quantification and data analytics. I describe recent successes of these technologies in large-scale DOE applications where we have provided foundations of new codes, increased application robustness, and/or decreased time to solution. I briefly describe our plans for performance portability and interoperability of our libraries.

Lori A. Diachin
Lawrence Livermore National Laboratory
diachin2@llnl.gov

MS39

ExaGraph: Graph Algorithms Enabling Exascale Computations

Graph algorithms play a critical enabling role in modern scientific applications, but the low communication to computation ratio and the irregular memory access of these algorithms make them hard to implement on parallel systems. We develop several graph algorithms chosen from a set of exascale applications, including graph traversals, matching, edge cover, coloring, clustering and partitioning. Software technologies from CombBLAS, KokkosKernels and GMT are used to implement these algorithms. This talk will first discuss the scope of the Exagraph project. Then we focus on a new algorithmic paradigm, the design of approximation algorithms, used to develop parallel algorithms scalable to the exascale. We will illustrate this paradigm using matching, edge cover, and their variants.

Alex Pothen
Purdue University
Department of Computer Science
apothen@purdue.edu

Mahantesh Halappanavar
Pacific Northwest National Laboratory
hala@pnnl.gov

Aydin Buluc
Lawrence Berkeley National Laboratory
abuluc@lbl.gov

Erik G. Boman
Center for Computing Research
Sandia National Labs
egboman@sandia.gov

Siva Rajamanickam
Sandia National Laboratories
srajama@sandia.gov

Antonino Tumeo
Pacific Northwest National Laboratory
Antonino.Tumeo@pnnl.gov

Karen D. Devine
Sandia National Laboratories
kddevin@sandia.gov

MS39

An Overview of the SUNDIALS Suite of Time Integrators and Nonlinear Solvers with a Look Toward Exascale Computing

SUNDIALS is a suite of robust and scalable solvers for systems of ordinary differential equations, differential-algebraic equations, and nonlinear equations. The suite consists of six packages: CVODE(S), ARKode, IDA(S), and KINSOL. Each package is built on a common vector and linear solver API allowing for application-specific and user-defined linear solvers and data structures, encapsulated parallelism, and algorithmic flexibility. As part of the DOEs Exascale Computing Program and FASTMath Institute, SUNDIALS is enabling time integrators for exascale architectures. In this presentation we will summarize capabilities of the SUNDIALS suite, overview current development efforts, and discuss incorporation of new work in multirate time integration methods. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-744969.

Carol S. Woodward
Lawrence Livermore National Laboratory
woodward6@llnl.gov

Daniel R. Reynolds
Southern Methodist University
Mathematics
reynolds@smu.edu

David J. Gardner
Lawrence Livermore National Laboratory
gardner48@llnl.gov

Alan Hindmarsh
Lawrence Livermore National Laboratory
Center for Applied Scientific Computing
alanh@llnl.gov

Slaven Peles
Lawrence Livermore Natinoal Laboratory
peles2@llnl.gov

John Loffeld
Center for Applied Scientific Computing
Lawrence Livermore National Laboratory
loffeld1@llnl.gov

MS40

Large Scale Analysis of Unreliable Stochastic Networks

Abstract not available at time of publication.

Reza Aghajani
Department of Mathematics, University of California San Dieg
maghajani@ucsd.edu

MS40

Gradient Flows of Wasserstein Spaces on Random

Geometric Graphs and their Continuum Limits

Abstract not available at time of publication.

Nicolas Garcia-Trillos
Brown University
nicolas_garcia_trillos@brown.edu

MS40

Local Dynamics of Interacting Stochastic Processes on Sparse Graphs

Abstract not available at time of publication.

Kavita Ramanan
Brown University
kavita_ramanan@brown.edu

MS40

Analysis of Allocation Algorithms in a Large Urn Model

The urn model we investigated is a closed system consists of N urns, βN balls, a symmetric graph and an allocation algorithm. Balls are stored in urns. Urns are placed on the nodes of the symmetric graph. The edges of the graph represent the connections between the urns. Each urn has an independent exponential empty time with unit mean: at such a moment, the urn throws all balls within it into other urns, following an allocation algorithm only based on the connections and loads of the urns. We study the long time behaviors of a class of allocation algorithms in this large system. We prove that when the number of connections of a given urn goes to infinity along with the total number of urns, the asymptotic loads on each urn can be described by non-linear jump diffusions. Propagation of chaos holds when the initial condition is symmetric. We give the stationary distributions of these non-linear jump diffusions for several algorithms. We discuss the properties of these stationary distributions when the loads are heavy. We also prove the convergence of the stationary distributions from the N-urn system to the mean-field system under some addition assumptions. The main difficulties in our model are: 1) the interactions are of unbounded sizes and occur among random subsets of urns; 2) the empirical measures do not have self-contained evolution equations.

Wen Sun
Inria Paris
wen.sun@inria.fr

Robert Philippe
INRIA Paris
philippe.robert@inria.fr

MS41

Forward Uncertainty Propagation in Cardiac Electrophysiological Model

Patient-specific cardiac electrophysiological models have shown promising potential in predicting the risk of lethal arrhythmia. However, the construction of a personalized 3D anatomical model of the heart from magnetic resonance imaging (MRI) scans involves several semi-automatic steps that can introduce uncertainty in final model predictions. To quantify this uncertainty, Monte Carlo simulation of the cardiac model on the distribution of uncertain inputs is popular. This can be computationally expensive given that the simulation of a single heartbeat can take up to 0.5 hour, especially if the uncertain input is high in dimension. In this study, we focus specifically on the uncertainty in model prediction as a result of the uncertainty in classification of myocardial tissue properties in relation to myocardial infarction. To study this, we first quantify the uncertainty in model construction arising from segmenting MRI images into major myocardial tissue categories: healthy, infarct core, and gray zone. Next, to reduce the computational cost for Monte Carlo simulation of the cardiac model, we reduce the input dimensions from pixel space to a small number of clusters on the distribution of tissue types. Each tissue type will be assigned a specific model parameter from literature during simulation. Finally, we study how this uncertainty propagates to the model predictions.

Kesavan Kushalnagar, Jwala Dhamala, Linwei Wang
Rochester Institute of Technology
krk4565@rit.edu, jd1336@rit.edu, linwei.wang@rit.edu

MS41

Convolution Quadrature Methods for Time-domain Scattering by Unbounded Material Interfaces

We present a class of flexible, robust and easy-to-implement boundary integral equation methods for the numerical solution of acoustic and electromagnetic time-domain scattering problems in the presence of unbounded penetrable media in two-spatial dimensions. The proposed methodology relies on Convolution Quadrature (CQ) methods in conjunction of the recently introduced Windowed Green Function (WGF) method. As in standard time-domain scattering problems by bounded obstacles, a CQ method of the user's choice is utilized to transform the problem into a finite number of (complex) frequency-domain problems posed on the unbounded material interfaces. Each one of these is then formulated as a second-kind integral equation that is effectively reduced to a bounded interface by means of the WGF method, which introduces errors that decrease super-algebraically fast as the window size increases. The resulting windowed integral equations can then be solved by means of any (accelerated or unaccelerated) Helmholtz boundary integral equation solver capable of handling complex wavenumbers. A high-order Nystrm method based on Alpert's quadrature rules is utilized here. A variety of numerical examples including wave propagation in open waveguides as well as scattering by multiply layered media and infinite wedges, demonstrate the capabilities of the proposed approach.

Ignacio Labarca Figueroa
Pontificia Universidad Católica de Chile
ijlabarca@uc.cl

Carlos Pérez Arancibia
Massachusetts Institute of Technology
cperezar@mit.edu

Luiz M. Faria
KAUST
lfaria@mit.edu

MS41

On a Navier-Stokes-Fourier-like System Capturing Transitions between Viscous and Inviscid Fluid Regimes and between No-slip and Perfect-slip

Boundary Conditions

We study a model with implicit constitutive relations that captures non-Newtonian fluids with temperature-dependent coefficients, in particular those which are able to describe the threshold slip phenomenon with the temperature-dependent activation criteria. Such a model is able to describe all states of the fluid from the yield stress, through the Newtonian fluid up to the inviscid case only by the temperature change. Also, concerning the boundary conditions, we are able to capture the standard Navier's slip, but also the threshold slip case, i.e. the stick-slip or the perfect slip-slip condition. These models always include the activation, however, the standard constitutive relations (yield stress, inviscid fluid, no slip or perfect slip boundary conditions) are the limit cases when certain activating coefficient tends to infinity for some temperature. Finally, also the large-data and the long-time existence analysis is provided. [E. Maringová and J. Žabenský: On a Navier-Stokes-Fourier-like system capturing transitions between viscous and inviscid fluid regimes and between no-slip and perfect-slip boundary conditions, Nonlinear Anal. RWA, 41 (2018), pp. 152-178.]

Erika Maringová
Charles University
maringova@karlin.mff.cuni.cz

Josef Zabensky
University of Wuerzburg
josef.zabensky@gmail.com

MS41

Goal-oriented Adaptivity using Gerenalized Multiscale Finite Element Method

Goal-oriented adaptivity is introduced within the framework of the generalized multiscale finite element method (GMsFEM) for high-contrast flow. GMsFEM is a systematic approach for approximation to multiscale problems. The methodology is based on a coarse mesh for global solution and a subordinate fine mesh over which local problems are considered. In this research, we will discuss the formulation of goal-oriented a posteriori error indicators within GMsFEM. The techniques will be illustrated with numerical examples.

Sai-Mang Pun
The Chinese University of Hong Kong
smpun@math.cuhk.edu.hk

Eric Chung
CUHK
tschung@math.cuhk.edu.hk

Sara Pollock
Wright State University
sara.pollock@wright.edu

MS41

Valuing Structures of Optionality

Usually banks provide differents optionalities in corporate and mortgage loans. Among the most common one, prepayment of monthly payment is given as a facility to borrowers breaking the natural cash flows associated with a loan. However banks provide a much broader range of optionalities to borrower trying to balance risk and value in inherently expensive options. Therefore it is important for corporate lenders to properly price the economic impact associated with those optionalities. Through the theory of term structure, stochastic processes and finance I will present a methodology to price different optionalities considering the issues from both a practitioner and academic perspective.

Alberto Rubio, Ronny Vallejos
Universidad Técnica Federico Santa María
alberto.rubio@alumnos.usm.cl, ronny.vallejos@usm.cl

MS41

Exact Reconstruction of Euclidean Distance Geometry Problem using Low-rank Matrix Completion

The Euclidean distance geometry problem arises in a wide variety of applications, from determining molecular conformations in computational chemistry to localization in sensor networks. When the distance information is incomplete, the problem can be formulated as a nuclear norm minimization problem. In this paper, this minimization program is recast as a matrix completion problem of low rank r Gram matrix with respect to a suitable basis. The well known restricted isometry property can not be satisfied in the scenario. Instead, a dual basis approach is introduced to theoretically analyze the reconstruction problem. If the Gram matrix satisfies certain coherence conditions with parameter ν, the main result shows that the underlying configuration of n points can be recovered with very high probability from $O(nr\nu\log^2(n))$ uniformly random samples. Computationally, simple and fast algorithms are designed to solve the Euclidean distance geometry problem. Numerical tests on different three dimensional data and protein molecules validate effectiveness and efficiency of the proposed algorithms [https://arxiv.org/abs/1804.04310].

Abiy Tasissa, Rongjie Lai
Rensselaer Polytechnic Institute
tasisa@rpi.edu, lair@rpi.edu

MS42

Cell-to-cell Variability in Collective Gradient Sensing

When cells cooperate to sense a signal, such as a cluster of cells performing collective chemotaxis, they must deal with cell-to-cell variability: even genetically identical cells can have differing responses to chemical signals. We show theoretically and computationally that variability in signaling can limit collective chemotaxis. This occurs because when a strongly responding cell is at one end of a cell cluster, cluster motion is biased toward that cell. These errors can be mitigated if clusters average measurements over times long enough for cells to rearrange - fluid clusters are better able to sense gradients. We develop a bound controlling cluster accuracy as a function of cell-to-cell variation and cluster rheology. We also discuss methods to more accurately infer cell-to-cell variability in both motility and signaling properties from cell trajectories, as well as applying our theory to experimental measurements of cluster rearrangement.

Brian Camley
University of California, San Diego
bcamley@jhu.edu

MS42

Continuum Approximations to Systems of Inter-

acting Particles

Collective behavior of many biological cells leads to many striking phenomena and promising applications. Study of systems of many interacting biological cells requires development of new mathematical tools. Specifically, in this talk I will focus on modeling correlations in such systems. I will introduce an individual based model (IBM) for many interacting cells and several continuum approximations to this IBM via truncations of the BBGKY hierarchy. The Mean Field Approximation (MFA), the Kirkwood Superposition Approximation (KSA), and a more recent truncation of the BBGKY hierarchy - Truncation Approximation (TA) - will be described. Properties of these approximations are compared showing that TA is less computationally expensive than KSA. MFA is the least computationally expensive of the three but does not capture evolution of correlations. In addition, these continuum approximations are compared to Monte Calro simulations of the IBM numerically, showing that both TA and KSA are more accurate than MFA

Robby Creese
Pennsylvania State University
rec5208@psu.edu

MS42

Cell Packing in the Drosophila Melanogaster Egg Chamber Directs Extracellular Signaling Critical for Clustered Cell Migration

Diffusible messengers are necessary activators of many biological processes. The extracellular space conducting these messengers are often spatially restricted by neighboring cells. We consider two processes in the fruit fly egg chamber: A) Secretion induced asymmetric epithelial cell activation prior to cell clustering and B) Chemoattractant distribution throughout the cell-packed egg chamber, which directs clustered cell migration. Each of these is significantly effected by an extracellular space with high cell density. We model each scenario with reaction-diffusion PDEs in a spatially heterogeneous cell-packed environment to relate diffusible messenger distribution and action. We then show how gradients of chemoattractants may impact clustered cellular migration across the egg chamber through an agent-based simulation of the eight cell cluster in the cell-packed domain. We show the extracellular domain may direct which border cells become activated in forming the cluster as well as where gradients of chemoattractant fluctuate and possibly impact the pacing and trajectory of clustered cell migration.

Bradford E. Peercy
Department of Mathematics and Statistics
University of Maryland, Baltimore County
bpeercy@umbc.edu

Michelle Starz-Gaiano
Dept. of Biological Sciences
UMBC
starz@umbc.edu

MS42

Sharp Interface Limit in a Phase Field Model of Cell Motility

In this talk, I will first present a hierarchy of mathematical models of eukaryotic cell motility in order of decreasing computational complexity, ranging from free boundary to agent based models. Then I will focus on a phase field model of cell motility which was studied in collaboration with L. Berlyand and V. Rybalko. The model consists of two coupled parabolic PDEs describing cell shape and actin filament network. The asymptotic behavior of solutions in the limit of a small parameter related to the width of the interface will be discussed. Derivation of an equation of motion of the interface, which is mean curvature motion with an additional nonlinear term, will be presented. In a 1D model parabolic problem we rigorously justified the sharp interface limit. To this end, a special representation of solutions was introduced, which reduced analysis of the system to a single nonlinear PDE that describes the interface velocity. Further stability analysis reveals a qualitative change in the behavior of the system for small and large values of the coupling parameter. Results of numerical simulations which show discontinuities of the interface velocity and hysteresis will be also presented.

Mykhailo Potomkin
Department of Mathematics
Penn State University
mup20@ucs.psu.edu

MS43

Ordering Heuristics for Tensor Decomposition

The efficiency of low-rank tensor decompositions relies on the existence of low-rank approximations of different unfoldings. The order in which these different dimensions are considered, can lead to dramatically different ranks between dimensions, and deteriorate the compression level which scales polynomially with the ranks. We will present a viable heuristic which could be used to select sub-optimal orderings at the expenses of limited pre-processing costs.

Daniele Bigoni, Alessio Spantini, Youssef M. Marzouk
Massachusetts Institute of Technology
dabi@mit.edu, spantini@mit.edu, ymarz@mit.edu

MS43

Approximation and Sampling of Multivariate Probability Distributions by Tensor Decompositions

General multivariate distributions are notoriously expensive to sample from, particularly the posterior distributions in PDE-constrained inverse problems. We develop a black-box sampler for arbitrary continuous multivariate distributions that is based on low-rank tensor surrogates in the tensor-train (TT) format. We build upon recent developments of the cross approximation algorithms in linear algebra in order to construct a TT approximation of the target probability density function using a small number of function evaluations. The storage required for accurate TT approximations is moderate, scaling linearly with dimension. In turn, the particular structure of the TT surrogate allows sampling by an efficient conditional distribution method since the required one-dimensional conditional-marginals, are computable with linear complexity in dimension. Transformed independent samples serve as optimal quadrature points for integrating non-smooth quantities of interest. Unbiased samples from the target may be generated by utilizing samples from the TT surrogate as independent proposals in a Metropolis-Hastings algorithm. We show that this Metropolised TT-surrogate sampler can lead to significant computational gains compared to the delayed rejection adaptive Metropolis (DRAM) algorithm

and the direct quasi Monte Carlo integration.

Sergey Dolgov
University of Bath
Department of Mathematical Sciences
s.dolgov@bath.ac.uk

Colin Fox
University of Otago, New Zealand
fox@physics.otago.ac.nz

Karim Anaya-Izquierdo
University of Bath
Department of Mathematical Sciences
k.anaya-izquierdo@bath.ac.uk

Robert Scheichl
University of Bath
r.scheichl@bath.ac.uk

MS43

Weak Separability of Symmetric Qubit Density Tensors is Polynomial-time

In STOC 2003 L. Gurvits showed that the separabilty problem for bipartite density tensors, i.e., to decide if a given density matrix correspondin to biparttie state is separable, is NP-hard. This result follows from a stronger result that weak separability problem for bipartite tensors is NP-hard. In this paper we show that the weak separability of symmetric d-partite density tensors corresponding to qubits is polynomial-time computable. The proof uses recent results of Friedland-Lim, Friedland-Wang and Derksen-Friedland-Lim-Wang: arXiv:1410.6072, arXiv:1601.07629, arXiv:1608.01354, arXiv:1705.07160

Shmuel Friedland
Department of Mathematics ,University of Illinois, Chicago
friedlan@uic.edu

MS43

Stability of Low-Rank Tensor Representations and Structured Multilevel Preconditioning for Elliptic PDEs

Folding grid-value vectors into high-dimensional tensors of mode sizes $2 \times 2 \times \cdots \times 2$, combined with low-rank representation in the tensor-train format, affords highly efficient approximations for various classes of functions. These include solutions of elliptic PDEs on nonsmooth domains or with oscillatory data. This tensor-structured approach is attractive because it leads to highly compressed, adaptive approximations based on simple discretizations. Straightforward choices of the underlying basis lead to the well-known *matrix ill-conditioning* of discrete operators. In this work, we demonstrate that the use of tensor structure leads to *representation ill-conditioning*, a new effect specific to computations in tensor networks. We construct an explicit tensor-structured representation of a BPX preconditioner with ranks independent of the number L of discretization levels. However, the application of the preconditioner in this representation introduces representation ill-conditioning. To remedy this, we obtain a reduced-rank decomposition, which turns out to be free of both matrix and representation ill-conditioning. For an iterative solver based on the soft thresholding of low-rank tensors, we obtain convergence and complexity estimates and demonstrate its reliability and efficiency for discretizations with up to 2^{50} nodes in each dimension. This is a joint work with Markus Bachmayr (University of Bonn).

Vladimir Kazeev
Stanford University
kazeev@stanford.edu

MS44

Nonlinear PDE Control using the Koopman Operator Theory

The Koopman operator theory is an increasingly popular formalism of dynamical systems theory which enables analysis and prediction of the state space dynamics from measurement data. In this talk, we discuss the application of this theory for designing controllers for systems governed by nonlinear partial differential equations. The design process includes identifying the Koopman-linear representation of the system using variations of dynamic mode decomposition and then applying model predictive control to the linear system. This methodology is illustrated in several examples including the Burgers and 2D Navier-Stokes equations.

Hassan Arbabi
University of California, Santa Barbara
harbabi@engr.ucsb.edu

Milan Korda
University of California at Santa Barbara
USA
korda.m@gmail.com

Igor Mezic
University of California, Santa Barbara
mezic@engineering.ucsb.edu

MS44

Koopman Spectra in Reproducing Kernel Hilbert Spaces

Every invertible dynamical system induces a Koopman operator, which is a linear, unitary operator acting on the space of observables. Koopman eigenfunctions represent the periodic or non-mixing component of the dynamics. The extraction of these eigenfunctions from a given time-series is a non-trivial problem when the underlying system has a continuous spectrum, which behaves like a strong noisy component to the signal. This paper describes methods for identifying Koopman eigenfrequencies and eigenfunctions from a discretely sampled time-series generated by an unknown dynamical system. Given the values of a function at these time samples, our main result gives necessary and sufficient conditions under which these values can be extended to a functional space called a reproducing kernel Hilbert space or RKHS. An RKHS is a dense subset of the space of continuous functions and is very useful for out-of-sample extensions. We take a data-driven approach, in which given a sequence of N time samples of the dynamical system through some observation map, one fits an RKHS function for every candidate eigenfrequency ω and calculate its RKHS norm $w_N(\omega)$. We establish conditions based on this norm to characterize the discrete spectrum, and one of our main results is that $\lim_{N\to\infty} w_N(\omega) = \infty$ iff $i\omega$ is not a Koopman eigenvalue.

Suddhasattwa Das, Dimitrios Giannakis
Courant Institute of Mathematical Sciences
New York University

dass@cims.nyu.edu, dimitris@cims.nyu.edu

MS44

Using Deep Learning to Discover Koopman Eigenfunctions for Nonlinear Dynamics

Koopman operator theory transforms any autonomous non-linear dynamical system into an infinite-dimensional linear system. Since linear systems are well-understood, a mapping of non-linear dynamics to linear dynamics provides a powerful approach to understanding and controlling fluid flows. However, finding the correct change of variables remains an open challenge. We present a strategy to discover an approximate mapping using deep learning. Our neural networks find this change of variables, its inverse, and a finite-dimensional linear dynamical system defined on the new variables. Our method is completely data-driven and only requires measurements of the system, i.e. it does not require derivatives or knowledge of the governing equations. We find a minimal set of approximate Koopman eigenfunctions that are sufficient to reconstruct and advance the system to future states. We demonstrate the method on several dynamical systems.

Bethany Lusch
University of Washington
herwaldt@uw.edu

J. Nathan Kutz
University of Washington, Seattle
Dept of Applied Mathematics
kutz@uw.edu

Steven Brunton
University of Washington
sbrunton@uw.edu

MS44

Perspectives on Koopman Spectral Specification

Abstract not available at time of publication.

Huaijin Yao
University of Minnesota
yaoxx368@umn.edu

Maziar Hemati
Department of Aerospace Engineering and Mechanics
University of Minnesota
mhemati@umn.edu

MS45

Low-rank Projector-Splitting for the Vlasov-Poisson Equation

Many problems encountered in plasma physics require a kinetic description. The associated partial differential equations are posed in an up to six-dimensional phase space. A direct discretization of this phase space, often called the Eulerian approach, has many advantages but is extremely expensive from a computational point of view. In this talk, we propose a dynamical low-rank approximation to the Vlasov–Poisson equation. This approximation is derived by constraining the dynamics to a manifold of low-rank functions via a tangent space projection and by splitting this projection into the subprojections from which it is built. This reduces a time step for the six- (or four-) dimensional Vlasov–Poisson equation to solving two systems of three- (or two-) dimensional advection equations. By a hierarchical dynamical low-rank approximation, a time step for the Vlasov–Poisson equation can be further reduced to a set of six (or four) systems of one-dimensional advection equations. The resulting systems of advection equations can then be solved by standard techniques such as semi-Lagrangian or spectral methods. We highlight the favorable behavior of the proposed numerical method by performing numerical simulation of linear Landau damping and the two-stream instability. These simulation show that that the proposed algorithm is able to drastically reduce the required computational effort. This talk is based on [L. Einkemmer, C. Lubich, arXiv:1801.01103].

Lukas Einkemmer
University of Innsbruck
lukas.einkemmer@uibk.ac.at

MS45

Concurrent Implicit Spectral Deferred Correction Scheme for Low-mach Number Combustion with Detailed Chemistry

We present a parallel high-order implicit-explicit time integration scheme for the advection-diffusion-reaction systems arising from the equations governing low-Mach number combustion with complex chemistry. Our strategy employs parallelization across the method to accelerate the serial Multi-Implicit Spectral Deferred Correction (MISDC) scheme used to couple the advection, diffusion, and reaction processes. In our approach, referred to as Concurrent Implicit Spectral Deferred Correction (CISDC), the diffusion solves and the reaction solves are performed concurrently by different processors. Our analysis shows that the proposed parallel CISDC scheme is stable for stiff problems and that the sweeps converge to the fixed-point solution at a faster rate than with serial MISDC. We present numerical examples to demonstrate that the new algorithm is high-order accurate in time, and achieves a parallel speedup compared to serial MISDC.

Francois Hamon
Lawrence Berkeley National Laboratory
fhamon@lbl.gov

Marc Day
Lawrence Berleley National Laboratories
MSDay@lbl.gov

Michael Minion
Lawrence Berkeley National Lab
Stanford University
mlminion@lbl.gov

MS45

New KIOPS Algorithm for Estimating Exponential-type Matrix Functions Inside Exponential Integrators

In recent years exponential integrators attracted attention of the numerical analysis and scientific computing communities as an efficient alternative to implicit methods for integrating large scale stiff systems of differential equations. The most computationally expensive component of an exponential integrator is evaluation of products of exponential-type matrix functions and vectors. It has been shown that for a general problem where no information is available about the spectrum of the Jacobian, the most efficient algorithm to evaluate these products is the adaptive

Krylov method of Niesen and Wright [Niesen and Wright, ACM 505 Transactions on Mathematical Software (2012)]. In this talk we present a new KIOPS algorithm for approximating the exponential-type matrix functions products with vectors. The new algorithm builds on ideas in [1] but employs completely different components such as incomplete orthogonalization and new adaptivity process to offer significant computational savings compared to the adaptive Krylov method *phipm* of Niesen and Wright. Using a suite of test problems we show how optimized exponential EPIRK methods [Tokman, Loffeld, Tranquilli, SISC (2012); Rainwater, Tokman, JCP (2016)] used in conjunction with KIOPS are both more accurate and more efficient then previously proposed methods.

Stephane Gaudreault
Environment Canada
stephane.gaudreault2@canada.ca

Greg Rainwater
CSU Monterey Bay
grainwater@csumb.edu

Mayya Tokman
University of California, Merced
School of Natural Sciences
mtokman@ucmerced.edu

MS45

Semi-Lagrangian Solution of the Gyrokinetic Vlasov Equation in Tokamak Geometry

In the context of turbulence simulations of magnetic fusion devices, we consider the gyrokinetic Vlasov equation for ions in the drift-kinetic limit, coupled to a quasi-neutrality equation with adiabatic electrons. For this purpose, a semi-Lagrangian simulation code is currently under development within the framework of the SeLaLib object-oriented Fortran library [http://selalib.gforge.inria.fr/]. The code employs field-aligned interpolation and splitting to reduce significantly the number of poloidal planes and hence the memory footprint of the simulations. The curvature of the background magnetic field in toroidal geometry poses challenges in setting up initial conditions corresponding to a stable kinetic equilibrium, in applying non-constant boundary conditions for the interpolation in the radial and the velocity domains, and in the treatment of the O-point. Possible solutions to these problems are presented and discussed, including the development of the corresponding computational tools in SeLaLib. Verification tests in cylindrical geometry with a screw-pinch magnetic field configuration as well as preliminary results of standard test-cases in toroidal geometry are presented.

Edoardo Zoni
Max-Planck-Institut für Plasmaphysik, NMPP division, and
Technische Universität München, Department of Mathematics
edoardo.zoni@ipp.mpg.de

Yaman Güçlü
Department of Mathematics
Michigan State University
yaman.guclu@ipp.mpg.de

Eric Sonnendrücker
Max-Planck-Institut für Plasmaphysik, NMPP division, and
Technische Universität München, Department of Mathematics
eric.sonnendruecker@ipp.mpg.de

MS46

Combining Photoacoustic and Optical Coherence Tomography

We discuss a multi-modal imaging system consisting of an optical coherence tomography measurement, which we want to model as an inverse electromagnetic scattering problem, and a photoacoustic setup, where the acoustic response induced by a short laser pulse is measured and which provides us, after tracing back the pressure wave, with internal data describing the absorbed energy inside the medium. In a Born approximation setting, the inverse problem of recovering the absorption and scattering parameters and the thermoacoustic Grüneisen parameter (which describes the conversion of absorbed electromagnetic energy into pressure) from these two sets of measurement data can be reduced to a Fredholm integral equation. We want to show that this allows us at least in simple cases to obtain a quantitative reconstruction for all the involved physical parameters.

Peter Elbau
University of Vienna
peter.elbau@univie.ac.at

Leonidas Mindrinos, Otmar Scherzer
Computational Science Center
University Vienna
leonidas.mindrinos@univie.ac.at, otmar.scherzer@univie.ac.at

MS46

Multiscale Modeling and Computation of Optically Manipulated Nano Devices

We present a multiscale modeling and computational scheme for optical-mechanical responses of nanostructures. The multi-physical nature of the problem is a result of the interaction between the electromagnetic (EM) field, the molecular motion, and the electronic excitation. To balance accuracy and complexity, we adopt the semi-classical approach that the EM field is described classically by the Maxwell equations, and the charged particles follow the Schrdinger equations quantum mechanically. To overcome the numerical challenge of solving the high dimensional multi-component many- body Schr odinger equations, we further simplify the model with the Ehrenfest molecular dynamics to determine the motion of the nuclei, and use the Time-Dependent Current Density Functional Theory (TD-CDFT) to calculate the excitation of the electrons. This leads to a system of coupled equations that computes the electromagnetic field, the nuclear positions, and the electronic current and charge densities simultaneously. In the regime of linear responses, the resonant frequencies initiating the out-of-equilibrium optical-mechanical responses can be formulated as an eigenvalue problem. A self-consistent multiscale method is designed to deal with the well separated space scales. The isomerization of Azobenzene is presented as a numerical example.

Di Liu
Michigan State University
Department of Mathematics

richardl@math.msu.edu

MS46

Asymptotic Approaches for High Frequency Wave Propagation

In this talk we will present some asymptotic approaches for simulating high frequency wave propagation that is governed by Helmholtz equation, Maxwell's equations or Schrodinger equation. Instead of computing the oscillatory waves directly, asymptotic approximations such as geometrical-optics approximations are applied to approximate the waves, where non-oscillatory phase and amplitudes can be computed efficiently to reconstruct the waves for any high frequencies. Detailed formulations will be derived, and numerical schemes along with numerical examples will be presented.

Songting Luo
Department of Mathematics
Iowa State University
luos@iastate.edu

MS47

Forecast Sensitivity and Impact Estimation of a Correlated Observation Error Covariance Model

The value added by atmospheric measurements to the analyses and forecasts produced by data assimilation systems (DAS) is closely determined by the representation of the statistical properties of the errors in the prior forecast estimate (background) and observations. This work presents recent advances in the adjoint-based evaluation of the model forecast error sensitivity to observations, error covariance parameter specification, and impact estimation in a four-dimensional variational data assimilation system (4D-Var DAS). Equations are derived for the hyperparameter sensitivity analysis and assessment of error correlation structures in a 4D-Var DAS and a proof-of-concept is provided with Lorenz's 40-variable model. Practical issues of the implementation are discussed together with the current status of implementation at numerical weather prediction centers. Illustrative results are shown for inter-channel error correlations in the assimilation of radiance data from hyperspectral remote sensing instruments.

Dacian N. Daescu
Portland State University
Department of Mathematics and Statistics
daescu@pdx.edu

Rolf Langland
Naval Research Laboratory
Monterey, CA
rolf.langland@nrlmry.navy.mil

Ricardo Todling
NASA/GSFC Global Modeling and Assimilation Office
ricardo.todling@nasa.gov

MS47

Observability- and Forecast-sensitivity-based Path Planning for Lagrangian Data Assimilation

Observability-based path planning of autonomous sampling platforms for flow estimation is a technique by which candidate trajectories are evaluated based on their ability to enhance the observability of underlying flow-field parameters. Until now, observability-based path planning has focused primarily on forward-in-time integration, such as forecast-sensitivity-based approach. We present a novel approach that makes use of the background error covariance at the current time to account properly for uncertainty of the underlying flow, and compare the observability- and forecast-sensitivity-based path planning, with focus on Lagrangian data assimilation in the framework of observing system simulation experiments.

Kayo Ide
University of Maryland, College Park
ide@umd.edu

MS47

Comparing Adjoint and Ensemble-based Approaches to Observation Impact on Forecasts

For a number of years GMAO has been evaluating observation impact (OBSI) on the 24-hour forecasts using an adjoint-based approach implemented within its near-real time GEOS data assimilation system (DAS). This implementation involves the adjoint of the GEOS general circulation model (GCM) and the adjoint of the Grid-point Statistical Interpolation (GSI) analysis. Recently, GEOS DAS has evolved, first into ensemble hybrid 3dVar, and as of January 2017 into hybrid 4dEnVar. The adjoint-based OBSI tool is automatically available in systems implementing traditional or hybrid, 3D or 4D, variational methods. Hybrid DASs not having an adjoint of the GCM, have no ability to evaluate OBSI through the adjoint-based approach. In such systems, an argument can be made for deriving the OBSI using an ensemble-based approach. Unfortunately, typical hybrid systems use ensembles that operate at different resolution than the deterministic forecasting model thus with mean forecasts likely being misrepresentations of the quality of their corresponding full resolution forecasts. Moreover, in many hybrid systems, the ensemble analysis handles the observing system in substantially different ways than the way the hybrid, deterministic, analysis does. This particular issue is enough to argue that an ensemble-based approach to observation impact is bound to generate incorrect assessments of the observations, within hybrid systems. This presentation compares these approaches to OBSI using GEOS DAS.

Ricardo Todling
NASA/GSFC Global Modeling and Assimilation Office
ricardo.todling@nasa.gov

Fabio Diniz
National Institute for Space Research, Brazil
fabioluiz.rodriguesdiniz@nasa.gov

MS47

A Formulation of Forecast Error Covariance in High-dimensional Ensemble Data Assimilation Suitable for State Space Localization

In this work we examine a method for state space error covariance localization that can be used within ensemble data assimilation, with potential implications on the future development of hybrid variational-ensemble data assimilation. We will present theoretical and algorithmic description of this method and evaluate it in applications with the global Weather Research and Forecasting (WRF) model. Future development and possible further generalization of

the method will also be discussed.

Milija Zupanski
Cooperative Institute for Research in the Atmosphere
Colorado State University
Milija.Zupanski@colostate.edu

MS48

The MAA Guides: Evidence-Based Instructional Practices in Undergraduate Mathematics (2017) and the Curriculum CUPM Guide to Majors in the Mathematical Sciences (2015)

Every ten years the MAA, in collaboration with other professional societies, releases an updated curriculum guide that suggests what should be taught in the undergraduate program for mathematics majors and other students who need quantitative skills. The 2015 Curriculum CUPM Guide to Majors in the Mathematical Sciences is on-line and can be found by searching for the title. As this guide was nearing completion, a group was assembled to develop a companion guide with suggestions for how to best teach mathematics. The goal was to encourage best practices using up to date evidence based research on student learning. The resulting project was funded by the NSF through the MAA and is now available as the MAA Instructional Practices Guide, also freely available by searching for the title. We emphasize how mathematicians can use the guides to inform curriculum design and teaching practice, especially in applied mathematics and statistics.

Richard Cleary
Babson College
rcleary@babson.edu

MS48

Improving Students Understanding of Numerical Analysis and Mathematical Statistics through 3D Printing

In an undergraduate Numerical Analysis course, students learn many of the basics of scientific computing including: interpolating polynomials, numerical integration, and solving optimization problems. Different versions of these methods are also running in the background of many 3D design tools. In Fall 2016, I asked my students to implement these methods in MATLAB to design a bottle. Then, we used a 3D printer to create tangible versions of their bottles and check their calculations. At the end of the semester, students had an exhibit to show their bottles and they wrote a reflection paper on the process and challenges of the project. I will discuss the successes and pitfalls of this project as well as present another project I designed using a 3D printer to help my Mathematical Statistics students explore random samples and parameter estimation.

Bree Ettinger
Emory University
betting@emory.edu

MS48

Inquiry-based Learning in Financial Mathematics for Actuarial Science Students

Incorporating active learning techniques in actuarial science courses is challenging because the courses are tied to external exams that cover a great deal of content. However, an argument can be made that the flexible problem solving necessary for success on actuarial exams is well-served by active learning. In this talk, I will share how I balanced content coverage with inquiry-based learning in the Theory of Interest course designed to prepare students for the actuarial exam on financial mathematics. I will report preliminary analysis of the impact of the active learning as well as my reflections on the experience.

Victor Piercey
Ferris State University
victorpiercey@ferris.edu

MS48

Best Practices for Active Learning in the Applied Mathematics Classroom

Research in mathematics education has reliably shown that passive, lecture-dominated instruction is less effective than engaging students in active learning. What are the best alternatives to lecture? How can methods that may have been developed for proofs-based pure math courses be modified for an applied mathematics classroom? In this talk, we will explore pedagogical techniques including inquiry-based learning, problem-based learning, POGIL, and other general strategies. In addition to anecdotal experience, scholarly results for these teaching methods will be summarized. We hope to provoke a discussion that includes suggestions and experiences from audience members.

Haley Yaple
Carthage College
hyaple@carthage.edu

MS49

Mixture Models in Algebraic Statistics

This will be an introductory presentation to hidden variable statistical models. One of its common instances are mixture models, which have an easy description even though they carry already complex mathematical structure. They are also intimately connected to algebraic geometry objects such as secant varieties. Several relevant examples will be presented highlighting their study in algebraic statistics.

Carlos E. Amendola Ceron
Technical University Berlin
amendola@math.tu-berlin.de

MS49

Maximum Likelihood Estimation for the Latent Class Model through Model Boundary Decomposition

The Expectation-Maximization (EM) algorithm is routinely used for the maximum likelihood estimation in the latent class analysis. However, the EM algorithm comes with no guarantees of reaching the global optimum. We characterize the boundary stratification of the binary latent class model with a binary hidden variable. For small models, such as for three binary observed variables, we show that this stratification allows exact computation of the maximum likelihood estimator. We also analyze the EM fixed point ideal which provides an alternative method of studying the boundary stratification and maximizing the likelihood function. In particular, we compute the minimal primes of this ideal in the case of a binary latent class model

with a binary or ternary hidden random variable.

Serkan Hosten
Department of Mathematics
San Francisco State University
serkan@sfsu.edu

MS49

Dimensions of Group-based Phylogenetic Mixtures

Group-based phylogenetic tree models are statistical models that describe how genes change over an evolutionary tree. From an algebraic geometry perspective, these models are toric varieties and their mixtures are secants or joins. We would like to understand these mixture varieties for the purposes of model selection and determining parameter identifiability, and as a first step, we study their dimensions. We prove in a broad range of cases that such mixture models have the "expected" dimensions based on the dimensions of the constituent varieties. The proofs involve the combinatorics and convex geometry of toric varieties including tropical techniques.

Robert Krone
UC Davis
rkrone@math.ucdavis.edu

MS49

Mixtures and Products in two Graphical Models

In this talk I explore two statistical models. One is a mixture model and the other is a product of mixtures; a popular machine learning model called restricted Boltzmann machine. We derive relations between theoretical properties of restricted Boltzmann machines and several natural notions from discrete mathematics and convex geometry. We prove results on the relative representational power of the two modes, that formally justify widely held intuitions about distributed representations. In particular, we show that a mixture of products requiring an exponentially larger number of parameters is needed to represent the probability distributions which can be obtained as products of mixtures. We take a closer look at the first non-trivial case, with three observed binary variables. Although the two models look different from their parametrizations, we show that in this case they represent the same set of distributions on the interior of the probability simplex, and are equal up to closure. We give a semi-algebraic description of this model in terms of six binomial inequalities and obtain closed form expressions for the maximum likelihood estimates. This talk is based on joint work with Anna Seigal "Mixtures and products in two graphical models' https://arxiv.org/abs/1709.05276 and previous work with Jason Morton "When does a mixture of products contain a product of mixtures?' http://epubs.siam.org/doi/10.1137/140957081

Guido F. Montufar
UCLA
guidomontufar@gmail.com

MS50

How Deep are Deep Gaussian Processes?

Recent research has shown the potential utility of probability distributions designed through hierarchical constructions which are conditionally Gaussian. This body of work is placed in a common framework and, through recursion, several classes of deep Gaussian processes are defined. The resulting samples have a Markovian structure with respect to the depth parameter and the effective depth of the process is interpreted in terms of the ergodicity, or non-ergodicity, of the resulting Markov chain.

Mark Girolami
Imperial College London
m.girolami@imperial.ac.uk

Matt Dunlop
Caltech
mdunlop@caltech.edu

Andrew Stuart
Computing + Mathematical Sciences
California Institute of Technology
astuart@caltech.edu

Aretha L. Teckentrup
University of Edinburgh
a.teckentrup@ed.ac.uk

MS50

Machine Learning of Linear Fractional-order Differential Equations

The use of fractional-order operators in the recent field of machine learning of differential equations has two parallel objectives. First, to generate fractional-order models for systems driven by nonlocality or heavy-tailed stochastic processes. Fractional derivatives are in many cases the appropriate tool for the macroscopic description of such systems. Second, since fractional-order derivatives serve to continuously interpolate between integer-order derivatives, to allow for the discovery of differential equations (including integer-order equations) using regression/continuous optimization techniques rather than genetic/symbolic regression algorithms. In this talk, we will describe a Gaussian process based method for learning linear fractional-order equations from noisy data. We provide a uniform way of implementing a wide family of constant-coefficient linear operators (Fourier multipliers). We demonstrate our methodology on both synthetic data and data from such applications as finance.

Mamikon Gulian, Maziar Raissi
Brown University
mamikon_gulian@brown.edu, maziar_raissi@brown.edu

Paris Perdikaris
University of Pennsylvania
pgp@seas.upenn.edu

George E. Karniadakis
Brown University
Division of Applied Mathematics
george_karniadakis@brown.edu

MS50

Deep UQ: A Variational Reformulation of the Uncertainty Propagation Problems in Stochastic Elliptic PDEs using Deep Neural Networks

Stochastic partial differential equations (SPDE) have a ubiquitous presence in computational science and engineering. Stochasticity in SPDEs arises from unknown/random boundary/initial conditions or field parameters (e.g., the permeability of the ground in flow through porous media,

the thermal conductivity in heat transfer) and, thus, it is inherently high-dimensional. In this regime, traditional uncertainty propagation techniques fail because they attempt to learn the high-dimensional response surfaces (the curse of dimensionality). The only viable alternative is Monte Carlo (and advanced variants such as multi-level MC). However, as A. OHagan put in in his 1987 paper, Monte Carlo is fundamentally unsound because it fails to identify and exploit correlations between the samples. In this work, we focus on elliptic SPDEs. To overcome the curse of dimensionality, we represent the solution of the SPDE using a deep neural network (DNN) with spatial/time and stochastic inputs. However, contrary to the plethora of existing methodologies, we do not rely on observations of input-output examples from an external PDE solver. Our DNN is trained by minimizing a physics-informed loss function subject to constraints arising from the Dirichlet boundary conditions. We develop a stochastic gradient descent algorithm for the solution of the resulting variational problem, and we study its convergence and scalability.

Sharmila Karumuri, Ilias Bilionis
Purdue University
skarumur@purdue.edu, ebilionis@gmail.com

Jitesh Panchal
School of Mechanical Engineering
Purdue University, West Lafayette, Indiana, 47907
panchal@purdue.edu

MS50

Hidden Physics Models: Machine Learning of Nonlinear Partial Differential Equations

A grand challenge with great opportunities is to develop a coherent framework that enables blending conservation laws, physical principles, and/or phenomenological behaviours expressed by differential equations with the vast data sets available in many fields of engineering, science, and technology. At the intersection of probabilistic machine learning, deep learning, and scientific computations, this work is pursuing the overall vision to establish promising new directions for harnessing the long-standing developments of classical methods in applied mathematics and mathematical physics to design learning machines with the ability to operate in complex domains without requiring large quantities of data. To materialize this vision, this work is exploring two complimentary directions: (1) designing data-efficient learning machines capable of leveraging the underlying laws of physics, expressed by time dependent and non-linear differential equations, to extract patterns from high-dimensional data generated from experiments, and (2) designing novel numerical algorithms that can seamlessly blend equations and noisy multi-fidelity data, infer latent quantities of interest (e.g., the solution to a differential equation), and naturally quantify uncertainty in computations. The latter is aligned in spirit with the emerging field of probabilistic numerics.

Maziar Raissi
Brown University
maziar_raissi@brown.edu

MS51

Dynamic Contagion in an Eisenberg-Noe Clearing Network

We will consider an extension of the Eisenberg-Noe model of financial contagion to allow for time dynamics in both discrete and continuous time. Mathematical results on existence and uniqueness of firm wealths under discrete and continuous-time will be provided. The financial implications of time dynamics will be considered, with focus on how the dynamic clearing solutions differ from those of the static Eisenberg-Noe model.

Zachary Feinstein, Tathagata Banerjee
Washington University in St. Louis
zfeinstein@ese.wustl.edu, tbanerjee@wustl.edu

Alex Bernstein
University of California, Santa Barbara
bernstein@pstat.ucsb.edu

MS51

Sensitivity of the Eisenberg-Noe Clearing Vector to Individual Interbank Liabilities

The financial system is increasingly interconnected. Cyclical interdependencies among corporations may cause that the default of one firm seriously affects other firms and even the whole financial network. To describe financial networks, L. Eisenberg and T. Noe introduced network models that became popular among researchers and practitioners. To describe the connections between firms, they use the liabilities between two firms to construct relative liability matrices. Based on this description, they compute the payouts of firms to their counterparties. However, in practice, there is no accurate record of the liabilities and researchers have to resort to estimation processes. Thus it is very important to understand possible errors of payouts due to the estimation errors. In our research, we quantify the clearing vector's sensitivity to such estimation errors and show that its directional derivatives are, like the clearing vector itself, solutions of fixed point equations. We describe estimation errors utilizing a basis for the space of matrices representing permissible perturbations and derive analytical solutions to the maximal deviations of the Eisenberg-Noe clearing vector. Moreover, we quantify the probability of observing clearing vector deviations of a certain magnitude, for uniformly or normally distributed errors in the relative liability matrix.

Weijie Pang
Worcester Polytechnic Institute
wpang@wpi.edu

Stephan Sturm
WPI
ssturm@wpi.edu

Zachary Feinstein
Washington University in St. Louis
zfeinstein@ese.wustl.edu

Birgit Rudloff
Vienna University of Economics and Business
brudloff@wu.ac.at

Eric Schaanning
Risk Lab, ETH Zurich
eric.schaanning@math.ethz.ch

Mackenzie Wildman
University of California Santa Barbara

wildman@pstat.ucsb.edu

MS51

Consistent Inter-Model Specification for Stochastic Volatility and VIX Market Models

This talk addresses the following question: if a stochastic model is specified for the curve of VIX futures, what are the restrictions in order for it to be consistent with a stochastic volatility model? In other words, assuming that a stochastic volatility model is in place, a so-called market model will need to satisfy some conditions in order for there to not be any inter-model arbitrage or mis-priced derivatives. The present work gives such a condition, and also shows how to recover the correctly specified stochastic volatility function from the market model.

Andrew Papanicolaou
New York University
ap1345@nyu.edu

MS51

Risk Adjustment Processes

In the wake of the financial crisis factors commonly ignored in financial modeling got on the center stage: funding differentials and the absence of the postulated riskfree rate and counter party credit risk. These factors have been taken into account in derivatives pricing in the framework of value adjustments (also known as XVA). However, to the best of our knowledge this has so far not been accounted for in risk management. We are developing a theory of risk-adjustment processes incorporating funding spreads and credit risk to market risk evaluations based on BSDE representations of convex risk measures.

Stephan Sturm
WPI
ssturm@wpi.edu

MS52

Extremal Spectral Gaps for Periodic Schrödinger Operators

The spectrum of a Schrödinger operator with periodic potential generally consists of bands and gaps. In this talk, for fixed m, we discuss the problem of maximizing the gap-to-midgap ratio for the m-th spectral gap over the class of potentials which have fixed periodicity and are pointwise bounded above and below. We prove that the potential maximizing the m-th gap-to-midgap ratio exists. In one dimension, we prove that the optimal potential attains the pointwise bounds almost everywhere in the domain and is a step-function attaining the imposed minimum and maximum values on exactly m intervals. Optimal potentials are computed numerically using a rearrangement algorithm and are observed to be periodic. In two dimensions, we develop an efficient rearrangement method for this problem based on a semi-definite formulation and apply it to study properties of extremal potentials. We show that, provided a geometric assumption about the maximizer holds, a lattice of disks maximizes the first gap-to-midgap ratio in the infinite contrast limit. Using an explicit parametrization of two-dimensional Bravais lattices, we also consider how the optimal value varies over all equal-volume lattices.

Chiu-Yen Kao
Claremont McKenna College
ckao@cmc.edu

Braxton Osting
University of Utah
osting@math.utah.edu

MS52

Two-grid and Time Marching Methods for Interior Penalty Discretization of the Monge-Ampere Equation

The Monge-Ampère equation plays a role in applications in geometry, image processing, mesh generation and adaptivity. The most natural finite element discretization of the Dirichlet problem for the elliptic Monge-Ampère equation is with C^1 elements, which are often difficult to work with. We discretize the problem with a C^0 interior penalty method, allowing the use of simpler C^0 Lagrange elements. We then prove convergence for two methods for the resolution of the nonlinear discrete problem: an iterative time marching method that may capture more accurate results for nonsmooth solutions than does Newton's method, and a two-grid method which is computationally more efficient than Newton's method. The two-grid method is also applied to a mixed discretization.

Eric Malitz
University of Illinois, Chicago
eric.malitz@gmail.com

Gerard Awanou
University of Illinois at Chicago
awanou@uic.edu

Hengguang Li
Department of Mathematics
Wayne State University
hli@math.wayne.edu

MS52

A Phase Field Model for Polycrystallization Processes in Binary Mixtures

In this talk, we consider the phase field model for polycrystallization in the solidification of binary mixtures in the two dimensional bounded convex domain Ω. This model is based on a free energy functional in terms of three order parameters: the local crystallinity ϕ, the concentration c of one of the components of the binary mixture, and the local orientation Θ of the crystals. The equations of motion are given by an initial-boundary value problem for a coupled system of partial differential equations consisting of two quasilinear second order parabolic equations (in ϕ and Θ) and one quasilinear fourth order parabolic equation of Cahn-Hilliard type equation in c. We prove the existence of a weak solution by performing an implicit discretization in time and splitting of the equations. Using regularity results for quasilinear parabolic equations, it is shown that a solution of the time-discrete system converges to a weak solution of the original system.

Natasha S. Sharma
The University of Texas at El Paso
nssharma@utep.edu

Ronald H. Hoppe
University of Houston
Department of Mathematics
rohop@math.uh.edu

Rahul Kumar, James Winkle
University of Houston
rkumar@math.uh.edu, winkle@math.uh.edu

MS52

Error Analysis of a Numerical Method Applied to the Monge Ampere Equation

The Monge-Ampère equation is a prototype fully nonlinear elliptic equation, appearing in many applications such as optimal transport problem, nonlinear elasticity and etc.. In this talk, we will discuss a useful geometric tool in the error analysis of the numerical Monge-Ampère equation, namely a discrete Alexandroff estimate. Thanks to this estimate, we will show some recent results on the L_∞ and W_p^2 estimate of a numerical method applied to the Monge-Ampère equation.

Wujun Zhang
Rutgers University
wujun@math.rutgers.edu

Ricardo Nochetto
Department of Mathematics
University of Maryland, College Park
rhn@math.umd.edu

Michael J. Neilan
University of Pittsburgh
Department of Mathematics
neilan@pitt.edu

MS53

Global Sensitivity Analysis via Transductive Measure Transformation

Abstract not available at time of publication.

Doug Allaire
Texas A&M
dallaire@tamu.edu

MS53

Low-dimensional Ridge Approximations for High-dimensional Functions

Complex physical models contain many input parameters. When modeling the map from input parameters to output predictions, one may wish to exploit low-dimensional structures when present to enable UQ studies whose cost scales exponentially with dimension. Ridge functions are one type of approximation model with such exploitable low-dimensional structure. We discuss how to fit and exploit ridge functions from point queries of a function of several variables.

Paul Constantine, Jeffrey M. Hokanson
University of Colorado Boulder
pconstan@mines.edu, jeffrey.hokanson@colorado.edu

MS53

Rare Event Simulation for Dynamical Systems in the Presence of an Attractor

We focus on improving state-of-the-art rare event simulation methods for dynamical systems. Current methods focus on using dynamic importance sampling and particle splitting algorithms. Both approaches have been found to be improved by considering large deviations theory, in which finding biasing functions or choosing importance sets for splitting hinges upon finding solutions and subsolutions of a Hamilton-Jacobi equation. This task becomes increasingly difficult for high dimensional or highly nonlinear dynamical systems. In this talk we explore methods for accelerating rare event simulation in high dimensional, nonlinear dynamical systems by providing nonasymptotic bounds on their performance.

Benjamin J. Zhang
Massachusetts Institute of Technology
bjz@mit.edu

Tuhin Sahai
United Technologies Research Center
sahait@utrc.utc.com

Youssef M. Marzouk
Massachusetts Institute of Technology
ymarz@mit.edu

MS54

Non-newtonian Fluids Coupled with the Biot System

Computational algorithms for the generalized Stokes-Biot coupled system are proposed for the interaction of a free fluid with a poroelastic structure. The talk is focused on a decoupling scheme that allows the non-Newtonian fluid and the poroelastic structure computed independently using a common stress force along the interface. This approach is based on a nonlinear operator equation, where the operator measures violation of some interface conditions. Numerical algorithms based on a Newton-type updating technique are discussed and numerical results are provided to validate the accuracy and efficiency of the proposed algorithms.

Hyesuk Lee
Clemson University
Dep. of Mathematical Sciences
hklee@clemson.edu

MS54

Simplification, Superconvergence, and Discrete Maximum Principles for Weak Galerkin Finite Element Methods

In this talk, the speaker will introduced a simplified formulation for the weak Galerkin finite element method for model second order elliptic equations and the Stokes equation. The simplified form will be further studied for developing several new algorithms and results, including a new finite difference scheme for the Poisson and Stokes equations, a superconvergence for the weak Galerkin approximation in the energy norm for both the second order elliptic equation and the Stokes equation, and a discrete maximum principle for the WG approximations. Numerical results will be presented to confirm the theory on superconvergence and maximum principles.

Jun ping Wang
N S F
jwang@nsf.gov

Dan Li
The University of British Columbia
danli@cs.ubc.ca

Yujie Liu
School of Data and Computer Science, Sun Yat-sen University
Guangzhou, 510275, P. R. China.
liuyujie5@mail.sysu.edu.cn

Chunmei Wang
Texas State University
c_w280@txstate.edu

MS54

Dynamic Poroelasticity: Direct and Inverse Problems

The classic dynamic poroelastic theory of Biot, developed in 1950's, describes the propagation of elastic waves through a porous media containing a fluid. This theory has been extensively used in various fields dealing with porous media: continuum mechanics, oil/gas reservoir characterization, environmental geophysics, earthquake seismology, etc. In this work, we study the propagation of elastic waves in porous media governed by the Biot equations in the low and high-frequency ranges. In the low frequency limit we prove the existence and uniqueness result both for the direct problem and the inverse one, which consists in identifying the unknown scalar function $f(t)$ in the body density force $f(t)\mathbf{g}(\mathbf{x}, t)$ acting on a poroelastic body when some additional measurement is available. In the case of the high-frequency range (Biot-JKD approach), we prove the uniqueness and continuous dependence on the data of a weak solution both in unbounded and bounded time intervals and in all space dimensions. Additionally, we discuss the implementation of the matrix method to derive explicit formulas for the analysis of propagation of elastic waves through a stratified 3D porous media, where the parameters of the media are characterized by piece-wise constant functions of only one spatial variable, depth.

Viatcheslav I. Priimenko
North Fluminense State University Darcy Ribeiro
National Institute of Science and Technology-GP
slava@lenep.uenf.br, slava211054@gmail.com

Mikhail P. Vishnevskii
Sobolev Institute of Mathematics
North Fluminense State University Darcy Ribeiro
mikhail@uenf.br

MS54

Computational Challenges in Modeling Unsteady Landfill Methane Emissions

Short-term field measurements of landfill methane emissions reveal significant fluctuations in the magnitude of the emissions. Previous work with numerical simulations used steady landfill emissions to focus the modeling on investigating the accuracy of an emissions measurement technique, the tracer dilution method (Taylor et al., 2016). This work expands on the previous results by incorporating time-varying emissions into the existing model for a more realistic representation of the field emissions. This work uses the new unsteady emissions model to investigate the effects of those time-varying model emissions on the accuracy of tracer dilution method measurements. The first part of the investigation looks at how to simulate these time-varying emissions, including which physical processes to include in the model and how to balance the different drivers of emissions on the desired time scale of approximately one hour. The work also investigates the prospect that the variance seen in short-term field measured emissions could be due to measurement error, based on the results of the numerical simulations.

Diane M. Taylor
Santa Clara University
dtaylor2@scu.edu

Fotini K. Chow
University of California, Berkeley
tinakc@berkeley.edu

MS55

Adaptive Sampling Strategies for Stochastic Optimization

In this talk, we present a stochastic optimization method that adaptively controls the sample size used in the computation of gradient approximations. Unlike other variance reduction techniques that either require additional storage or the regular computation of full gradients, the proposed method reduces variance by increasing the sample size as needed. The decision to increase the sample size is governed by an inner product test that ensures that search directions are descent directions with high probability. We show that the inner product test improves upon the well-known norm test, and can be used as a basis for an algorithm that is globally convergent on nonconvex functions and enjoys a global linear rate of convergence on strongly convex functions. Numerical experiments on logistic regression problems illustrate the performance of the algorithm.

Raghu Bollapragada
Department of Industrial Engineering and Management Sciences
Northwestern University
raghu.bollapragada@u.northwestern.edu

Jorge Nocedal
Department of Electrical and Computer Engineering
Northwestern University
j-nocedal@northwestern.edu

Richard H. Byrd
University of Colorado
richard@cs.colorado.edu

MS55

Variance Reduction through Sample Partitioning for Sparse Tensor Analysis

The generalized canonical polyadic (GCP) decomposition is a particularly useful tool for extracting explanatory factors from tensors for data analysis. Unfortunately, ordinary optimization schemes become computationally intractable for large tensors. We explore the use of Stochastic Gradient Descent (SGD) to solve the GCP decomposition of large sparse tensors. This scenario exhibits unique challenges due to the unusual structure of the gradient in this case as well as potentially enormous variance in gradient approximations that arises using ordinary uniform sampling on sparse tensors. We solve this problem by constructing stratified samples that are tailored to the unique structure of the gradient of the GCP model.

Cliff Anderson-Bergman
Sandia National Labs
ciande@sandia.gov

Jed A. Duersch
University of California Berkeley
jaduers@sandia.gov

David Hong
University of Michigan
dahong@umich.edu

Tamara G. Kolda
Sandia National Laboratories
tgkolda@sandia.gov

MS55

Stochastically Miminizing Sum of Non-differentiable Convex Functions

With the advent of the big data era, stochastic gradient descent and its variants have enjoyed enormous popularity. Such methods have strong theoretical guarantees when applied to differentiable convex optimization problems. In contrast, stochastic methods for minimizing non-differentiable functions have received much less attention. In this talk, we present stochastic proximal point (SPP) and proximal-proximal-gradient (PPG) which stochastically minimize a sum of non-differentiable convex functions. We compare these to incremental proximal point and point SAGA, other methods applicable to the same setup. Finally, we relate PPG to varianced reduced stochastic gradient methods, which include Finito, SAG, and SAGA.

Ernest K. Ryu
University of California, Los Angeles
Department of Mathematics
eryu@math.ucla.edu

MS55

Autotuning the Learning Rate in Batch and Stochastic Gradient Descent

Choosing a proper learning rate in gradient descent and stochastic gradient descent can be difficult. If certain parameters of the loss function, .e.g. Lipschitz smoothness or strong convexity constant, are known a priori, optimal theoretical rates are known. However, in practice, these parameters are not known, and often the loss function is not convex, and only locally smooth. Thus, adjusting the learning rate is an important problem – a learning rate that is too small leads to painfully slow convergence, while a learning rate that is too large can cause the loss function to fluctuate around the minimum or even to diverge. Several methods have been proposed in the last few years to adjust the learning rate according to gradient data that is received along the way. We propose a new method along these lines, PolarGrad, and demonstrate its superior performance to previous methods. Unlike previous methods, we can prove that PolarGrad achieves optimal convergence rates in batch and stochastic settings, but without having to know e.g. Lipschitz constants or strong convexity parameters in advance.

Rachel Ward
Department of Mathematics
University of Texas at Austin
rward@math.utexas.edu

Xiaoxia Wu
UT Austin
xwu@math.utexas.edu

MS56

Clustering Massive Protein Similarity Networks using HipMCL

We present HipMCL, a high-performance parallel algorithm for large-scale network clustering. HipMCL parallelizes popular Markov Clustering algorithm (MCL) that has been shown to be one of the most successful and widely used algorithms to cluster sequence similarity or expression networks. HipMCL employs novel parallel algorithms for sparse matrix-matrix multiplication, k selection and finding connected components and can cluster large-scale networks 1000 times faster than the original MCL without any information loss. HipMCL can cluster a network with 70 million nodes and 68 billion edges in 2.4 hours using 2000 nodes of a Cray XC40 supercomputer, enabling unprecedented discoveries in network biology.

Ariful Azad
Lawrence Berkeley National Laboratory
azad@lbl.gov

Georgios Pavlopoulos
JGI
g.pavlopoulos@lbl.gov

Christos Ouzounis
CERTH
christos.ouzounis@me.com

Nikos Kyrpides
JGI
nckyrpides@lbl.gov

Aydin Buluc
Lawrence Berkeley National Laboratory
abuluc@lbl.gov

MS56

Spatial Kinetic Coupling Scheme of two Distinct Turbulence Codes using Adios Communication Technology

A general kinetic coupling scheme allowing for a consistent coupling of turbulence solutions between two adjacent spatial regions from two separate codes will be presented. Coupling of the core and edge adjacent regions is enabled through an overlap layer. The correctness of this scheme will be demonstrated by spatially coupling a core XGC simulation with an edge XGC simulation. Using the same code for both sides permits to focus on the validity of the model. It will thus be shown that the coupling scheme allows the turbulence to propagate freely from one side to the other, i.e., from one executable to the other. As a second exercise, this new scheme will be applied to the coupling of a core GENE simulation with an edge XGC simulation. During this second exercise the accuracy, stability, and convergence of the solution will be studied in detail. In both cases, the ADIOS technology is used to allow the two executables to run on separate sets of nodes for in-memory coupling, and to enable communication between the two executables.

Julien Dominski
PPPL
jdominsk@pppl.gov

Gabriele Merlo
University 0f Texas Austin
gmerlo@ices.utexas.edu

Jong Choi
ORNL
choij@ornl.gov

Seung-Hoe Ku
Princeton Plasma Physics Laboratory
sku@pppl.gov

Eric Suchyta
ORNL
suchytaed@ornl.gov

CS Chang
PPPL
cschang@pppl.gov

Frank Jenko
University of Texas Austin
jenko@physics.ucla.edu

Scott Klasky
Oak Ridge National Laboratory
Oak Ridge, TN
klasky@ornl.gov

Scott Parker
University of Colorado at Boulder
sparker@colorado.edu

Amitava Bhattacharjee
PPPL
amitava@pppl.gov

MS56

Sympack: An Overview

The package symPACK is designed to solve sparse symmetric linear systems using Cholesky factorization on distributed-memory platforms. It differs from most of the existing solvers in that our implementation is task based, and uses 1-sided communication and dynamic scheduling. We will provide preliminary results to demonstrate the performance of symPACK.

Mathias Jacquelin
Lawrence Berkeley National Lab
mjacquelin@lbl.gov

Esmond G. Ng
Lawrence Berkeley National Laboratory
egng@lbl.gov

MS56

Using MPI-3.0 Shared Memory in PETSc

The recent computer hardware trend toward large shared memory multi- and many-core architectures pushes software developers to mix MPI with different shared-memory model for optimal performance and low memory consumption. The release of MPI-3.0 standard supports a process-level shared-memory interface which enables processes on the same node to have direct access to each other's memory. It can be intergrated into the Portable, Extensible Toolkit for Scientific Computation (PETSc) library with minimum API changes. While this approach is simple, requires minimal changes from the exiting PETSc MPI code with a great deal of flexibility, making it competitive over the existing pure MPI message-passing in PETSc is challenging. In this talk, we will present our recent work on using MPI-3.0 shared memory in PETSc. We will show our algorithms and demonstrate the performance on extreme-scale many-core computers.

Hong Zhang
MCS, Argonne National Laboratory
hzhang@mcs.anl.gov

MS57

Modeling How Temperature Affects the Dynamics of the Human Sleep/Wake Cycle

Sleep is a behavioral state in which we spend nearly one third of our lives. This biological phenomenon clearly serves an important role in the lives of most species. While much effort has been put forth in understanding the nature of sleep, many aspects of sleep are still not well understood. Here, we present a Morris-Lecar type, ODE model of human sleep-wake regulation with thermoregulation and temperature effects. Simulations of this model show features previously presented in experimental data such as elongation of duration and number of REM bouts across the night as well as the appearance of awakenings due to deviations in body temperature from thermoneutrality. The model highlights how temperature effects interact with sleep history to effect sleep regulation. We will discuss the dynamics associated with the model as well as how the model could be used as a foundation for experimental simulations pertaining to jet lag, sleep deprivation, and temperature effects on sleep.

Selenne Banuelos
California State University - Channel Islands
selenne.banuelos@csuci.edu

MS57

Pattern Formation Mechanism for Homeostatic Control of Synapse Density During C. Elegans Growth

We propose a novel mechanism for Turing pattern formation that provides a possible explanation for the regular spacing of synapses along the ventral cord of C. elegans during development. The model consists of two interacting chemical species, where one is passively diffusing and the other is actively trafficked by molecular motors; we identify the former as the kinase CaMKII and the latter as the glutamate receptor GLR-1. We use linear stability analysis to derive conditions on the associated nonlinear interaction functions for which a Turing instability can occur. We find that the dimensionless quantity γ, the ratio of switching rate and diffusion coefficient to motor transport velocity, must be sufficiently small for patterns to emerge. One consequence is that patterns emerge outside the parameter regime of fast switching where the model effectively reduces to a two component reaction-diffusion system. Furthermore, these patterns are also maintained during domain growth. We discuss selection and stability of patterns for this mechanism in both 1- and 2-dimensional domains.

Heather Z. Brooks
University of Utah

heather@math.utah.edu

Paul C. Bressloff
University of Utah
Department of Mathematics
bressloff@math.utah.edu

MS57

Deep Neural Networks for Low-resolution Photon-limited Imaging

Photon-limited imaging is prevalent in many applications such as night vision, astronomy, and medical imaging. Recovering the true signal from low-photon low-dimensional observations is particularly challenging because the measurements are inherently noisy and the problem is ill-posed. This work proposes deep learning architectures as an alternative to existing reconstruction algorithms based on sparsity regularization. By training on existing data, the neural networks circumvent the costs of iterative numerical optimization algorithms. We demonstrate the efficiency and accuracy of autoencoders and convolutional neural networks (CNNs) through numerical experiments.

Omar DeGuchy, Fabian Santiago
Applied Mathematics Unit
University of California, Merced
odeguchy@ucmerced.edu, fsantiago3@ucmerced.edu

Mario Banuelos, Roummel F. Marcia
University of California, Merced
mbanuelos4@ucmerced.edu, rmarcia@ucmerced.edu

MS57

Data-driven Validation of Predator-prey Dynamics in an Agroecosystem

Faced with shifting global landscapes, there is need for models which can describe the effect of changing ecological communities on the provision of beneficial ecosystem services. In particular, we are interested in the biological control of agricultural pests, which is driven by the structure of predator communities. We therefore consider the utility of the Allometric Trophic Network (ATN) model in describing predator-prey interactions in an agroecosystem. The model assumes Lotka-Volterra dynamics parameterized by body mass, and we motivate a variation on this model accounting for species habitat use as well as intraguild interference. We then evaluate model performance using the results from greenhouse experiments explicitly designed for the validation of this model. We conclude with some discussion of the field-level design of experiments for model validation. This is a joint work with collaborators at the Swedish University of Agricultural Sciences in Uppsala and California State University, Monterey Bay.

Amanda Laubmeier
North Carolina State University
anlaubme@ncsu.edu

MS58

Eigenvalue Problems in Inverse Scattering Theory

We investigate the development of target signatures in order to detect changes in the material properties of an inhomogeneous medium from its measured scattering data. After an overview of this qualitative approach to inverse scattering theory, we present some recently developed eigenvalue problems arising from acoustic scattering that provide useful target signatures, and we briefly discuss the extension of these ideas to electromagnetic scattering. Our presentation includes both theoretical results and numerical experiments.

Samuel Cogar
University of Delaware
cogar@udel.edu

MS58

Preconditioning Weak Constraint Variational Data Assimilation Problems

Weak constraint four-dimensional variational data assimilation is an important method for incorporating data (typically observations) into a model. The linearised system arising within the minimisation process can be formulated as a saddle point problem. Unlike many saddle point problems, the expensive parts of the system are the (1,2) and (2,1) blocks. Here we consider the requirements which this places on the choice of preconditioner and compare the efficacy of different choices, including inexact constraint and Schur complement preconditioners. When additionally considering a low-rank solution to the system, further constraints to the preconditioners are added and the efficacy also changes. We apply these preconditioners to the data assimilation saddle point problem for the linear advection-diffusion equation, and the non-linear Lorenz-95 model, considering a traditional GMRES solver, and a low-rank inexact GMRES.

Daniel Green, Melina Freitag
University of Bath
D.L.H.Green@bath.ac.uk, m.a.freitag@bath.ac.uk

MS58

Ecological Invasions by Fat-tailed Dispersers

Integrodifference equations (IDEs) are used in ecology to model the growth and spread of populations. With IDEs, dispersal of offspring is specified with a probability density function whose shape influences how rapidly invasions progress. We apply tail additivity, a property of regularly varying probability densities, to model invasions with fat-tailed dispersal in one dimension. We analyze invasions from newly- and well-established populations and show that invasions progress at exponential rates that depend on the degree of tail fatness of the kernel.

Benjamin R. Liu
University of Washington
Applied Mathematics
benliu@uw.edu

Mark Kot
University of Washington
mark_kot@comcast.net

MS58

A Stochastic Model for High Performance Computing of Viscoelastic Polymer Behavior

Hydrogels have attracted attention as "smart" materials for their tunable mechanical properties that respond to environmental stimuli such as pH, UV, or temperature; making them ideal for a variety of biomedical and sensor technology applications. Consisting of mostly water,

the viscoelastic properties of hydrogels are the product of a network of polymer chains attaching and detaching at various entanglement points. Due to this complexity at the micro-scale, many previous polymer simulations rely on mathematical simplifications of chain dynamics to produce results. In this poster we explore the potential for a mean-field model to capture the properties that emerge from a mixture of hydrogels using massively parallel computation on graphics processing units. This approach abstracts away the network positions and uses stochastic differential equations derived from physical properties to capture the breaking and reforming behavior of network segments, thereby keeping the non-linear micro-scale polymer dynamics intact.

Erik Palmer
Department of Mathematics
University of South Carolina
etpalmer@math.sc.edu

Paula A. Vasquez
University of South Carolina
paula@math.sc.edu

MS58

Fundamental Limits on Distributed Statistical Learning with Constrained Heirarchical Communication

There have been a number of recent results on the fundamental limits of distributed statistical learning problems with communication constraints. We extend these results to the setting of hierarchical communication architecture. Afterwards, we discuss some applications of these results to distributed machine learning and sensor networks.

Dmitry Shemetov
UC Davis Mathematics
rbassett@math.ucdavis.edu

James Sharpnack
University of California Davis
jsharpna@ucdavis.edu

MS58

Battery Modelling: Why 2D Matters, and How Asymptotics can Help

Batteries are the most promising technology for off-grid energy storage, but must be managed optimally in order to maximise their lifetime. Mathematical modelling of the underlying chemical processes provides a mechanism to identify these optima. We use asymptotic methods to obtain a simplified one-dimensional model for a lead-acid battery that captures all of the fundamental physical behaviour of the battery. We then investigate the more physically realistic case in which current enters the battery from the tops of the electrodes, rather than the sides. Since the aspect ratio of height to width is large, we can again use asymptotic methods to simplify the model, and we find that the impact of the vertical dimension on the voltage is significant. We compare the one- and two-dimensional models with data from lead-acid batteries provided by BBOXX, and find good agreement.

Valentin Sulzer
University of Oxford
sulzer@maths.ox.ac.uk

Jon Chapman
Mathematical Institute
The University of Oxford
chapman@maths.ox.ac.uk

Colin Please
Mathematical Institute
University of Oxford
please@maths.ox.ac.uk

David Howey, Charles Monroe
University of Oxford
david.howey@eng.ox.ac.uk, charles.monroe@eng.ox.ac.uk

MS60

Sobol Tensor Trains for Sensitivity Analysis

Low-rank decompositions are highly suitable for the Sobol method of analysis of variance, which is one of the most successful approaches for global sensitivity analysis. Given a low-rank tensor train (TT) surrogate model we compute its Sobol TT, a representation that gathers its Sobol indices for all orders of interaction in the TT format. Due to its multilinear nature we can efficiently query and aggregate the Sobol TT's entries as well as produce related quantities such as the total, closed, and superset indices. Furthermore, thanks to an interpretation in terms of discrete finite automata, the TT format lends itself very well to error-free compression of mask tensors that allow us to select, count and weigh Sobol indices in various ways. We use these to extract advanced sensitivity metrics from any TT model, including the effective dimensions, the full dimension distribution and arbitrary semivalues, particularly the Shapley values.

Rafael Ballester
Visualization and MultiMedia Lab
University of Zurich
rballester@ifi.uzh.ch

MS60

Deep Learning for Partial Differential Equations

The curse of dimensionality is commonly encountered in numerical partial differential equations (PDE), especially when uncertainties have to be modeled into the equations as random coefficients. However, very often the variability of physical quantities derived from PDE can be captured by a few features on the space of random coefficients. Based on such observation, we propose using neural-network, a technique gaining prominence in machine learning tasks, to parameterize the physical quantity of interest as a function of random input coefficients. The simplicity and accuracy of the approach are demonstrated through notable examples of PDEs in engineering and physics.

Yuehaw Khoo
Stanford University
yuehaw.khoo@gmail.com

Lexing Ying
Stanford University
Department of Mathematics
lexing@stanford.edu

MS60

Multivariate Low-rank Approximation using Ma-

chine Learning

Approximating a multivariate function using a low number of parameters is an important problem which appears in many areas of numerical mathematics. To solve this task several approaches such as cross-approximation exist. We will discuss possible ways to speed up construction of such an approximation using machine learning techniques.

Valentin Khrulkov
Skoltech
valentin.khrulkov@skolkovotech.ru

MS60

Time Integration for Rank Structured Tensors

We present discrete methods for computing low-rank approximations of time-dependent tensors that are the solution of a differential equation. The approximation format can be Tucker, tensor trains, MPS or hierarchical tensors. We will consider two types of discrete integrators: projection methods based on quasi-optimal metric projection, and splitting methods based on inexact solutions of substeps. For both approaches we show numerically and theoretically that their behaviour is superior compared to standard methods applied to the so-called gauged equations. In particular, the error bounds are robust in the presence of small singular values of the tensors matricisations. Based on joint work with Emil Kieri, Christian Lubich, and Hanna Walach.

Bart Vandereycken
University of Geneva
bart.vandereycken@unige.ch

MS61

Granger Nets for Spatio-temporal Stochastic Inference: Predicting Earthquakes, Weather, and Crime

Abstract not available at time of publication.

Ishanu Chattopadhyay
University of Chicago
ishanu@uchicago.edu

MS61

Transfer Operators in Reproducing Kernel Hilbert Spaces

Transfer operators such as the Perron-Frobenius or Koopman operator play an important role in the global analysis of complex dynamical systems. We extend transfer operator theory to reproducing kernel Hilbert spaces and show that these operators are related to Hilbert space representations of conditional distributions, known as conditional mean embeddings in the machine learning community. Moreover, numerical methods to compute empirical estimates of these embeddings are akin to data-driven methods for the approximation of transfer operators such as extended dynamic mode decomposition and its variants. One main benefit of the presented kernel-based approaches is that these methods can be applied to any domain where a similarity measure given by a kernel is available. We illustrate the results with the aid of guiding examples and highlight potential applications in molecular dynamics as well as video and text data analysis.

Stefan Klus
Freie Universitaet Berlin
stefan.klus@fu-berlin.de

MS61

Local Characterization of Feedback Control Laws for Unsteady Wake Flows

A data-driven approach leveraging unsupervised clustering is developed for controlling complex unsteady wake flows. The flow physics consists of many degrees of freedom leading to a high computational cost for numerical simulations, which is challenging for control design. Data-driven clustering and optimization techniques enable local characterization of control laws in a tractable manner. In particular, the aerodynamic force history is partitioned into few clusters which correspond to a characteristic coarse-grained phase in feature space. Coupling flow control simulations with an optimization strategy, the amplitude (and spanwise wavenumber in 3D flows) for actuation input in each of these clusters is optimized to minimize aerodynamic power and actuation power. Reclustering the control trajectories enables further drag reduction. The approach is demonstrated for two and three-dimensional large-eddy simulations (LES) for a spanwise-periodic compressible flow over a NACA 0012 airfoil at an angle of attack of 9° and Reynolds number $Re = 23000$. The feedback control consists of event-based control in transient stage and phasor control at steady state. The optimal control suppresses flow separation and von Karman wake structures in 3D flows with a preference towards lower spanwise wavenumbers. The analysis performed provides insights for feedback flow control of complex systems characterizing local cluster-based control laws based on feature space trajectories.

Aditya G. Nair
Florida State University
Mechanical Engineering
agn13@my.fsu.edu

Bernd Noack
LIMSI-CNRS
Technical University Braunschweig
bernd.noack@limsi.fr

Chi-An Yeh
Florida State University
cy13d@my.fsu.edu

Eurika Kaiser, Steven Brunton
University of Washington
eurika@uw.edu, sbrunton@uw.edu

Kunihiko Taira
Florida State University
Mechanical Engineering
ktaira@fsu.edu

MS61

Data-driven Computational Optimal Control for Stochastic Nonlinear Systems

State-of-the-art computational optimal control methods for stochastic dynamical systems rely on sample trajectories to evaluate performance metrics. As the number of such trajectories increases, the dimension of the optimal control problem rapidly becomes intractable. In this talk, I will present a new paradigm for computational optimal control that emphasizes the role of data-driven probability density

function (PDF) equations instead of nonlinear dynamics in the control loop. Such paradigm opens the possibility to integrate advanced numerical methods for high-dimensional PDF equations with optimization algorithms to quantify the effects of uncertainty in nonlinear control systems.

Tenavi Nakamura-Zimmerer
University of California, Santa Cruz
tenakamu@ucsc.edu

Daniele Venturi
Department of Applied Mathematics and Statistics
University of California Santa Cruz
venturi@ucsc.edu

Qi Gong
University of California, Santa Cruz
qigong@soe.ucsc.edu

MS62

A Low-rank Splitting Integrator for Large-scale Problems

The efficient numerical integration of large-scale matrix differential equations is an important and extensively studied problem in numerical analysis. Large-scale matrix differential equations typically arise from the space discretization of semi-linear partial differential equations. Examples include evolution equations in two space dimensions and differential Lyapunov and Riccati equations. The problems are usually stiff and standard numerical methods require a large amount of computing time and memory. In his talk we propose a numerical low-rank approximation that is based on splitting methods. In particular, we split the linear, stiff part of the vector field from the non-stiff, non-linear one and integrate the former one by employing the action of the matrix exponential function. This action is approximated numerically by an interpolation at Leja points. On the other hand, the non-stiff, non-linear part is integrated by a projector-splitting method. This provides a dynamical low-rank approximation that does not suffer from possible small singular values. We carry out a rigorous stiff error analysis of the proposed method and illustrate its benefits by several numerical examples. This is joint work with Chiara Piazzola (University of Innsbruck) and Hanna Walach (University of Tübingen).

Alexander Ostermann
University of Innsbruck
alexander.ostermann@uibk.ac.at

MS62

High-order Relaxed Multirate Infinitesimal Step Methods for Multiphysics Applications

Increasingly, computational science requires large-scale simulations that consistently and accurately couple distinct physical processes. While the mathematical models for specific processes often have a well-known type (hyperbolic, parabolic, etc.) and are suitable for classical numerical integrators, the same cannot be said for the coupled models. These multiphysics models are often of mixed type, may have limited differentiability, and involve processes that evolve at dissimilar rates. As such, many multiphysics simulations require more flexible time integrators that may be tuned for these complex problems. In this talk, we discuss recent work on constructing novel 'multirate' time integration methods for such applications. While integrators that utilize different stepsizes for distinct processes are not new, traditional approaches suffer from nonrobust stability or low accuracy. The proposed class of 'relaxed multirate infinitesimal step methods' pushes the limits of multirate integration, allowing for fourth-order accuracy, robust theory, and temporal error estimators to enable stepsize adaptivity. This talk focuses on the theoretical construction of explicit-explicit RFSMR methods (both fast and slow components are integrated explicitly), and presents convergence and efficiency results for such methods applied to a set of standard multirate test problems.

Daniel R. Reynolds
Southern Methodist University
Mathematics
reynolds@smu.edu

Jean Sexton
Lawrence Berkeley National Laboratory
jmsexton@lbl.gov

MS62

Strong Stability Preserving Multiderivative Time Integrators for Systems of Equations

In this talk, we explore the strong stability preserving (SSP) properties of multistage multiderivative methods. This class of methods is an umbrella class that encompasses all Taylor as well as Runge-Kutta solvers. In place of exclusively introducing additional stages as is done in a Runge-Kutta method to obtain higher order accuracy, multiderivative methods permit the evaluation of derivatives of the solution in addition to the right hand side function. In the context of partial differential equations, when such a method is based upon a Taylor series expansion it is called a Lax-Wendroff type of method. However, unlike strict Taylor discretizations, these methods introduce greater flexibility by introducing stages that can be used to modify the region of absolute stability as well as reduce the total number of derivatives required to obtain a desired order of accuracy. In this work we give a brief overview of one option for implementing these methods, and we describe sufficient conditions for a two-derivative multistage method to be SSP. We present two different options for defining what it means to be SSP, one based on a second-derivative condition, and a second based upon a Taylor series condition. Numerical examples demonstrate how optimal time integrators can be optimized once characteristics of the spatial discretization are known.

Sigal Gottlieb
Department of Mathematics
University of Massachusetts Dartmouth
sgottlieb@umassd.edu

Zachary J. Grant
University of Massachusetts at Dartmouth
zgrant@umassd.edu

David C. Seal
United States Naval Academy
seal@usna.edu

MS62

Fractional Order Convergence of Time-discretizations for Semilinear PDEs

We study semilinear evolution equations $\frac{\mathrm{d}U}{\mathrm{d}t} = AU + B(U)$ posed on a Hilbert space $\mathcal{Y}$, where A is normal and generates a strongly continuous semigroup, B is a smooth non-

linearity from $\mathcal{Y}_\ell = D(A^\ell)$ to itself, and $\ell \in I \subseteq [0, L]$, $L \geq 0$, $0, L \in I$. In particular the one-dimensional semilinear wave equation and nonlinear Schrödinger equation with periodic, Neumann and Dirichlet boundary conditions fit into this framework. We discretize the evolution equation with an A-stable Runge-Kutta method in time, retaining continuous space, and prove convergence of order $O(h^{p\ell/(p+1)})$ for non-smooth initial data $U^0 \in \mathcal{Y}_\ell$, where $\ell \leq p + 1$, for a method of classical order p, extending a result by Brenner and Thomée for linear systems. Our approach is to project the semiflow and numerical method to spectral Galerkin approximations, and to balance the projection error with the error of the time discretization of the projected system. Numerical experiments suggest that our estimates are sharp.

Claudia Wulff
University of Surrey
Dept. of Math and Statistics
c.wulff@surrey.ac.uk

MS63

Atmosphere-ocean Coupled Data Assimilation using Nasa Geos: Estimation of Air-sea Interface State Variables

Air-sea interface variables, such as the skin Sea Surface Temperature (SST) are essential for atmosphere-ocean coupling. In the NASA GMAO Data Assimilation System (DAS), the skin SST and 3-D atmospheric state are jointly estimated [S. Akella, et al. (2017), doi:10.1002/qj.2988]. This presentation is focussed on the prior or *background* error covariance that is used in this analysis. The GEOS DAS uses an ensemble-variational assimilation strategy. In that, specification of a climatological background (CB) error covariance for SST relies on the NOAA's OI SST, with estimates of standard deviation and correlation length scales based on weekly analyses of the *bulk* SST at 1 degree resolution. However, present analysis system is striving to resolve SST diurnal variability with six hourly analyses and assimilates a vast number of in-situ and satellite observations. The first part of this presentation re-derives the CB error covariance using OSTIA SST analyses and illustrates the impact of this update on assimilating satellite observations. In a hybrid assimilation system the CB error covariances are appended with a flow-dependent background error covariance estimate implied by the underlying ensemble. The second part of this presentation refers to: a. treatment of the skin SST in the ensemble members, b. corresponding ensemble spread, and c. impact of these additions on the data assimilation system.

Santha Akella, Ricardo Todling
NASA/GSFC Global Modeling and Assimilation Office
santha.akella@nasa.gov, ricardo.todling@nasa.gov

MS63

Data Assimilation for the Radiation Belt Environment

The Earth's radiation belts experience significant and abrupt changes due to acceleration, loss, and transport processes of the trapped energetic electrons in Earth's magnetic field. Since high-energy particles can potentially damage space infrastructure, understanding and predicting the dynamics of the radiation belts is of particular importance. In this work we implement a four dimensional variational data assimilation (4D-Var) to a radial diffusion equation and its parameterizations modeling the radiation belt environment. Specifically, we use the 4D-Var to determine transport coefficients (D_{LL}, and τ) within the model that control how particles are distributed throughout Earth's magnetic environment. A series of assimilation experiments are perform to not only estimate the correct radiation belt environment, but also estimate the appropriate value of the various parameterization commonly used in the models. The results are compared with other assimilation techniques to assess the effectiveness of the 4D-Var for this problem.

Humberto C. Godinez
Los Alamos National Laboratory
Applied Mathematics and Plasma Physics
hgodinez@lanl.gov

Michael Henderson
Los Alamos National Laboratory
mghenderson@lanl.gov

MS63

The Complexity and Pitfalls of Comparing Different Data Assimilation Algorithms for Terrestrial Model Predictions

In order to optimally merge measurement data and terrestrial model predictions in near real-time, different data assimilation (DA) algorithms have been proposed in the literature. It is important to find out which algorithm performs best for a given problem, and therefore several comparison studies of DA-algorithms have been performed and published. We compared eight different DA-algorithms for two different cases, with 1000 synthetic experiments per case, and seven different ensemble sizes per synthetic experiment. Results show that the ranking of the performance of DA-algorithms is strongly dependent on the specific synthetic experiment and the specific case. Therefore, comparison of DA-algorithms requires a large number of synthetic tests for different cases.

Harrie Jan Hendricks-Franssen
Agrosphere (IBG-3)
Forschungszentrum Jülich
h.hendricks-franssen@fz-juelich.de

Johannes Keller, Gabriele Marquart
RWTH Aachen
jkeller@eonerc.rwth-aachen.de, gmarquart@eonerc.rwth-aachen.de

MS63

A New Framework for Land Data Assimilation by Evolutionary Particle Filter

Particle Filters have received increasing attention in hydrogeosciences, as an effective tool to improve model predictions in nonlinear and non-Gaussian dynamical systems. The implication of dual state and parameter estimation using the PFs in hydrology has evolved since last decade and now we are proposing a more effective and robust framework through evolutionary PF based on Genetic Algorithm and MCMC, the so-called EPFM. In this framework, the prior distribution undergoes an evolutionary process based on the designed mutation and crossover operators. The merit of this approach is that the particles move to an appropriate position and then the ensemble spread is improved by means of MCMC. We report the usefulness and effectiveness of the proposed EPFM on conceptual and highly nonlinear hydrologic models over different climate

and geographical regions in the US. In addition, we elaborate on our recent development in model uncertainty characterization within data assimilation. Traditional methods rely on subjective, ad-hoc tuning factors or parametric distribution assumptions that may not always be applicable. We present a data-driven approach to model uncertainty characterization that makes no assumption about the form of the distribution. In the experiments, it is shown that the proposed method leads to substantial improvements in estimation of both the latent states and observed system outputs over a standard method involving perturbation with Gaussian noise.

Hamid Moradkhani
University of Alabama
hmoradkhani@ua.edu

MS64

Supervised Learning for High Frequency Trade Execution

We introduce a high frequency trade execution model which treats price movement in reduced form. This model is used to assess the ability of a market making strategy to avoid adverse price selection, given conditional fill probabilities at each level of the limit order book and the price movements. We apply the trade execution model to Level II E-mini S&P 500 futures history and develop a Recurrent Neural Network to forecast the price distribution. Results characterize the resilience of various market making strategies under execution latency and prediction error.

Matthew F. Dixon
Illinois Institute of Technology
mdixon7@stuart.iit.edu

MS64

Financial Correlation Clustering

We discuss some problems related to the clustering of high dimensional financial data.

Damir Filipovic
EPFL
damir.filipovic@epfl.ch

MS64

Welfare Analysis of Central Bank Digital Currency: Privacy versus Efficiency

A Central Bank Digital Currency (CBDC) is electronically transacted and stored money, similar to existing cryptocurrencies like Bitcoin, but guaranteed by a central bank. If a central bank introduced a CBDC, it could provide the public with a cheaper payment system, leading to efficiency gains compared to a traditional currency. However, a CBDC may compromise users' privacy because transactions could be monitored by the state's authority. In several countries (e.g., Japan), central banks have already made steps toward a CBDC by establishing digital payment platforms, but it is an open debate whether central banks should introduce their own digital currencies. In this talk, we present a model featuring the trade-off between efficiency and privacy faced by people who decide between different payment methods, and analyze the welfare implications of a CBDC.

Christoph Frei
University of Alberta
cfrei@ualberta.ca

Agostino Capponi
Columbia University
agcappo@gmail.com

MS64

Monopoly Without a Monopolist: An Economic Analysis of the Bitcoin Payment System

Owned by nobody and controlled by an almost immutable protocol, the Bitcoin cryptocurrency payment system is a platform with two main constituencies: users, who make and receive payments; and profit-seeking miners, who maintain the system's infrastructure. We seek to understand the economics of the system: How does the system raise revenue to pay for its infrastructure? How are usage fees determined? How much infrastructure is deployed? What are the implications of changing parameters in the protocol? To address these questions, we offer and analyze an economic model of a cryptocurrency system featuring user-generated transaction fees, and focus on Bitcoin as the leading example. These fees, as well as the systems infrastructure level (number of servers in use), are determined in an equilibrium of a congestion-queueing game derived from the system's limited throughput. The system eliminates dead-weight loss from monopoly, but introduces other inefficiencies. Namely, the system requires significant congestion to raise revenue and fund infrastructure. In the absence of significant congestion, meaningful transaction-fee generation will cease, and in the long-term the cryptocurrency system will risk collapse. Moreover, the current design of the system, specifically the processing of large but infrequent blocks of transactions, makes the system less efficient at raising revenue.

Gur Huberman, Jacob Leshno, Ciamac C. Moallemi
Graduate School of Business
Columbia University
gh16@gsb.columbia.edu, jleshno@columbia.edu, ciamac@gsb.columbia.edu

MS65

Kinematic Design with Numerical Algebraic Geometry

Precision-point synthesis problems for design of four-bar linkages have typically been formulated using two approaches. The exclusive use of path-points is known as "path synthesis", whereas the use of poses, i.e. path-points with orientation, is called "rigid-body guidance" or the "Burmester problem". We consider the family of "Alt-Burmester" synthesis problems, in which some combination of path-points and poses are specified, with the extreme cases corresponding to the typical approaches. The Alt-Burmester problems that have, in general, a finite number of solutions include Burmesters original fivepose problem and also Alts problem for nine path-points. The elimination of one path-point increases the dimension of the solution set by one, while the elimination of a pose increases it by two. Using techniques from numerical algebraic geometry, we tabulate the dimension and degree of all problems in this Alt-Burmester family, and provide more details concerning all the zero- and one-dimensional cases.

Dani Brake
University of Notre Dame
Dept. of App. Comp. Math. and Stats.

brakeda@uwec.edu

MS65

Exact Reconstruction of Euclidean Distance Geometry Problem using Low-rank Matrix Completion

The Euclidean distance geometry problem arises in a wide variety of applications, from determining molecular conformations in computational chemistry to localization in sensor networks. When the distance information is incomplete, the problem can be formulated as a nuclear norm minimization problem. In this paper, this minimization program is recast as a matrix completion problem of low rank r Gram matrix with respect to a suitable basis. The well known restricted isometry property can not be satisfied in the scenario. Instead, a dual basis approach is introduced to theoretically analyze the reconstruction problem. If the Gram matrix satisfies certain coherence conditions with parameter ?, the main result shows that the underlying configuration of n points can be recovered with very high probability from O(nr?log2(n)) uniformly random samples. Computationally, simple and fast algorithms are designed to solve the Euclidean distance geometry problem. Numerical tests on different three dimensional data and protein molecules validate effectiveness and efficiency of the proposed algorithms [https://arxiv.org/abs/1804.04310].

Rongjie Lai
Rensselaer Polytechnic Institute
lair@rpi.edu

MS65

Numerical Differential Geometry

This will be an introductory talk to Numerical Differential Geometry. In particular connections between manifold optimization, polynomial optimization, and matrix completion will be discussed.

Jose Rodriguez
University of Chicago
jose.israel.rodriguez.math@gmail.com

MS65

Fiber Product Homotopies for Multi-parameter Eigenvalue Problems

We develop a homotopy to solve multi-parameter eigenvalue problems (MEP). Our numerical experiments show that our method outperforms the Δ method in terms of memory management and outperforms previous homotopy based methods to find all eigenpairs in terms of timing. For generic-singular MEPs, we prove that our homotopy will have no paths going to infinity almost surely. This is in contrast to homotopy methods where for these singular MEPs there will always be paths diverging to infinity.

Yiling You
University of Chicago
Department of Statistics
ylyou@uchicago.edu

Jose I. Rodriguez
Department of Statistics
University of Chicago
joisro@uchicago.edu

Lek-Heng Lim
University of Chicago
lekheng@galton.uchicago.edu

MS66

Tomographic Reconstruction with Simultaneous Error Correction

The advanced imaging technique, which leads to unquestionable improved clarity of sample structure, however, is highly vulnerable to systematic and random errors. These errors are fundamental obstacles to a full realization of the next-generation photon science since they can lead to reduced spatial resolution and even misinterpretation of the underlying sample structures. In this work, we formulate new physical models to capture these experimental error, we devise new mathematical optimization formulations for robust inversion of complex sample. The numerical results are demonstrated on both synthetic and real data.

Zichao Di
Argonne National Lab
wendydi@mcs.anl.gov

MS66

Derivative Free Optimization with Integer Variables

Abstract not available at time of publication.

Sven Leyffer
Argonne National Laboratory
leyffer@anl.gov

MS66

Quasi-Newton Methods for Off-the-Shelf Machine Learning

Machine learning (ML) problems are often posed as highly nonlinear and nonconvex unconstrained optimization problems. Methods for solving ML problems based on stochastic gradient descent generally require fine-tuning many hyper-parameters. In this talk we discuss alternative approaches for solving ML problems based on a quasi-Newton trust-region framework that does not require extensive parameter tuning. We will present numerical results that demonstrate the potential of the proposed approaches.

Jennifer Erway
Wake Forest University
erwayjb@wfu.edu

Joshua Griffin
SAS Institute, Inc.
Joshua.Griffin@sas.com

Roummel F. Marcia
University of California, Merced
rmarcia@ucmerced.edu

Riadh Omheni
SAS Institute, Inc.
riadh.omheni@sas.com

MS66

A Scheduling Problem Motivated by Cybersecurity

We describe a scheduling problem motivated by cyberse-

curity. We briefly describe PLADD (Probabilistic Learning Attacker, Dynamic Defender), an abstract game introducted by Jones et. al. that approximates the competition for a resource between the resource owner (defender) and an attacker. PLADD is an extension of the FlipIt resource competition game, incorporating elements of moving-target defenses in cyber systems. The goal of these models is to develop optimal defender strategies. One way to study defense strategies is to sample attack scenarios from the probability distributions representing time to attacker success. We can then compute the optimal sequence of defender actions for that finite attack scenario set using stochastic programming. In this case, the stochastic program has a scheduling interpretation and an integer-programming formulation. One can also use the same abstractions to study machine-learning-based classifiers under concept drift. We will discuss progress towards formal complexity analysis, approximation algorithms, and report on computational experiments using cybersecurity data.

Ojas Parekh, Cynthia Phillips
Sandia National Laboratories
odparek@sandia.gov, caphill@sandia.gov

Vladlena Powers, Nouri Sakr, Cliff Stein
Columbia University
vp2342@columbia.edu, n.sakr@columbia.edu, cliff@ieor.columbia.edu

MS67

Photonic Bound States in the Continuum

Bound states in the continuum are solutions of wave equations that remain spatially localized with no radiation, even though their frequencies are embedded in the continuous spectra of spatially extended states. Photonic structures are highly tailorable and provide an attractive platform to realize these unique states. I will present theoretical and experimental data for the observation of bound states in the continuum in photonic crystal slabs, the vortices in the far-field polarizations for resonances surrounding such states, as well as prospects for realizing bound states in the continuum in optical fibers with periodic gratings.

Chia Wei Hsu
Yale University
chiawei.hsu@yale.edu

MS67

Irreducibility of the Fermi Surface for Planar Periodic Graphs

The reducibility of the Fermi surface for periodic graph operators is central to the construction of embedded eigenvalues supported by a localized defect. We conjecture that the Fermi surface of any planar doubly periodic graph is always irreducible except at finitely many energies. We prove this in the case of two vertices per period and nearest-period interactions. Reducibility is equivalent to the factorability of a polynomial in two variables. The proof involves construction of Groebner bases for the algebraic set in the coefficients of the periodic operator that describes when it the Fermi surface is factorable. This is joint work with Daniel Rockwell and Stephen Shipman.

Wei Li
Louisiana State University
liwei@lsu.edu

MS67

Generation of Bound States in the Continuum in a Second Order Nonlinear Process

For periodic structures sandwiched between two homogeneous media, a bound state in the continuum (BIC) is a guided mode above the light line that cannot couple with propagating plane waves in the surrounding media. This is no longer the case for nonlinear media. For structures with a second order nonlinearity, we show that some BICs can be generated by pumping the structure with an incident wave having one half the BIC frequency. It is, however, not a pure second harmonic generation process, since the third and fourth harmonics are also generated and they cannot be ignored. Using a perturbation method, we show that the amplitude of the BIC is proportional to A/δ, where A is the amplitude of the incident wave with frequency $\omega_*/2$ (ω_* is the frequency of the BIC), $\delta = \sqrt[3]{A\gamma_1}$ is a small dimensionless parameter, and γ_1 is the magnitude of a relevant element of the second order nonlinear susceptibility tensor. Our theoretical results are validated by direct numerical simulations.

Lijun Yuan
Chongqing Technology and Business University
ljyuan@ctbu.edu.cn

Ya Yan Lu
City University of Hong Kong
Dept of Mathematics
mayylu@cityu.edu.hk

MS67

An Integrated View of Complex Aspects of Bound States

This introductory talk will present an overview of the topic of the minisymposium. It will address modern interest in bound states of physical systems, especially at energies embedded in the continuum of radiation states. We will discuss the mechanisms for the creation of bound states and the associated resonant phenomena. Of particular importance today are spectrally embedded bound states that are not induced by symmetry.

Stephen Shipman
Louisiana State University
shipman@lsu.edu

MS68

Upwind Schemes for Maxwell's Equations in Second-order Form

High-order central upwind schemes for the second-order wave equation are derived from a conservative finite-difference approach. A formally exact differential-difference equation provides schemes of arbitrarily high order. Upwinding is incorporated by embedding an exact d'Alembert solution to a generalized Riemann problem into the numerical flux function. It is shown that the upwind dissipation appears as a modular term that can be easily added to neutrally stable centered schemes similar to common artificial dissipation with the advantage of not introducing a free-tuning parameter. The scheme is applied to Maxwell's equations in second-order form and high-order convergence is demonstrated for classical scattering prob-

lems.

Jordan B. Angel
Rensselaer Polytechnic Institute
angelj2@rpi.edu

MS68

A Kernel-based High Order Numerical Scheme

In this talk, I will introduce a novel numerical scheme, in which the spatial derivatives are represented as a special kernel based formulation of the solutions. We use this method to solve the nonlinear advection-diffusion equations and Hamilton-Jacobi equations. In such a framework, a high order weighted essentially non-oscillatory (WENO) methodology and a nonlinear filter are further employed to avoid spurious oscillations. Moreover, theoretical investigations indicated that the proposed scheme is unconditionally stable up to third order accuracy when combining with the explicit SSP-RK scheme. Evaluation of the kernel based approach is done with a fast O(N) summation algorithm. The new method allows for much larger time step evolution compared with other explicit schemes with the same order accuracy, leading to remarkable computational savings.

Andrew Christlieb
Michigan State University
christli@msu.edu

Wei Guo
Texas Tech University
weimath.guo@ttu.edu

Yan Jiang
Michigan State University
jiangyan@math.msu.edu

MS68

An Alternative Formulation of Discontinous Galerkin Schemes for Solving Hamilton-Jacobi Equations

The aim of this paper is to develop an alternative formulation of discontinuous Galerkin (DG) schemes for approximating the viscosity solutions to nonlinear Hamilton-Jacobi (HJ) equations. The main difficulty in designing DG schemes lies in the inherent non-divergence form of HJ equations. One effective approach is to explore the close relationship between HJ equations and hyperbolic conservation laws: the standard DG scheme is applied to solve a conservation law system satisfied by the derivatives of the solution of the HJ equation. In this paper, we consider an another approach to directly solving the HJ equations, motivated by a class of successful direct DG schemes by Cheng et al. [J. Comput. Phys., v223 (2009); J. Comput. Phys., 268(2014)]. The proposed schemes are derived based on the central-upwind scheme by Kurganov et al. [SIAM J. Sci. Comput., v23 (2001)]. In particular, we make use of precise information of the *local speeds of propagation* at the discontinuous element interface with the goal of adding adequate numerical viscosity and hence naturally capturing the viscosity solutions. A collection of numerical experiments is presented to demonstrate the robustness of the methods for solving general HJ equations with linear, nonlinear, smooth, non-smooth, convex, or non-convex Hamiltonians.

Guoyi Ke, Wei Guo
Texas Tech University
guoyi.ke@ttu.edu, weimath.guo@ttu.edu

MS68

Entropy-bounded Discontinuous Galerkin Method and its Application in High-fidelity CFD

This talk discusses the entropy-bounded discontinuous Galerkin (EBDG) scheme for nonlinear conservation laws. EBDG is an extension of the postivity-preserving DG by Zhang & Shu. Specifically, EBDG scheme provides simple implementation to enforce the boundedness of pressure; avoids use of particular quadrature rules; and enables the solution limiting on multidimensional settings with arbitrary element shape. After outlining the theoretical foundation and algorithmic implementation of EBDG scheme, the focus will be placed on applying EBDG in high-fidelity numerical simulations of multiphysics flow problems. First of all, a benchmark study of the EBDG method against the state-of-the-art finite-volume solver will be reported with particular emphasis on simulations of compressible turbulence. Furthermore, we will discuss the efforts for enabling DG-based large-eddy-simulation capability for predictions of turbulent reacting flows. Validation studies with the consideration of a bluff-body stabilized premixed flame and a partially-premixed jet flame will be presented. The talk will finish with some concluding remarks highlighting the overarching challenges that face the research community on leveraging the high-order DG methods for practical applications.

Yu Lv
Mississippi State University
ylv@ae.msstate.edu

MS69

Combinatorial Properties of Expansion Complexes

This talk will give a broad overview of expansion complexes—what they are, where they come from, their uses, their properties. In particular, we will show how an expansion complex gives rise to a bi-infinite hierarchy of planar polygonal complexes, the one in the sequence related to the next by subdivision, and with all in the hierarchy locally isomorphic with one another. We will see that some of these hierarchies—a countably infinite few among an uncountable number—admit a nontrivial combinatorial symmetry, and we will show how to construct all of these. We will examine some the properties that these hierarchies share with the traditional hierarchical euclidean tilings like the famous Penrose tilings. These include, aside from local isomorphism, finite local complexity interpreted as satisfying an appropriate isoperimetric inequality, compactness of its pointed local isomorphism space, combinatorial repetitiveness, and exponential expansivity.

This lecture will serve to set up the remaining lectures in this session.

Philip L. Bowers
FSU
bowers@math.fsu.edu

MS69

Expansion Complexes in Exploring the Cannon Conjecture

Cannon's Conjecture is the statement that if G is a

Gromov-hyperbolic discrete group whose space at infinity is a 2-sphere, then G acts properly discontinuously, cocompactly, and isometrically on hyperbolic 3-space. Following pioneering work by Cannon, Cannon and Swenson showed that the conjecture follows for a group G by showing that a certain recursive sequence of covers of the space at infinity is (combinatorially) conformal. Cannon, Floyd, and Parry introduced finite subdivision rules as a toy model for the sequences of covers of the space at infinity. Following the Bowers-Stephenson work on the expansion complex for the pentagonal subdivision rule, they formulated a more general theory of expansion complexes for finite subdivision rules. In this talk I'll discuss finite subdivision rules and expansion complexes, how they arose in our approach to resolving Cannon's Conjecture, and the role of expansion complexes in an attempt to pursue this approach. This is joint work with James Cannon and Walter Parry.

William Floyd
Virginia Tech
wfloyd@math.vt.edu

MS69

Solving the Type Problem for Rotationally Symmetric, Single Tile-type Expansion Complexes

If a subdivision rule τ with one face type is dihedrally symmetric (plus other mild conditions), then any expansion complex associated to τ necessarily admits a hierarchical structure known as a conformal hierarchy. Bowers & Stephenson have shown that the conformal tiling for any expansion complex in this setting is parabolic—that is, it tiles the complex plane $\mathbb{C}$. In this talk I will detail a more general type of hierarchical structure—a fractal hierarchy—which is created through the use of the Cannon-Floyd-Kenyon-Parry idea of using a hyperbolic branched covering of a single-tile type conformal tiling, ultimately generalizing the Bowers-Stephenson result to subdivision rules that are merely rotationally symmetric.

Dane P. Mayhook
Iowa State University
dmayhook@iastate.edu

MS69

Geometrizing Expansion Complexes: Type and Visualization

We describe the transition from expansion complexes as combinatorial objects to their realizations as concrete conformal tilings. The underlying theory and many open questions are grounded in classical analytic function theory. However, the computational methods, based on circle packing, are new, and the resultant computer experiments and visualizations are the prime drivers of the topic. We outline the constructions and formualate the fundamental "type" problem, illustrating with several examples.

Kenneth Stephenson
University of Tennessee, Knoxville
Department of Mathematics
kstephe2@utk.edu

MS70

Session Cancelled

This session has been cancelled.

Paul Constantine
University of Colorado Boulder
pconstan@mines.edu

MS71

Multi-physics Finite Element Methods for a Dynamic Poro-elastic Model

In this talk I shall present some recent developments on multiphysics finite element methods for a poroelasticity model and for its limiting model (as the constrained storage coefficient tends to zero) which is known as Biot's consolidation problem in soil mechanics and is also known as Doi's model for polymer gels. In particular, a new approach based on a multiphysics reformulation of the poroelasticity model will be discussed in detail. The idea of the approach is to introduce an "pseudo-pressure" and to show that such a pressure is governed by a diffusion process. Based on this new formulation various fully discrete finite element methods for approximating the model have been proposed and analyzed. A common feature of these methods is that at each time step two simple sub-problems need to be solved: one of which is a generalized Stokes-type problem for the displacement vector field and another is a diffusion problem for the "pseudo-pressure" field. The convergence and stability of these methods will be discussed and numerical experiment results will also be presented to demonstrate the efficiency of the approach, in particular, to show that the so-called "locking phenomenon" is naturally avoided.

Xiaobing H. Feng
The University of Tennessee
xfeng@math.utk.edu

MS71

Mechanics and Mathematics of Multicomponent Multiphase Flows in Porous Media

This talk will review structural properties of the equations used to model geophysical flows which involve multiple components undergoing phase transitions. Simulations of these problems only model the gross properties of these flows since a precise description of the physical system is neither available nor computationally tractable. Macroscopic models utilize classical thermodynamics to characterize phase formation in the constitutive relations of the classical balance laws. Convexity (concavity) of the free energy (entropy) functions appearing in classical thermodynamics plays an essential role in the development of stability estimates of solutions to the equations modeling these flows.

Noel J. Walkington
Department of Mathematical Sciences
Carnegie Mellon University
noelw@andrew.cmu.edu

MS71

Nonlinear Poro-visco-elasticity

We consider a nonlinear elliptic-parabolic system of PDEs that models fluid flow through poro-visco-elastic material. The ability of the fluid to flow within the solid is described by the permeability tensor which varies nonlinearly with the structural dilation. We study the existence of weak solutions in bounded domains with physical, mixed-type boundary conditions, and we account for non-zero volumetric and boundary sources. One principal aim is to investigate the influence of viscoelasticity on the qualitative prop-

erties solution. Our analysis shows that different time regularity requirements are needed for the volumetric source of linear momentum and the boundary source of traction depending on the presence of viscoelasticity. Theoretical results are further investigated via numerical simulations; when data are appropriately regular, numerical simulations show that the solutions satisfy the predicted energy estimates. Simulations also show that, in the purely elastic case, the Darcy velocity and the related fluid energy may become unbounded if the data do not enjoy the time regularity required by the theory. These results are interpreted in the context of pressure changes in lamina cribrosa (in the human eye), and the connection between these biomechanics and the development of glaucoma.

Justin T. Webster
Department of Mathematics and Statistics
University of Maryland, Baltimore County
websterj@umbc.edu

Lorena Bociu
NC State University
Raleigh, NC
lvbociu@ncsu.edu

Giovanna Guidoboni
Indiana University-Purdue University at Indianapolis
Department of Mathematical Sciences
gguidobo@math.iupui.edu

Riccardo Sacco
Politecnico di Milano
riccardo.sacco@polimi.it

MS72

Homeostasis as a Network Phenomenon

Homeostasis occurs when an output variable remains approximately constant as an input parameter varies over an interval. We formulate homeostasis in the context of singularity theory by replacing 'approximately constant over an interval' with 'zero derivative of the output with respect to the inputs at a point'. Unfolding theory then classifies all small perturbations of the input-output function. In particular, in one input systems the 'chair' singularity of Best, Nijhout, & Reed is especially important in applications. We discuss several applications in biochemical and gene regulatory motifs. We show that the hyperbolic umbilic can also organize evolution to homeostasis in two input systems. This work is joint with Ian Stewart, Mike Reed, Janet Best, Fred Nijhout, and Fernando Antoneli.

Martin Golubitsky
The Ohio State University
Department of Mathematics
golubitsky.4@osu.edu

MS72

Shifting Attention to Neuronal Network Dynamics: Self-reprogramming on top of Reference States

Flexible function is essential for the brain to cope with varying environments, changing quality of sensory information as well as context dependency. This requires organized communication and flexible information processing among the different sub-circuits in neuronal networks. While state-of the art artificial networks already exceed human performance in many specialized tasks, general intelligence solving generic tasks or being able to bootstrap function from a small set of samples likely requires the interaction of a larger number of sub-networks which must coordinate communication and computation. Here we discuss how the structure of an information processing circuit might be dynamically affected by its own operation similar to field-programmable gate arrays (FPGAs) in which logic gates can be dynamically re-linked on the fly by setting specialized memory-bits. We argue that in a neuronal circuit an underlying reference dynamical state, such as a neuronal oscillation, is capable of performing such a function. We outline some implications for neuronal data analysis. To demonstrate the utility of this approach, we further show that in oscillatory Hopfield networks this mechanism enables believe propagation like context dependent pattern-recognition.

Christoph Kirst
Center for Studies in Physics and Biology
Rockefeller University, US
Christoph.Kirst@Rockefeller.edu

MS72

New States in Complex Systems

The dynamics of complex systems and networks are often described by simple equations which nevertheless can admit a rich variety of disparate solutions. Discovering and understanding the full spectrum of solutions that correspond to stable states is at the forefront of current research. Recent work by our group and others has presented us with a myriad of stable or metastable states with remarkable properties, which were previously assumed to be impossible. In this presentation, I will discuss symmetric states requiring system asymmetry, chimera states in continuous locally-coupled media, and states remotely synchronized by uncorrelated intermediates. The presentation will include a discussion of applications and implications for natural and technological network systems.

Adilson E. Motter
Northwestern University
motter@northwestern.edu

MS72

Collective Phenomena Emerging from Intertwined Dynamical Processes in Multiplex Networks

Dynamical processes on complex networks play a vital role in shaping the world around us. Some examples of such dynamical processes include synchronization, transport, spreading, etc. Over the last few decades the study of dynamical processes on network have garnered a great deal of attention from the mathematics, physics, and other scientific communities due to their application to a wide range of phenomena. Despite this progress, the vast majority of work considers dynamics that act on a network in isolation. In this work we present a general framework for modeling and studying the intertwined dynamics of multiple dynamical processes acting in parallel on interconnected networks. As a specific example inspired by brain dynamics, we consider the case of intertwined synchronization and transport dynamics, using the framework of multiplex networks as a structural connection. In particular, the dynamics of the synchronization process depends on the dynamics of the transport process and vice-versa. We show using numerical and analytical methods that the connections between these two dynamical processes induces spontaneous explosive synchronization and switch-like transitions between homogeneous and heterogenous transport dynamics,

otherwise not present in the two systems each acting in isolation. We hypothesize that such novel dynamical effects may arise in a wide range of other intertwined dynamical processes, for which our general framework may be useful.

Per Sebastian Skardal
Trinity College
Department of Mathematics
persebastian.skardal@trincoll.edu

MS73

Computational Affordable Approach to Calculate Computationally Expensive Properties of Chemical Reaction on Surfaces

With the recent explosion in computational catalysis and related microkinetic modeling, the need for a fast, yet accurate, way to predict equilibrium and rate constants for surface reactions has become more important. In this work, we present a computationally efficient method to calculate partition functions and entropy of adsorbed species and equilibrium constants.

Líney Arnadottir
Oregon State University
liney.arnadottir@oregonstate.edu

MS73

Nonlinear Filtering Problems for Systems Governed by PDEs

The Kalman filter is one of the very essential discovery for the last century and provides estimate of state and parameters. It works well if the dynamics are nearly linear but it requires improvements for significantly nonlinear and non-Gaussian system. In this presentation we introduce an improved variation of the Kalman filter for large scale nonlinear stochastic systems based on the Gaussian filter. This is an approach based on the optimal filtering theory; i.e., the optimal filter based on the Bayes' formula for discrete time dynamics and the Zakai equation for continuous time. That is, we develop the filtering update via the assumed Gaussian density filter. A key step is that we update the covariance in the square root factors form and thus we update the square root factors of the Gaussian covariance. This evolves into the reduced Gaussian filter based on the reduced factor updates. For dissipative system, we develop an alternative to the reduced Gaussian filter, by the assumed covariance filter. For systems that are time reversible, we use the time reversal filter and use the quasi reversible method for mildly diffusive system which are systems that are not time reversible.

Melissa Ngamini
Morehouse College
melissa.ngamini@morehouse.edu

MS73

Parametric Linear System Solving with Error Correction

Consider solving a black box linear system, where the entries are univariate polynomials over a field and the matrix is full rank. The solution can be recovered even if some evaluations are erroneous. In [Boyer and Kaltofen, Proc. SNC 2014] the problem is solved with an algorithm that generalizes Welch/Berlekamp decoding of an algebraic Reed-Solomon code. We describe an algorithm that given the same inputs uses possibly fewer evaluations to compute the solution. We introduce a second count for the number of evaluations required to recover the solution based on work by Stanley Cabay. Assuming we have the actual degrees for all necessary input parameters, we give the criterion that determines when the Cabay count is fewer than the generalized Welch/Berlekamp count. We then specialize the algorithm for parametric linear system solving to the recovery of a vector of rational functions. If the rational function vector is the solution to a full rank linear system we may recover it from fewer evaluations than generalized Welch/Berlekamp decoding. We then show that if entries in our rational function vector are polynomials, then the vector can be viewed as an interleave Reed-Solomon code. Thus, if the errors occur in bursts we can again do better than generalized Welch/Berlekamp decoding. Finally, we present an algorithm for parametric linear system solving with errors when the matrix is rank deficient.

Cleveland Waddell, Erich Kaltofen
North Carolina State University
cawaddel@ncsu.edu, kaltofen@ncsu.edu

Arne Storjohann
D. Cheriton School of C.S.
Univ of Waterloo, ON, Canada
astorjoh@uwaterloo.ca

Clément Pernet
INRIA/LIG-MOAIS
Grenoble Université
clement.pernet@imag.fr

MS73

A New Iterative Method for Solving Non-square Systems of Linear Equations

This talk presents a new iterative procedure for solving systems of m linear equations in n variables under a sufficient condition that is practical. We show how this procedure may utilize elementary row operations to meet its sufficient condition. In this iterative procedure, the approximate solution obtained in each iteration is a convex combination of some l_∞-norm projections of the previous approximate solution. Under a regularity condition, this procedure converges quadratically. Application examples are given that show how this procedure can generate desired non-basic solutions and how it can be applied to solve linear programming problems and nonlinear systems of equations.

Ira Wheaton
Morehouse College
ira.wheaton@morehouse.edu

Samuel Awoniyi
FAMU/FSU College of Engineering
sawoniyi@fsu.edu

MS75

Macroscopic Models of Human Circadian Rhythms

Disrupted circadian rhythms have been implicated in a vast array of both mental and physical health maladies including heart disease, diabetes, addiction, depression and sleep disorders. Therefore, it is a matter of vital importance to understand and predict human circadian dynamics. Increasing knowledge of the molecular details of the circadian clock has induced a divergence in the modeling approaches employed in the field. Detailed high-dimensional models have been created to explain and predict the molecular

data sets measured in model organisms. While models of human circadian data have remained phenomenological and low-dimensional to avoid over-fitting the available data. However, these two modeling approaches have not been integrated to allow for the exchange of knowledge between the molecular and human paradigms. In order to incorporate molecular data, models of human circadian dynamics need to derived systematically from more detailed high-dimensional models of the master circadian clock. In this presentation we demonstrate the use of the recently proposed m^2 ansatz for modeling the light-response of human circadian rhythms. Starting from a phase oscillator description of the clock neurons we derive a low-dimensional model for the human circadian clock and fit the parameters to available data. We validate these parameter fits against additional data, and compare the predictions of our models against the predominant human models currently used in the literature.

Kevin Hannay
Schriener University
khannay@schreiner.edu

Victoria Booth
University of Michigan
Depts of Mathematics and Anesthesiology
vbooth@umich.edu

Daniel Forger
University of Michigan
forger@umich.edu

MS75

Modeling Circadian Chronotypes, Sleep, Light, and Schedules

Dynamic mathematical models of the effects of light on the human circadian system and of the effects of circadian rhythms and length of time awake on objective performance and subjective alertness can be used to predict the effects of different sleep/wake and work schedules on objective performance, subjective alertness, and also sleep timing and duration. Individuals with different preferences for early- or late- schedules (chronotypes) may self-select different sleep/wake timing, especially on non-work days, with associated different light exposure patterns that may feedback on their circadian oscillator. We explored the effects of self-selected schedules and lighting on circadian rhythms and sleep timing and duration; the effects of different chronotypes on self-selected lighting conditions; the effects of different rotating shift work schedules on performance, alertness, and sleep timing and duration; and the interactions of these factors. The results may be used to explain physiological observations and to plan individual and group work schedules to improve performance, alertness, and sleep.

Elizabeth B. Klerman
Brigham and Women's Hospital & Harvard Medical School
ebklerman@hms.harvard.edu

MS75

Quantifying the Role of Interindividual Variability in Circadian Data Collection and Analysis

Adult humans have an intrinsic circadian rhythm of ∼24.2 h that is entrained to the 24 h day by external factors (e.g. light, eating, exercise). To assess characteristics of the intrinsic circadian rhythm, participants undergo experimental protocols that impose specific light/dark (L/D) schedules. Ultradian forced desynchrony (FD) protocols are used to assess the intrinsic period of the circadian clock, and phase response curve (PRC) protocols are used to determine the phase dependence of the clock's response to light. Interindividual differences among participants complicate the interpretation of the data collected under these protocols. Our aim was to quantify the contribution of these interindividual differences to the variability observed in estimates of intrinsic periods and PRCs. Using a mathematical model of the human circadian pacemaker we simulated ultradian FD and PRC protocols for participants with heterogeneous circadian characteristics and assessed the dependence of the estimated intrinsic periods and PRCs on interindividual differences. Furthermore, we sought to identify protocol designs that minimize variability associated with interindividual differences and to develop novel methodologies to mine PRC data. This work informs interpretation of experimental characterization of intrinsic periods and PRCs and identifies features of protocol design that lead to robust estimates of phase dependence in the circadian system's response to light.

Nora Stack
Department of Applied Mathematics and Statistics
Colorado School of Mines
nstack@mymail.mines.edu

Cecilia Diniz Behn
Colorado School of Mines
Applied Math & Statistics
cdinizbe@mines.edu

MS75

The Entrain Project: Using Circadian Rhythms to Understand Real-world Sleep

Circadian clocks govern biological functions that repeat with a period of approximately 24 hours, with light as the primary synchronizer of the human circadian clock. Using techniques from optimal control, we can generate schedules of light and dark that shift a model of the circadian clock to a new time zone as quickly as possible. In 2014, we released a mobile application, Entrain, for relaying these optimal schedules to travelers crossing multiple time zones. Since the release, significant updates have been made to the modeling underlying the app. Here I will discuss those updates, which include adapting the optimal schedules to make them robust to real world constraints, incorporating wearable data in the circadian estimates, and an increased focus on detailed sleep modeling. I'll also discuss future directions for the work, and persistent challenges that come with modeling clocks in the wild.

Olivia Walch
Univeristy of Michigan
ojwalch@umich.edu

MS76

Simplicial Closure and Higher-order Link Prediction

Networks are a fundamental abstraction of complex systems throughout the sciences and are typically represented by a graph consisting of nodes and edges. However, many systems have important higher-order interactions, where groups of nodes interact simultaneously, and such higher-order relations are not captured by a graph containing only

pairwise connections. While there are certainly mathematical formalisms for expressing higher-order interactions (such as hypergraphs and simplicial complexes), we lack a systematic way to evaluate higher-order network models. Here, we evaluate higher-order network models through a new prediction problem for the temporal evolution of higher-order structure, which we call "higher-order link prediction". The central idea of this task is to predict which new sets of node will interact in the future given the history of the system. We develop a number of algorithms for higher-order link prediction and use them to predict group interactions in systems from biomedicine, social media, human collaboration, and communications. These algorithms use several large-scale sparse matrix computations that bring a number of scalability challenges.

Austin Benson, Rediet Abebe
Cornell University
arb@cs.cornell.edu, red@cs.cornell.edu

Michael Schaub
Massachusetts Institute of Technology
mschaub@mit.edu

Ali Jadbabaie
MIT
jadbabaie@mit.edu

Jon M. Kleinberg
Cornell University
Dept of Computer Science
kleinber@cs.cornell.edu

MS76

Local Spectral Methods, Variational Perspective, and Local Graph Clustering of Large Graphs

Local spectral methods such as the Approximate Personalized PageRank (APPR) algorithm have proven to be a powerful tool for the analysis of large data graphs. They are defined operationally, and while they come with strong theory, there is no a priori notion of objective function/optimality condition that characterizes the steps taken by them. We discuss a novel variational formulation which makes explicit the actual optimization problem solved by the APPR algorithm. This viewpoint builds a bridge across two seemingly disjoint fields of graph processing and numerical optimization, and it allows one to leverage well-studied, numerically robust, and efficient optimization algorithms for processing today's large graphs. Based on this and related connections, we have developed a code base for local graph clustering of large informatics graphs.

Meng Liu
Purdue University
liu1740@purdue.edu

Kimon Fountoulakis
UC Berkeley
kfount@berkeley.edu

David F. Gleich
Purdue University
dgleich@purdue.edu

Michael Mahoney
UC Berkeley
mmahoney@stat.berkeley.edu

MS76

Dynamic Analysis of Katz Centrality in Graphs

Dynamic graph data can represent the changing relationships in a variety of different fields. A common problem of interest is to identify the most important vertices in a graph. Vertex importance is calculated using centrality metrics, where a centrality metric assigns a value to each vertex in the graph and these values can then be turned into rankings indicating relative importance. To calculate the centrality values of vertices in a dynamic graph, the most naive method is to recompute the scores from scratch every time the graph is changed. However, as the graph grows larger, recomputing from scratch quickly becomes intractable. It is therefore preferable to have algorithms that can update in real-time given updates to the graph without needing to perform a full static recomputation. We focus on Katz Centrality, a linear-algebra based metric that ranks vertices by counting the number of walks of different lengths starting at each vertex and penalizing longer walks with a user-chosen parameter. We present a dynamic algorithm to incrementally update centrality scores in evolving networks. Comparing our algorithm to a pure static recomputation, we see significant performance improvements while maintaining good quality of the centrality scores. We are able to reduce the computation time in the dynamic setting compared to statically recomputing the scores. The quality of our method never deteriorates over time, proving it can be used for a large number of updates.

Eisha Nathan
Georgia Institute of Technology
enathan3@gatech.edu

MS76

Eigenvector-based Centrality Measures for Multiplex and Temporal Networks

Quantifying the importances of nodes in biological, technological and social networks is a central data-science pursuit with numerous applications, and it is important develop improved techniques for more comprehensive data structures such as multilayer network models in which layers encode different edge types, such a network at different instances in time or data obtained from complementary sources. In this work, we present a principled generalization of eigenvector-based centralities – which includes pagerank, hub/authority scores and non-backtracking centrality– for the analysis of multiplex and temporal networks. A key aspect of this approach involves studying joint, marginal and conditional centralities, which are derived from the dominant eigenvector of a supracentrality matrix. We characterize these centralities in the strong and weak-coupling limits using singular perturbation theory and apply this approach to empirical and synthetic datasets.

Dane Taylor
University at Buffalo
danet@buffalo.edu

Mason A. Porter
University of Oxford
Mathematical Institute
mason@math.ucla.edu

Peter J. Mucha
University of North Carolina
mucha@unc.edu

MS77

Discontinuous Galerkin Schemes for Maxwells Equations in Nonlinear Optical Media

The propagation of electromagnetic waves in general media is modeled by the time-dependent Maxwells partial differential equations (PDEs), coupled with constitutive laws that describe the response of the media. In this work, we focus on nonlinear optical media whose response is modeled by a system of first order nonlinear ordinary differential equations (ODEs), which include a single resonance linear Lorentz dispersion, and the nonlinearity comes from the instantaneous electronic Kerr response and the residual Raman molecular vibrational response. To design efficient, accurate, and stable computational methods, we apply high order discontinuous Galerkin discretizations in space to the hybrid PDE-ODE Maxwell system with several choices of numerical fluxes, and the resulting semi-discrete methods are shown to be energy stable. Under some restrictions on the strength of the nonlinearity, error estimates are also established. When we turn to fully discrete methods, the challenge to achieve provable stability lies in the temporal discretizations of the nonlinear terms. To overcome this, novel strategies are proposed to treat the non- linearity in our model within the framework of the second-order leap-frog and implicit trapezoidal time integrators. The performance of the overall algorithms are demonstrated through numerical simulations of kink and antikink waves, and third-harmonic generation in soliton propagation.

Vrushali A. Bokil
Oregon State University
bokilv@math.oregonstate.edu

Yingda Cheng
Department of Mathematics
Michigan State University
ycheng@math.msu.edu

Yan Jiang
Michigan State University
jiangyan@math.msu.edu

Fengyan Li
Rensselaer Polytechnic Institute
lif@rpi.edu

MS77

Recent Advances in Numerical Analysis and Modeling of Invisibility Cloak

In the June 23, 2006's issue of Science magazine, Pendry et al and Leonhardt independently published their papers on electromagnetic cloaking. In Nov.10, 2006's Science magazine, Pendry et al demonstrated the first practical realization of such a cloak with the use of artificially constructed metamaterials. Since then, there is a growing interest in using metamaterials to design invisibility cloaks. In this talk, I will focus on some time-domain cloaking models we studied recently. Well-posedness study and time-domain finite element method for these models will be presented. Finally, I will show some numerical simulations of time-domain cloaking. I will conclude the talk with some open issues.

Jichun Li
Department of Mathematical Sciences
University of Nevada, Las Vegas, NV 89154-4020
jichun.li@unlv.edu

Yunqing Huang
Xiangtan University, China
Department of Mathematics
huangyq@xtu.edu.cn

Wei Yang
Xiangtan University, China
yangweixtu@126.com

MS77

Finite-Difference Time-Domain Method for Electrically and Magnetically Anisotropic Media

In this talk, we report the recent developments on the Anisotropic Finite-Difference Time-Domain (AFDTD) Method for solving Maxwells equation of electrodynamics. To model curved geometry and to eliminate staircasing error, Transformation Optics (TO) can be applied to map non-orthogonal mesh to Cartesian mesh and the resulting anisotropic Maxwells equations are solved using the Anisotropic FDTD algorithm. A temporal subcycling technique based on iteration algorithm is developed to further improve the computational efficiency. Applications to scattering problem and radar imaging will be presented.

Jinjie Liu
Delaware State University
jliu@desu.edu

Moysey Brio
ACMS at Department of Mathematics
The University of Arizona
brio@math.arizona.edu

MS77

Unconditionally Stable FDTD Operator Splitting Methods for the Maxwell-Landau-Lifshitz-Gilbert Equations

We develop and analyze operator splitting methods for the Maxwell-Landau-Lifshitz-Gilbert system in two spatial dimensions: Sequential (SS) and Strang-Marchuck (SM) splitting methods. In one time step, each splitting scheme involves the solution of several, decoupled 1D Maxwell systems. We prove that both splitting schemes are unconditionally stable, preserve the modulus of the discrete magnetization, and satisfy a discrete energy decay property that mimics those of the continuum solution. The SS scheme is first (second) order accurate in time (space), while SM is second order accurate in both time and space. Numerical experiments and examples are given that illustrate and confirm our theoretical results.

Puttha Sakkaplangkul
Michigan State University
sakkapla@math.msu.edu

Vrushali A. Bokil
Oregon State University

bokilv@math.oregonstate.edu

MS78

Estimating the Error in Matrix Function Approximations using the Lanczos Algorithm

The evaluation of matrix functions f(A)v, where A is a large symmetric matrix, f is a function, and v is a vector, may be prohibitively expensive. It is well known that the Lanczos algorithm can be used to determine inexpensive approximations of f(A)v. This talk is concerned with estimating the error in the computed approximations

Nasim Eshghi, Lothar Reichel
Kent State University
Neshghi@kent.edu, reichel@math.kent.edu

MS78

Rapid Modification of Orthogonal Polynomials by Rational Weight Functions

Given a Jacobi matrix for some measure, the modified Jacobi matrix corresponding to the measure obtained through multiplication by a polynomial weight function can be obtained in linear time. The case of a rational weight function, however, is considerably more difficult. The Minimal Solution method of Gautschi, and the Inverse Cholesky method due to Elhay and Kautsky, require substantially more computational effort, and also perform best in complementary scenarios. In this talk, we explore an alternative approach based on the attempted reversal of the procedure for polynomial modification. This reversal introduces unknown parameters, which are obtained through a rapidly convergent iteration. The cases of division by linear and irreducible quadratic factors will be considered.

Amber C. Sumner
William Carey University
asumner@wmcarey.edu

James V. Lambers
University of Southern Mississippi
Department of Mathematics
James.Lambers@usm.edu

MS78

Modified Block Full Orthogonalization Methods

We begin with an overview of a comprehensive block Krylov subspace framework, which encompasses a variety of block methods for solving linear systems and computing matrix functions. Within this framework, we establish the block full orthogonalization method (BFOM). We show that block GMRES (BGMRES) and a newer method, known as block Radau-Lanczos (BRL), are modified versions of BFOM, in a particular sense that draws on low-rank matrices, matrix polynomials, and block Gauss-Radau quadrature. We examine how BFOM, BGMRES, and BRL behave by looking at their associated residual matrix polynomials and convergence plots.

Kathryn Lund, Daniel B. Szyld
Temple University
katlund@temple.edu, szyld@temple.edu

Andreas J. Frommer
Bergische Universitaet Wuppertal
Fachbereich Mathematik und Naturwissenschaften
frommer@math.uni-wuppertal.de

MS79

A Distributed Buchberger's Algorithm

Many open problems in computational algebraic geometry and computational commutative algebra require the calculation of a Grbner basis. Buchberger's algorithm, a generalization of Gaussian elimination, provides a general framework for constructing such a basis from a generating set. The algorithm, however, is sequential and, therefore, not well suited to modern computers, which rely on parallel computing. In this talk, we describe a parallelized form of Buchberger's algorithm and contrast it with the classical algorithm as well as Faugre's F4 algorithm.

Sara Jamshidi
Pennsylvania State University
sxj937@psu.edu

MS79

Generalized Tensor Decomposition for Non-normal Data

Tensor decomposition is a fundamental method in the data sciences for latent factor analysis, multidimensional scaling, clustering, outlier identification, missing data interpolation, etc. It has found application in a broad range of areas including neuroscience, chemometrics, network analysis, signal processing, sensor characterization, and function approximation. The standard formulation of canonical tensor decompositions uses squared error as the goodness-of-fit metric. We propose a generalized canonical polyadic (GCP) tensor decomposition using a generic goodness-of-fit function. This unifies the standard approach with other methods such as Poisson tensor decomposition for count data using Kullback-Leibler (KL) divergence, and enables new formulations such as Bernoulli tensor decomposition for binary data based on estimating odds. Moreover, we have a straightforward approach for handling weights and for inferring missing entries. We show that the gradient has a simple formulation, even in the case of missing data, enabling the use of standard optimization methods for fitting the GCP model. In the case of large-scale and/or sparse data, we recommend using stochastic gradient descent. We demonstrate the flexibility of GCP on several real-world examples, including binary data corresponding to transactions on a social network and nonnegative data corresponding to neural activity in a mouse.

Tamara G. Kolda
Sandia National Laboratories
tgkolda@sandia.gov

David Hong
University of Michigan
dahong@umich.edu

Jed A. Duersch
University of California Berkeley
jaduers@sandia.gov

Cliff Anderson-Bergman
Sandia National Labs

ciande@sandia.gov

MS79

Orthogonalized ALS: A Theoretically Principled Tensor Decomposition Algorithm for Practical Use

The popular Alternating Least Squares (ALS) algorithm for tensor decomposition is efficient and easy to implement, but often converges to poor local optima—particularly when the weights of the factors are non-uniform. We propose a modification of the ALS approach that is as efficient as standard ALS, but provably recovers the true factors with random initialization under standard incoherence assumptions on the factors of the tensor. We demonstrate the significant practical superiority of our approach over traditional ALS for a variety of tasks on synthetic data—including tensor factorization on exact, noisy and over-complete tensors, as well as tensor completion—and for computing word embeddings from a third-order word tri-occurrence tensor.

Vatsal Sharan
Stanford University
vtsl30@gmail.com

MS80

Human-machine Interactions in Dynamic Portfolio Management

We introduce a model of autonomous portfolio management that explicitly accounts for the dynamic nature of the investor's preferences towards risk. We evaluate the usefulness of using an equilibrium human-machine policy over standard practice. Our framework allows to answer questions such as "Why would an investor choose to use the machine', and "What is the added benefit in terms of performance and efficiency?'

Agostino Capponi
Columbia University
agcappo@gmail.com

MS80

DGM: A Deep Learning Algorithm for Solving Partial Differential Equations

High-dimensional PDEs have been a longstanding computational challenge. We propose to solve high-dimensional PDEs by approximating the solution with a deep neural network which is trained to satisfy the differential operator, initial condition, and boundary conditions. Our algorithm is meshfree, which is key since meshes become infeasible in higher dimensions. Instead of forming a mesh, the neural network is trained on batches of randomly sampled time and space points. The algorithm is tested on a class of high-dimensional free boundary PDEs (American options), which we are able to accurately solve in up to 200 dimensions. In addition, we prove a theorem regarding the approximation power of neural networks for quasilinear PDEs.

Justin Sirignano
Imperial College London
University of Illinois at Urbana-Champaign
jasirign@illinois.edu

Konstantinos Spiliopoulos
Boston University
Department of Mathematics and Statistics
kspiliop@bu.edu

MS80

Liquidation Game: Investor vs. Intermediaries

We analyze a dynamic liquidation game where both liquidity demand and supply are endogenous. A large uninformed investor strategically liquidates a position, fully cognizant of the optimal response of competitive market makers. The Stackelberg game solution shows that the investor chooses to sell at higher intensity when he has less time to trade. This enables market makers to predict when execution ends, which helps them provide liquidity and thus reduces the liquidity premium they charge. The model explains several empirical facts: order duration and participation rate correlate negatively, price impact is concave in order size, and price pressure subsides before execution ends.

Agostino Capponi
Columbia University
agcappo@gmail.com

Albert Menkveld
VU University Amsterdam
albertjmenkveld@gmail.com

Hongzhong Zhang
Industrial Engineering and Operations Research
Columbia University
hz2244@columbia.edu

MS81

Consistent Bayesian Inference with Push-Forward Measures: Theoretical Developments

It is common that critical parameters in computational models of physical phenomena have significant uncertainties that must be quantified by solving an inverse problem using observable (noisy) data of model outputs. Statistical Bayesian inference is the most common approach for quantifying uncertainties in parameters using an assumed error model to inform posterior distributions of model inputs and model discrepancies. We have recently developed an alternative Bayesian solution to the stochastic inverse problem based on measure-theoretic principles. We prove that this approach, which we call consistent Bayesian inference, produces a posterior distribution that is consistent in the sense that the push-forward probability density of the posterior through the model will match the density on the observable data. Our approach only requires approximating the push-forward probability density of the prior through the computational model, which is fundamentally a forward propagation of uncertainty. We highlight various theoretical aspects of this approach including existence, uniqueness, and stability of posteriors. We also briefly discuss the theory of convergence when using surrogate models, which requires a generalization of the Arzela-Ascoli theorem and a converse of Scheffe's theorem. Numerical results will highlight various aspects of this approach including a comparison to the statistical Bayesian approach and discussing advantages and challenges.

Troy Butler
University of Colorado Denver
troy.butler@ucdenver.edu

Timothy Wildey

Sandia National Laboratories
tmwilde@sandia.gov

John D. Jakeman
Sandia National Labs
jdjakem@sandia.gov

MS81

Opportunities for Uncertainty Quantification in Shallow Geophysical Flows

Shallow geophysical flows represent a large class of natural hazards that share the common characteristic that the length scale of the flow is much longer than the depth of the flow. These are classically modeled using the shallow water equations however there have been a number of extensions to the shallow water equations that allow for the modeling of much more complex phenomena such as debris flow. One of the key difficulties in modeling shallow flows is that either the initial condition is poorly constrained or parameterizations (physics based or empirical) are poorly known. This difficulty is of course at the heart of uncertainty quantification. In this talk I will introduce the basic framework of shallow flows with some examples from the literature where problems exist along with some lessons from the application of uncertainty quantification to these flows.

Kyle T. Mandli
Columbia University
Applied Physics and Applied Mathematics
kyle.mandli@columbia.edu

MS81

Dimensionality Reduction of Wave-like Phenomena through Monotone Rearrangement

When approximating responses from geophysical flows, linear interpolation or linear approximation with respect to the input parameters often prove ineffective. For example, standard linear regression tools are not effective when used to predict inundation patterns resulting from tsunamigenic earthquakes. This is in general true for responses from hyperbolic partial differential equations (PDEs) where linear, low-dimensional bases are difficult to construct. We propose the use of displacement interpolation where the interpolation is done on the optimal transport map between the functions at nearby parameters, to achieve an effective dimensionality reduction of wave-like phenomena, such as inundations from tsunamis or storm surges.

Donsub Rim
Columbia University
dr2965@columbia.edu

Kyle T. Mandli
Columbia University
Applied Physics and Applied Mathematics
kyle.mandli@columbia.edu

MS81

Consistent Bayesian Inference with Push-forward Measures: Scalable Implementations and Applications

Uncertainty quantification is challenging for large-scale multiphysics applications where the number of uncertain parameters may be large, the number of high-fidelity model evaluations may be limited, and the available data may be corrupted by significant noise. The recently developed consistent Bayesian approach solves a specific stochastic inverse problem based on the measure-theoretic principles. This approach produces a posterior distribution that is consistent in the sense that the push-forward probability density of the posterior through the model will match the distribution on the observable data. While the consistent Bayesian approach is theoretically sound and conceptually simple, it does require approximating the push-forward of the prior through the computational model. While this is certainly nontrivial, we can leverage advanced approaches for forward propagation of uncertainty to reduce the online computational burden. In this presentation, we discuss some of the challenges in forward and inverse propagation of uncertainty in large-scale applications and some of the advanced approaches for forward propagation of uncertainty that can be leveraged within the consistent Bayesian framework to efficiently and accurately solve the stochastic inverse problem. We will also discuss why these challenges are different from those typically encountered in standard Bayesian inference. Numerical results will be presented to demonstrate the consistent Bayesian approach.

Tim Wildey
Optimization and Uncertainty Quantification Dept.
Sandia National Laboratories
tmwilde@sandia.gov

Troy Butler
Dept. of Mathematics and Statistics
University of Colorado - Denver
butler.troy.d@gmail.com

John D. Jakeman
Sandia National Labs
jdjakem@sandia.gov

MS82

Therapy Response Prediction using Deformable Image Registration Based CT Ventilation Imaging

Computed tomography derived functional imaging (CT-FI) is a novel image processing based modality that employs motion recovery algorithms to generate high-resolution pulmonary ventilation and perfusion images from dynamic computed tomography (often referred to as 4DCT). Considering that 4DCT imaging is standard of care for thoracic radiation oncology, CT-FI is ideal for 1) functional avoidance radiotherapy planning and 2) developing predictive radiotherapy response models. The mathematical derivation and clinical validation of CT-FI, as well as its current applications in radiation oncology will be presented.

Edward Castillo
Rice University
ec@rice.edu

MS82

Model Validation for Therapy Response Prediction in Liver

I will present the development of a mathematical model for predicting hepatocellular carcinoma (HCC) lesion response to transcatheter arterial chemoembolization (TACE) therapy. TACE treatment outcome information was obtained from a database of 113 HCC lesions (derived from 105 patients), receiving first line treatment with TACE. An au-

tomated segmentation program was developed using deep learning and random forest classification (RF) methods to parse out each HCC lesion. The Dice similarity coefficient (DSC) was calculated to compare the automated segmentation accuracy versus a manually validated process. The primary clinical endpoint was the time to progression (TTP) based on follow up CT radiological criteria, the median was calculated to be 28 weeks and was used to classify the patients as responders (>28 weeks) or non-responders (<28 weeks). A boruta feature selection algorithm was used for data reduction of quantitative image features considered. Model prediction accuracy was greatest at 66.7% when considering a combination of CLIP score + quantitative imaging features. This study demonstrates the feasibility of predicting treatment response of HCC to TACE therapy using quantitative imaging feature obtained prior to therapy. The approach is likely to provide useful information for assisting in patient selection for TACE therapy.

David Fuentes
University of Texas MD Anderson Cancer Center
dtfuentes@mdanderson.org

MS82

Predicting Distant Failure in Early Stage NSCLC Treated with SBRT

Stereotactic body radiation therapy (SBRT) has become the standard of care for medically inoperable early stage non-small cell lung cancer (NSCLC) with very high (95%) local control rates. However, distant failure after SBRT is common, with a 3-year actuarial rate of about 25%. For patients at high-risk of distant failure, intensified treatment with systemic therapy may lead to a reduced risk of distant relapse and improve overall survival. As this patient population is generally in poor health and the toxicity of systemic therapy could contribute to increased morbidity and mortality, a predictive model with both high sensitivity and specificity is needed to stratify high-risk patients to receive additional systemic therapy. Radiomics, which involve extracting a large number of quantitative imaging features and mining them, has shown promise in predicting treatment response for various diseases. Most of current radiomic models use a single objective (e.g., overall accuracy) during model training. However, for imbalanced data, a single objective based model may result in misleading results. In this talk, we will examine the influence of objective function used in model training to the model performance in validation. We will introduce a multi-objective radiomic predictive model that simultaneously consider both sensitivity and specificity during model training. We will also evaluate input features (e.g., CT, PET and clinical parameters) to the model performance.

Jing Wang
UT Southwestern
jing.wang@utsouthwestern.edu

MS83

Optimizing Time-limited Waveforms for Non-invasive, Focal Neural Stimulation

Clinical brain stimulation is most commonly implemented through invasive paradigms, whereby electrodes are surgically implanted deep within the brain. Such implantation allows for the delivery of current to focal deep brain regions. Recently, a technique has been proposed to enable focal stimulation non-invasively. The strategy works by placing multiple stimulators on the scalp surface, each delivering a periodic waveform of frequency that exceeds the bandwidth of typical neurons. When added together, however, these waveforms produce a periodic interference envelope (or, beats) of frequency low enough to promote neuronal spiking. In this work, we consider the optimization of waveforms for this type of interference-based, non-invasive stimulation. Our goal is to construct time-limited inputs that when added, interfere to produce a slowly varying envelope function maximally contained in a frequency range that activates neurons. The individual waveforms, however, must have minimal energy in such frequencies. We solve this problem by first computing a set of optimal envelope functions, which turn out to be modulated prolate spheroidal wave functions. In the second step, we minimize the difference between the envelope (extracted by Hilbert transform) of the summated individual waveforms and the optimal one, subject to the aforementioned high-frequency constraint. Properties of the resultant family of input waveforms are highlighted for different design specifications.

Sruti Mallik
Washington University in st. Louis
sruti.mallik@wustl.edu

ShiNung Ching
Washington University in St. Louis
shinung@wustl.edu

MS83

Controlling Populations of Neural Oscillators

Some brain disorders are hypothesized to have a dynamical origin; in particular, it has been been hypothesized that some symptoms of Parkinson's disease are due to pathologically synchronized neural activity in the motor control region of the brain. This talk will describe several different approaches for desynchronizing the activity of a group of neurons, including maximizing the Lyapunov exponent associated with their phase dynamics, optimal phase resetting, controlling the phase density, and controlling the population to have clustered dynamics. It is hoped that this work will ultimately lead to improved treatment of Parkinson's disease via targeted electrical stimulation.

Jeff Moehlis
Dept. of Mechanical Engineering
University of California – Santa Barbara
moehlis@engineering.ucsb.edu

Bharat Monga
Mechanical Engineering
UC Santa Barbara
monga@umail.ucsb.edu

Timothy Matchen
Dept. of Mechanical Engineering
University of California – Santa Barbara
tmatchen@umail.ucsb.edu

MS83

Cluster-synchronization in Networks of Oscillators: Analysis and Control of Dynamic Functional Connectivity

Synchronized behaviors among the nodes of a network are ubiquitous in nature and in several man-made systems. While some systems require complete synchroniza-

tion among all the parts to function properly, others rely on cluster or partial synchronization, where subsets of nodes exhibit coherent behaviors that remain independent from the evolution of other nodes in the network. For example, while patterns of partial synchronization have been observed in healthy individuals, complete synchronization in neural systems is often associated with degenerative diseases including Parkinsons and Huntingtons diseases, and epilepsy. In this talk, I present novel network-theoretic methods to predict and control the formation of synchronization patterns within a network of Kuramoto oscillators. I will show that exact patterns of synchronized oscillators are possible if and only if the interconnection structure and the oscillators satisfy certain stringent conditions. On the other hand, approximately synchronized patterns, which often appears in experimental time series, can emerge more easily depending on a graded combination of the interconnection structure and the intrinsic properties of the oscillators. Further, I will present structural control schemes to enforce the emergence of a desired synchronization landscape and, lastly, I will show how the proposed techniques find applicability in the analysis and control of dynamic functional connectivity in neural systems.

Fabio Pasqualetti
Department of Mechanical Engineering
University of California, Riverside, CA
fabiopas@engr.ucr.edu

MS83

A New Perspective on Brain Data: Modeling, Analysis, and Control

Abstract not available at time of publication.

Sergio Pequito
Department of Industrial and Systems Engineering
Rensselaer Polytechnic Institute
goncas@rpi.edu

MS84

An Ultra-weak Discontinuous Galerkin Method for Schrdinger Equation in One Dimension

In this paper, we develop an ultra-weak discontinuous Galerkin (DG) method to solve the one-dimensional nonlinear Schrödinger equation. Stability conditions and error estimates are derived for the scheme with a general class of numerical fluxes. The error estimates are based on detailed analysis of the projection operator associated with each individual flux choice. Depending on the parameters, we find out that in some cases, the projection can be defined element-wise, facilitating analysis. In most cases, the projection is global, and its analysis depends on the resulting 2×2 block-circulant matrix structures. For a large class of parameter choices, optimal *a priori* L^2 error estimates can be obtained. Numerical examples are provided verifying theoretical results.

Anqi Chen
Michigan State University
chenanq3@msu.edu

Fengyan Li
Rensselaer Polytechnic Institute
lif@rpi.edu

Yingda Cheng
Michigan State University
ycheng@msu.edu

MS84

Asymptotic Preserving IMEX-LDG Schemes for Kinetic Transport Equations in a Diffusive Scaling

We develop a family of high order asymptotic preserving (AP) local discontinuous Galerkin (LDG) schemes for kinetic transport equation in a diffusive scaling. Our approach is based on macro-micro decomposition and a reformulation of the decomposed system. With a proper application of globally stiffly accurate high order implicit-explicit Runge-Kutta (IMEX-RK) time integrator and a local discontinuous Galerkin spatial discretization, our scheme is unconditionally stable in the diffusive regime. In hyperbolic regime, our scheme has a time step restriction on the same level as the one for explicit upwind scheme solving transport equation. With energy analysis, we establish uniform stability and rigorously prove the AP property for schemes with first order IMEX-RK time integrator. Our scheme is implicit, but the underlying algebra system is sparse, positive definite and symmetric. The performance of the proposed schemes is demonstrated through a set of numerical examples.

Zhichao Peng
RPI
pengz2@rpi.edu

Fengyan Li
Rensselaer Polytechnic Institute
lif@rpi.edu

Yingda Cheng
Michigan State University
ycheng@msu.edu

Jingmei Qiu
University of Daleware
jingqiu@udel.edu

MS84

A Sparse Grid Discontinuous Galerkin Method for the Vlasov-Maxwell Equations

In this work, we develop a sparse discontinuous Galerkin (DG) scheme for the Vlasov-Maxwell equations in plasma simulations. Traditional DG scheme has too many degrees of freedom for high-dimensional simulations. To break the curse of dimensionality, the sparse grid method we developed is based on multiwavelets on tensorized nested grids and can significantly reduce the numbers of degrees of freedom. The accuracy and robustness of the scheme are validated by several numerical tests for Vlasov-Maxwell equations in up to four dimensions.

Zhanjing Tao
Michigan State University
tzjnchy555@math.msu.edu

Wei Guo
Texas Tech University
weimath.guo@ttu.edu

Yingda Cheng
Department of Mathematics
Michigan State University

ycheng@math.msu.edu

MS84

A Primal-dual Weak Galerkin Finite Element Method for Fokker-Planck Type Equations

The speaker will introduce a primal-dual weak Galerkin (PD-WG) finite element method for a class of second order elliptic equations of Fokker-Planck type. The method is based on a variational form where all the derivatives are applied to the test functions so that no regularity is necessary for the exact solution of the model equation. The numerical scheme is designed by using locally constructed weak second order partial derivatives and the weak gradient commonly used in the weak Galerkin context. Optimal order of convergence is derived for the resulting numerical solutions. Numerical results are reported to demonstrate the performance of the numerical scheme.

Chunmei Wang
Texas State University
c_w280@txstate.edu

Jun ping Wang
N S F
jwang@nsf.gov

MS85

Invariant Conformal Structures in Subdivision Tilings

A Euclidean subdivision rule, or self-similar tiling, is a tiling of the plane with a homothety which maps tiles over tiles. Examples include the square tilings, "chair" tilings, Penrose tilings, pinwheel tilings and many tilings with fractal boundaries. We show in what respects the underlying conformal structure is uniquely defined by the combinatorics of the subdivision.

Richard Kenyon
Brown University
rkenyon@math.brown.edu

MS85

The Space of Planar Polygonal Complexes and Local Isomorphism Classes

In this talk I will describe the metric space **RC** of all rooted planar polygonal complexes and articulate some of its properties. In this space **RC** each rooted expansion complex is represented, and all rooted expansion complexes locally isomorphic to a fixed one forms a local isomorphism class. The salient features of the local isomorphism class will be exposed. I will define various combinatorial properties that an expansion complex may or may not have—properties like repetitiveness, finite local complexity, isoperimetric inequalities—and show how these determine various desirable properties of the topology of the local isomorphism class. Some of this development may be thought of as a combinatorial version of constructions in the space of aperiodic tilings, where not only combinatorics, but also the Euclidean geometry of the tilings comes into play in determining topological properties of spaces of tilings. In the purely combinatorial setting of expansion complexes, we lose the tools of Euclidean geometry, and the spaces are thus less rigid, or more flexible than their tiling counterparts.

Thanittha Kowan
Department of Mathematics
Florida State University
tk14b@my.fsu.edu

MS85

From Traditional Substitution Tilings to Conformal Tiling

Under suitable conditions, a substitution tiling gives rise to a Smale space, from which three equivalence relations can be constructed, namely the stable, unstable, and asymptotic equivalence relations. We denote with S, U, and A their corresponding C*-algebras in the sense of Renault. In this talk I will show that the K-theories of S and U can be computed from the cohomology and homology of a single cochain complex with connecting maps for tilings of the line and of the plane. Then I will explain the complications that arise when leaving the traditional world and entering the world of conformal tilings and combinatorial tilings.

Maria Ramirez-Solano
Syddansk Universitet
maria.r.solano@gmail.com

MS85

Using Combinatorial Extremal Length to Determine Type

We consider different models of combinatorial extremal length to define and determine the discrete type of a planar triangulation. We will see to what extent type is preserved under combinatorial refinement and how these discrete notions pass to the classical setting.

Bill Wood
University of Northern Iowa
bill.wood@uni.edu

MS86

Using Theory to Reduce Uncertainty in High-dimensional Learning

Abstract not available at time of publication.

Symons Christopher
CSMD Science Council
Oak Ridge National Laboratory
symonsct@ornl.gov

MS86

Calibrating Expensive Codes against Expensive Data: New UQ Efforts at the National Ignition Facility

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Jim Gaffney
Lawrence Livermore National Laboratory
gaffney3@llnl.gov

MS86

Adaptive Sparse Quadrature for Multifidelity

Scramjet Flow Simulations

The development of scramjet engines is an important research area for advancing hypersonic and orbital flights. Progress towards optimal engine designs requires accurate and computationally affordable flow simulations, as well as uncertainty quantification (UQ). While traditional UQ techniques can become prohibitive under expensive simulations and high-dimensional parameter spaces, polynomial chaos (PC) surrogate modeling is a useful tool for alleviating some of the computational burden. However, non-intrusive quadrature-based constructions of PC expansions relying on a single high-fidelity model can still be quite expensive. We thus introduce a two-stage numerical procedure for constructing PC surrogates while making use of multiple models of different fidelity. The first stage involves an initial dimension reduction through global sensitivity analysis using compressive sensing. The second stage utilizes adaptive sparse quadrature on a multifidelity expansion to compute PC surrogate coefficients in the reduced parameter space where quadrature methods can be more effective. The overall method is used to produce accurate surrogates and to propagate uncertainty induced by uncertain boundary conditions and turbulence model parameters, for performance quantities of interest from large eddy simulations of supersonic reactive flows inside a scramjet engine.

Xun Huan
Sandia National Laboratories
xhuan@sandia.gov

Gianluca Geraci
Sandia National Laboratories, NM
ggeraci@sandia.gov

Cosmin Safta
Sandia National Laboratories
csafta@sandia.gov

Michael S. Eldred
Sandia National Laboratories
Optimization and Uncertainty Quantification Dept.
mseldre@sandia.gov

Khachik Sargsyan, Zachary Vane
Sandia National Laboratories
ksargsy@sandia.gov, zvane@sandia.gov

Joseph C. Oefelein
Sandia National Laboratories
Combustion Research Facility
oefelei@sandia.gov

Habib N. Najm
Sandia National Laboratories
Livermore, CA, USA
hnnajm@sandia.gov

MS86

A New Model Reduction Technique for Convection-Dominated PDEs with Random Velocity Fields

Abstract not available at time of publication.

Guannan Zhang
Oak Ridge National Laboratory
zhangg@ornl.gov

MS87

Coupled System for Biofilm/ Nutrient Involving a Parabolic Variational Inequality

We consider a coupled system of nonlinear parabolic equations with one of them subject to constraints. The model has an application to biofilm growth in porous media. We present our recent work on the well-posedness and numerical approximation with finite elements.

Azhar Alhammali
Oregon State University
alhammaz@oregonstate.edu

Malgorzata Peszynska
Department of Mathematics
Oregon State University
mpesz@science.oregonstate.edu

MS87

Fluid Flows through Deformable, Porous Media: Analysis and Applications in Biomechanics

Modeling of fluid flows through porous deformable media is relevant for many applications in biology, medicine and bioengineering, including tissue perfusion and fluid flow inside cartilages and bones. These fluid-structure mixtures are described mathematically by nonlinear poro-visco-elastic systems in bounded domains, with mixed boundary conditions, which are the drivers of the systems. I will present a novel hypothesis concerning the causes of damage in biological tissues, and discuss applications of our results to ocular perfusion and its the connections to the development of glaucoma, as well as confined compression tests for biological tissues.

Lorena Bociu
NC State University
Raleigh, NC
lvbociu@ncsu.edu

Giovanna Guidoboni
Indiana University Purdue University Indianapolis
gguidobo@iupui.edu

Riccardo Sacco
Politecnico di Milano
riccardo.sacco@polimi.it

Maurizio Verri
Dipartimento di Matematica
Politecnico di MIlano
maurizio.verri@polimi.it

MS87

A Compactness Lemma for Problems on Moving Domains

This talk addresses an extension of the Aubin-Lions-Simon compactness result to generalized Bochner spaces $L^2(0,T;H(t))$, where $H(t)$ is a family of Hilbert spaces, parameterized by t. A compactness result of this type is needed, e.g., in the study of the existence of weak solutions to a class of nonlinear evolution problems governed by partial differential equations defined on moving domains. We

identify the conditions on the regularity of the domain motion in time, i.e., on the dependence of the function spaces on time, under which our extension of the Aubin-Lions-Simon compactness result holds. Concrete examples of the application of the result will be presented. They include fluid-structure interaction problems for the incompressible, Navier-Stokes equations, coupled, e.g., to the elastodynamics of a Koiter shell.

Suncica Canic
Department of Mathematics
University of Houston
canic@math.uh.edu

Boris Muha
Department of Mathematics, Faculty of Science
University of Zagreb
borism@math.hr

MS87

Displacement Constraints in Biot Systems

A fully-saturated poroelastic medium is deformed by internal pressure-driven fluid flow coupled on its boundary to the stress of the external fluid and the constraints of a bounding surface. The formulation leads to a well-posed unilateral initial-boundary-value problem for the Biot - fluid system and the unknown contact surface of the medium.

Ralph Showalter, Alireza Hosseinkhan
Oregon State University
show@oregonstate.edu, hosseina@math.oregonstate.edu

MS88

Pulse Dynamics in Reaction-diffusion Equations with Strong Spatially Localised Impurities

In this talk we consider the impact of strong, spatially localised, impurities on the existence, stability and bifurcations of localised structures in systems of reaction-diffusion equations. By assuming that the system is linear, but may respond nonlinearly to inhomogeneities and by taking advantage of the multiple-scale nature of the problem we set up a general geometric singular perturbation framework by which the existence and stability of pinned single- and multi-pulse solutions can be determined. Our methods enable us to explicitly control the spectrum associated to (multi-)pulse structures and thus to study – and also 'tune' – their bifurcations.

Arjen Doelman
Mathematisch Instituut
doelman@math.leidenuniv.nl

Peter van Heijster
Mathematical Sciences School
Queensland University of Technology
petrus.vanheijster@qut.edu.au

Jianhe Shen
Fujian Normal University
China
jhshen@fjnu.edu.cn

MS88

Traveling Waves in Dimers

Consider an infinite chain of masses, each connected to its nearest neighbors by a (nonlinear) spring. This is a Fermi-Pasta-Ulam-Tsingou lattice. We prove the existence of traveling waves in the setting where the masses alternate in size. In particular we address the limit where the mass ratio tends to zero. The problem is inherently singular and we find that the traveling waves are not true solitary waves but rather "nanopterons", which is to say, waves which asymptotic at spatial infinity to very small amplitude periodic waves. Moreover, we can only find solutions when the mass ratio lies in a certain open set. The difficulties in the problem all revolve around understanding Jost solutions of a nonlocal Schrödinger operator in its semi-classical limit.

Aaron Hoffman
Franklin W. Olin College of Engineering
aaron.hoffman@olin.edu

J. Douglas Wright
Drexel
jdw66@drexel.edu

MS88

Water Transport in Dryland Ecosystems: Shaping Banded Vegetation Patterns

In dryland ecosystems, water can be thought of as a limiting resource. In an apparent response to water scarcity, two phase mosaics of vegetation and bare ground often develop in these regions. In some locations, the mosaic forms as bands or arcs of vegetations tens of meters wide and up to a kilometer in length, separated by bare ground. Observations suggest that topography may influence the bands. In patterned regions, slopes are about 1%, and cross-slope inhomogeneities can manifest as variation of just 5 meters per kilometer. In PDE models of the system, depending on the structure of the water transport term, inhomogeneity of the surface can lead to bands and band arcing as well as to predictions about when bands, versus bare soil or uniform vegetation, might appear.

Sarah Iams
Harvard University
Cambridge, MA
siams@seas.harvard.edu

Punit Gandhi
Mathematical Biosciences Institute, Ohio State University
gandhi.138@mbi.osu.edu

Mary Silber
University of Chicago
msilber@uchicago.edu

MS88

Synchronization of Coupled Oscillators with Symmetry

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Petko Kitanov
University of Guelph

pkitanov@uoguelph.ca

MS89

Deferred Correction Methods for Time Dependent Differential Equations

A major avenue of research in numerical analysis is creating algorithms to timely obtain high-order approximations to temporal differential equation systems. This is especially relevant for stiff systems, which are known to be difficult for numerical solvers. Deferred correction methods are an alternative numerical scheme for iteratively solving time dependent differential equations while obtaining high-order solutions. This talk will do two things. First, it will present deferred correction methods, focusing on properties of both the converged solution and the convergence procedure itself when applied to non-stiff and stiff systems. Second, this talk will introduce a novel Jacobian-free Newton-Krylov method capable of enhancing the performance of deferred correction methods in stiff systems.

Namdi Brandon
Department of Mathematics,
University of North Carolina, Chapel Hill
namdi.brandon@gmail.com

MS89

Hydrodynamic Synchronization in Models of Internally-driven Cilia

Cilia play an important role in many biological processes, including the transport of mucus in the lungs and the locomotion of micro swimmers. Whether occurring in pairs as on a single algal cell or arrays on epithelial cells, their beat pattern is self-organized. Minimal models of colloidal particles driven by optical traps have been used to shed light on the hydrodynamics of synchronization. Here we extend the minimal model that represents a cilium by a bead to one that represents the cilium as an elastic filament. The beat angle of this filament switches between two traps, driving the motion of the power and recovery strokes. The cilia are coupled to a viscous fluid using a centerline distribution of regularized Stokeslets. We also present a more detailed model of a cilium that tracks individual dynein molecular motors that are themselves driven by a geometric switch. The action of these motors is realized as forces between neighboring microtubules that comprise the cilium. While each model of a single cilium captures a realistic beat form, the emergent behavior of pairs of cilia are surprisingly different.

Lisa J. Fauci
Tulane University
Department of Mathematics
fauci@tulane.edu

MS89

Reconstructing Inclusions from Electrostatic Data

In this talk, we will discuss the use of a Sampling Method to reconstruct impenetrable inclusions from Electrostatic Cauchy data. Sampling Methods allow one to recover unknown obstacles with little to no a prior information. These methods are computationally simple to implement and analytically rigorous. We consider the case of an Impedance (Robin) inclusion where we show that the Dirichlet-to-Neumann mapping can be used to reconstruct such impenetrable sub-regions. We also propose a non-iterative method based on Boundary Integral Equations to reconstruct the impedance parameter from the knowledge of multiple Cauchy pairs. Some numerical reconstructions will be presented in two dimensions. This is joint work with W. Rundell.

Isaac Harris
Texas A&M University
Department of Mathematics
iharris@math.tamu.edu

MS89

Heterogeneities in Oscillatory Media

We look at the role of heterogeneities in shaping patterns in oscillatory media. We concentrate in the case when and impurities act as a pacemakers generating concentric waves that propagate away from the defect, i.e. generating target patterns. In particular, we study the specific example of a two dimensional array of oscillators with nonlocal coupling. The phase dynamics of this system is then described using an integro-differential equation and the heterogeneity is modeled as a localized perturbation. Using this model we then show the existence of target patterns using a combination of matched asymptotics to derive a good ansatz and the implicit function theorem to prove the results.

Gabriela Jaramillo
The University of Arizona
gjaramillo@math.arizona.edu

MS91

Fast Methods for Nonsmooth, Nonconvex Optimization

Abstract not available at time of publication.

Sasha Aravkin
University of Washington
tba@uw.edu

Peng Zhang
University of Washington, USA
tba@uw.edu

MS91

Analysis of Scaled Memoryless BFGS on a Class of Nonsmooth Convex Functions

The limited memory BFGS (L-BFGS) method is widely used for large-scale unconstrained optimization, but its behavior on nonsmooth problems has received little attention. L-BFGS can be used with or without "scaling"; the use of scaling is normally recommended. An important special case of L-BFGS is when just one BFGS update is stored and used at every iteration, sometimes also known as memoryless BFGS. In previous work, we gave an analysis of the gradient method using an Armijo-Wolfe inexact line search on the nonsmooth convex function $f(u,v) = a|u|+v$, where $a \geq 1$, showing that if $a \geq a_G$, where a_G depends only on the Armijo parameter, then, when the method is initiated at any point (u_0, v_0) with $u_0 \neq 0$, the iterates converge to a point $(0, \bar{v})$, although f is unbounded below. In this paper we analyze memoryless BFGS with scaling on a more general function, $f(x) = a|x^{(1)}|+\sum_{i=2}^{n} x^{(i)}$, where $x \in^n$. We show that if $a \geq \sqrt{4(n-1)}$, in the limit the the absolute value of the normalized search direction generated by this method converges to a constant vector, and further-

more for $n = 2$, if $a \geq a_L$, where $a_L < a_G$, the method converges to a non-optimal point. In other words, scaled memoryless BFGS fails under *weaker* conditions than the gradient method.

Azam Asl
Courant Institute of Mathematical Sciences - NYU
aa2821@nyu.edu

Michael L. Overton
Courant Institute of Mathematical Sciences- NYU
mo1@nyu.edu

MS91

Foundations of Gauge and Perspective Duality

Abstract not available at time of publication.

James V. Burke
University of Washington
Department of Mathematics
jvburke@uw.edu

MS91

Optimizing the Polynomial Abscissa Subject to Affine Constraints

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Julia Eaton
University of Washington
Department of Mathematics
jreaton@u.washington.edu

Sara Grundell
New York University
sara.grundel@gmail.com

Mert Gurbuzbalaban
Massachusetts Institute of Technology
mert.gurbuzbalaban@gmail.com

MS92

****LQ: Iterative Methods for Linear Systems with Error Minimization and Estimation Properties**

We discuss recent iterative methods for linear least-squares and least-norm problems, LSLQ and LNLQ, based on the Golub-Kahan process. In exact arithmethic, they are equivalent to SYMMLQ applied to the corresponding normal equations. Recent work gives Euclidean norm error bounds for SYMMLQ iterates on positive definite systems, and hence error bounds for CG. We extend these results to LSLQ and LNLQ and hence to LSQR and CRAIG respectively. We report numerical experiments on linear systems arising in certain penalty methods for optimization. The error bounds lead to bounds on the inexactness of the penalty function gradients, enabling optimization with inexact gradients.

Ron Estrin
ICME
Stanford University
restrin@stanford.edu

Dominique Orban
GERAD and Dept. Mathematics and Industrial Engineering
Ecole Polytechnique de Montreal
dominique.orban@gerad.ca

Michael A. Saunders
Systems Optimization Laboratory, Stanford University
saunders@stanford.edu

MS92

SPMR: A Family of Saddle-point Minimum Residual Solvers

We introduce SPMR, a new family of methods for iteratively solving saddle-point systems using a minimum or quasi-minimum residual approach. No symmetry assumptions are made. The basic mechanism underlying the method is a novel simultaneous bidiagonalization procedure that yields a simplified saddle-point matrix on a projected Krylov-like subspace, and allows for a monotonic short-recurrence iterative scheme. We develop a few variants, demonstrate the advantages of our approach, derive optimality conditions, and discuss connections to existing methods. Numerical experiments illustrate the merits of this new family of methods.

Chen Greif
Department of Computer Science
The University of British Columbia
greif@cs.ubc.ca

Ron Estrin
ICME
Stanford University
restrin@stanford.edu

MS92

Block Preconditioners Informed by Physical Timescales

Multiphysics simulations often involve the complex nonlinear coupling of many physical processes involving a range of different length- and time-scales. Implicit time integration of multiphysics systems allows resolution of slow time-scales of interest with fast time-scales manifesting in stiff modes in the resulting linear systems. An effective linear solver must account for fast time-scales for good performance, and should be resilient to time-scales changing throughout a simulation while remaining cheap to apply. This talk discusses block preconditioning as a general methodology for addressing the linear systems arising in complex multiphysics applications, focusing specifically on how time-scales can inform choices of sub-solver and Schur complement approximations. By considering CFL numbers related to important time-scales, we determine how fast physics are relative to the time-step. This indicates when to use lower fidelity approximations for slower physics and reserve expensive tools for fast subsystems. To illustrate this methodology, we consider a multifluid plasma system. The equations consist of a set of Euler equations for each tracked species coupled to the Maxwell equations. We show how a preconditioner that is adaptive to the many CFLs of this system can perform well in regimes where light waves are resolved but plasma and cyclotron frequencies may be fast, and also in the MHD limit where light waves are stepped over by orders of magnitude.

Edward G. Phillips
Sandia National Laboratories
egphill@sandia.gov

John Shadid
Sandia National Laboratories
Albuquerque, NM
jnshadi@sandia.gov

Eric C. Cyr
Computational Mathematics Department
Sandia National Laboratotories
eccyr@sandia.gov

Sean Miller
Sandia National Laboratories
seamill@sandia.gov

MS92
Preconditioning for Data Assimilation Problems

The 4D-Var method is frequently used for variational data assimilation problems in applications like numerical weather prediction and oceanographic modelling. One key challenge is that the state vectors used in realistic applications contain a very large number of unknowns so it can be impossible to assemble, store or manipulate the matrices involved explicitly. We present a multilevel limited-memory approximation to the inverse Hessian and illustrate its effectiveness as a preconditioner within a Gauss-Newton iteration.

Alison Ramage, Kirsty Brown
University of Strathclyde
A.Ramage@strath.ac.uk, kirsty.l.brown@strath.ac.uk

Igor Gejadze
IRSTEA-Montpellier
igor.gejadze@irstea.fr

MS93
Multiscale Modeling to Capture Near-fields in Plasmonic Structures

Plasmonic structures are commonly made of dielectrics and metals, and at optical frequencies metals exhibit unusual electromagnetic properties like a dielectric permittivity with a negative real part whereas dielectrics have a positive one. This change of sign allows the propagation of electromagnetic surface waves strongly oscillating at the metal-dielectric interface, and hyper-oscillating if the interface presents corners. Standard methods to study surface plasmons excitation do not always take into account the multiple scales inherent in electromagnetic problems which may lead to inaccurate predictions. In this presentation we present some techniques to accurately compute and efficiently take into account the multiple scales of 2D light scattering problems in plasmonic structures with corners.

Camille Carvalho
UC Merced
ccarvalho3@ucmerced.edu

MS93
Numerical Methods for Dispersive Electromagnetics with Distributions of Parameters

Electromagnetic wave propagation in complex dispersive media is governed by the time dependent Maxwell's equations coupled to auxiliary differential equations that describe the evolution of the induced macroscopic polarization. We consider polydispersive materials represented by distributions of dielectric parameters in a polarization model. Polynomial Chaos Expansions are used to approximate the resulting random polarization ODEs with systems of deterministic ODEs, providing a computational framework amenable to standard time and spatial discretization methods. We show how stability and dispersion analyses are affected by the presence of variability.

Nathan L. Gibson
Oregon State University
gibsonn@math.oregonstate.edu

MS93
Coulomb Force Effects in Multimaterial Continuum Plasmas

Magnetohydrodynamics (MHD) models have historically been critical in the computational analysis of high energy density pulsed power physics. Recent evidence in the pulsed power community suggests that low density regions can significantly affect the dynamics of high density target physics. However, many of the assumptions of MHD do not hold in low density regimes and MHD codes must find ways to work around the limitations of the model equations. This opens the door to a hierarchy of increasingly complex extended MHD models. We consider an incremental improvement of MHD, namely no longer neglecting electric displacements. We call the model Full Maxwell Hydrodynamics (FMHD). FMHD offers several advantages over MHD in low density regimes. First characteristic speeds do not become arbitrarily fast in the limit of low densities. Second it allows for the relaxation of charge quasi-neutrality assumed by MHD. This opens the door to Coulomb force effects in addition to Lorentz forces. In this talk we discuss the discretization and verification of FMHD in an indirect Arbitrary Lagrangian Eulerian (ALE) framework. We will discuss the Lagrangian discretization of the FMHD system using compatible finite elements and IMEX time integration and a compatible remap which discretizes the Lie derivative. This guarantees divergence free magnetic fields and preserves weak charge conservation. Code verification and qualitative demonstration will be provided.

Duncan A. McGregor
Sandia National Laboratories
Comptuational Multiphysics
damcgre@sandia.gov

Allen C. Robinson
Sandia National Laboratories
acrobin@sandia.gov

MS93
On Leap-frog-Chebyshev Methods

In this talk we consider wave-type problems of the form

$$u'' = -Lu + g(u),$$

where L is a symmetric, positive definite matrix stemming e.g. from the spatial discretization of the Laplacian, and g a is a "nice" non-linearity, which is expensive to evaluate. The most popular integrator for such problems is the leap-frog scheme

$$u^{n+1} - 2u^n + u^{n-1} = -\tau^2 L u^n + \tau^2 g(u^n),$$

which is stable under the CFL condition $\tau^2\|L\| < 4$. Typically the norm of L is very large which forces the use of a

tiny time step size τ. Thus, the scheme requires numerous evaluations of the non-linearity g. In order to overcome this issue we propose to modify the leap-frog scheme to

$$u^{n+1} - 2u^n + u^{n-1} = -P_p(\tau^2 L)u^n + \tau^2 g(u^n).$$

Here, P_p is a scaled and translated Chebyshev polynomial of degree p and thus we term this scheme leap-frog-Chebyshev method. In our talk we present a quite general stability result for such schemes. Moreover, we show that it is second order convergent similar to the leap-frog scheme but allows a time step size which is (almost) p times larger. Numerical examples show the improved properties and the higher efficiency of this novel scheme.

Andreas Sturm
Institute for Applied and Numerical Mathematics
Karlsruhe Institute of Technology, Karlsruhe, Germany
andreas.sturm@kit.edu

Marlis Hochbruck
Institute for Applied and Numerical Mathematics
Karlsruhe Institute of Technology
marlis.hochbruck@kit.edu

MS94

Krylov Subspace Spectral Methods for Navier-Stokes

Existing time-stepping methods for PDEs such as Navier-Stokes equations are not as efficient or scalable as they need to be for high-resolution simulation due to stiffness. The failure of existing time-stepping methods to adapt to changes in technology presents a dilemma that is becoming even more problematic over time. By rethinking approaches to time-stepping, dramatic gains in efficiency of simulation methods can be achieved. Krylov subspace spectral (KSS) methods have proven to be effective for solving time-dependent, variable-coefficient PDEs. The objective of this research is to continue the development of KSS methods to provide numerical solution methods that are far more efficient and scalable to high resolution for Navier-Stokes equations. So far, KSS methods have been applied only on 1-dimensional, 2-dimensional, and 3-dimensional rectangular domains, but current work is extending them to polar domains using polar coordinates and expansions in Legendre polynomials instead of Fourier series. We will utilize these techniques for compressible Navier-Stokes equations on rectangular domains as well as polar domains.

Brianna D. Bingham
The University of Southern Mississippi
brianna.bingham@usm.edu

James V. Lambers
University of Southern Mississippi
Department of Mathematics
James.Lambers@usm.edu

MS94

Multigrid Inspired Krylov Subspace Spectral Methods for Time-dependent PDEs

Krylov Subspace Spectral (KSS) methods are traditionally used to solve time-dependent, variable-coefficient partial differential equations. Lambers, Cibotarica, and Palchak improved the efficiency of KSS methods by optimizing the computation of high-frequency components. This talk will demonstrate how one can improve the efficiency of KSS methods further by using a multigrid-like approach for low-frequency components. The essential ingredients of multigrid, such as restriction, residual correction, and prolongation, are adapted to the time-dependent case. Numerical experiments demonstrate the effectiveness of this approach.

Haley Dozier
The University of Southern Mississippi
Haley.Dozier@usm.edu

James V. Lambers
University of Southern Mississippi
Department of Mathematics
James.Lambers@usm.edu

MS94

Approximate Analytical Solution for Modeling FRAP using Krylov Subspace Spectral Methods

We show how to solve the first order photobleaching kinetics partial differential equations with prebleach steady state initial conditions using a time-domain method known as a Krylov Subspace Spectral method (KSS method). KSS are explicit methods for solving time-dependent variable-coefficient partial differential equations(PDEs). KSS methods are advantageous compared to other methods because of its high resolution and its superior scalability. We will apply Gaussian Quadrature rules in the spectral domain developed by Golub and Meurant to solve PDEs. We present a simple rough analytical solution, as well as a computational solution that is first-order accurate. We then use this solution to examine short and long time behaviors.

Somayyeh Sheikholeslami
Beaumont Health System
sheikho.physics@gmail.com

James V. Lambers
University of Southern Mississippi
Department of Mathematics
James.Lambers@usm.edu

MS95

The EM Fixed Point Ideal and the Nonnegative Tensor Rank

The EM algorithm is commonly used for the maximum likelihood estimation on the latent class models. An EM fixed point for an observed data point is a parameter vector that stays fixed after one iteration of the EM algorithm. The EM fixed point ideal consists of all the polynomials that vanish on all the EM fixed points. We will explain how to employ the minimal prime decompositions of the EM fixed point ideals to describe the geometry of $2 \times 2 \times 2$ tensors of nonnegative rank 2 and 3, and to study the maximum likelihood estimation on these models. This talk is based on joint work with Elizabeth Allman, Hector Baños Cervantes, Robin Evans, Serkan Hoşten, Daniel Lemke, John Rhodes, and Piotr Zwiernik.

Kaie Kubjas
Aalto University
kaie.kubjas@aalto.fi

MS95

Factoring Graphs, Matrices, and Polynomials as

Tensor Products

The tensor or Kronecker product of two matrices is well-known. The tensor product of two graphs is one whose adjacency matrix is given by the tensor product of the adjacency matrices of the respective graphs. The tensor product of two (univariate) polynomials is one whose companion matrix is given by the tensor product of the companion matrices of the respective polynomials. These tensor products are category-theoretic products in the respective categories. We discuss how graphs, matrices, and polynomials may be factored into irreducible factors with respect to these tensor products. We use the Newton–Girard formulas and homotopy continuation to find the decomposition.

Lek-Heng Lim
University of Chicago
lekheng@galton.uchicago.edu

Jose I. Rodriguez
Department of Statistics
University of Chicago
joisro@uchicago.edu

MS95

On Linear Sections of Secant Varieties and its Applications in Tensors

Secant varieties are closely related to tensors. For example, the affine cone of the rth secant variety of a Segre variety is the set of tensors whose border ranks are $\leq r$. By studying the geometric property of the rth secant variety of a projective variety X, we can obtain interesting information of X-ranks. In this talk, we study linear sections of the rth secant variety of a Segre variety, in particular we focus on the influence of linear sections on the defining equations, and give some applications on the ranks of a general tensor.

Yang Qi, Lek-Heng Lim
University of Chicago
yangqi@galton.uchicago.edu,
lekheng@galton.uchicago.edu

MS95

Discovering Latent Factors using Tensor Decomposition

Latent variable models have a broad set of applications in domains such as social networks, natural language processing, computer vision and computational biology. Training them on a large scale is challenging due to non-convexity of the objective function. We propose a unified framework that exploits tensor algebraic constraints of the (low order) moments of the models. This versatile framework is guaranteed to estimate the correct model consistently and the spectral decomposition (matrix/tensor decomposition) proposed are embarrassingly parallel and has global convergence guarantees using SGD despite the non-convexity of the objective function. Topic Modeling will be discussed extensively, as well as user commonality inference in the large-scale social network using Mixed Membership Stochastic Blockmodel, and convolutional dictionary learning for text paraphrase embedding learning.

Furong Huang, Xuchen You
University of Maryland
furongh@cs.umd.edu, xyou@cs.umd.edu

MS96

Predictable Differences in the Intensity of Influenza Epidemics Among US Cities

The temporal dynamics of influenza epidemics are driven by climatic conditions and by antigenic evolution of the influenza virus. However, important spatial variation remains unexplained. I will discuss recent work that uses fine-grained insurance claims data to study differences in influenza dynamics across 603 US cities. The data reveal predictable spatial variation in epidemic intensity some cities consistently have more intense epidemics than others, including cities within the same climate and antigenic regimes. In particular, we find that incidence in smaller cities is consistently focused on shorter periods of the influenza season, while in larger cities, incidence is consistently more diffuse. We fitted a climate- and antigenically-forced SEIR model to the data in each city, which revealed that base transmission potential (transmission rate that is not modulated by climate) is positively correlated with population size and with spatiotemporal organization in population density. Counterintuitively, elevated base transmission rate produces a milder response to climate forcing in metropolises, by altering the spatiotemporal geometry of herd immunity.

Benjamin Dalziel
Oregon State University
benjamin.dalziel@oregonstate.edu

MS96

Using Ebola Genomes for Spatiotemporal Model Selection in the 2013-2016 Sierra Leone Epidemic

We discuss novel computational methods for tracking disease in human populations using pathogen genomes. Population models of disease are often studied as complex dynamical systems with many nonlinear interactions. A full mechanistic modeling perspective would incorporate all scales of the system from intra-host pathogen behavior to inter-host social network structure. We have instead concentrated on parsimonious models complemented by fast algorithms that can potentially enable meaningful intervention decisions. We built a likelihood-based nested model selection framework for virus mobility informed by linked pathogen genome sequences. Then we demonstrated our methodology on Ebola virus genomes collected from Sierra Leone during the 2013-2016 outbreak in West Africa. We discovered that the outbreak showed a temporal change in model preference coincident with a documented intervention, the Western Area Surge.

Kyle B. Gustafson
US Navy
gustafsonkyle@gmail.com

Joshua L. Proctor
Institute for Disease Modeling
JoshLProctor@gmail.com

MS96

Spatial Model for Risk Prediction and Sub-national Prioritization to aid Poliovirus Eradication in Pakistan

Background: Pakistan is one of only three countries where

poliovirus circulation remains endemic. For the Pakistan Polio Eradication Program, identifying high risk districts is essential to target interventions and allocate limited resources. Methods: Using a hierarchical Bayesian framework we developed a spatial Poisson hurdle model to jointly model the probability of one or more paralytic polio cases, and the number of cases that would be detected in the event of an outbreak. Rates of underimmunization, routine immunization, and population immunity, as well as seasonality and a history of cases were used to project future risk of cases. Results: The expected number of cases in each district in a 6-month period was predicted using indicators from the previous 6-months and the estimated coefficients from the model. The model achieves an average of 90% predictive accuracy as measured by area under the receiver operating characteristic (ROC) curve, for the past 3 years of cases. Conclusions: The risk of poliovirus has decreased dramatically in many of the key reservoir areas in Pakistan. The results of this model have been used to prioritize sub-national areas in Pakistan to receive additional immunization activities, additional monitoring, or other special interventions.

Laina Mercer, Steve Kroiss, Guillaume Chabot-Couture, Hil Lyons
Institute for Disease Modeling
lmercer@idmod.org, skroiss@idmod.org, gcouture@idmod.org, hlyons@idmod.org

MS96

Drivers of Cellular Proliferation in the HIV Latent Reservoir

HIV-1 persists within a slowly declining reservoir of approximately one million latently infected memory CD4+ T cells, despite decades of antiretroviral therapy (ART). When ART is stopped, abundant viral replication and progression to AIDS resume. The reservoir is therefore the major barrier to HIV cure. The HIV replication enzyme is extremely error prone creating new mutations with each cycle of infection. However, deep sampling of the HIV reservoir demonstrates the presence of multiple, large clones with identical genetic sequences. This provides strong evidence that these sequences were generated by the proliferation of memory CD4+ T cells using the DNA polymerase replication enzyme. Memory CD4+ T cells are known to proliferate in a homeostatic fashion to maintain organ size, but also more rapidly in response to foreign pathogens. Here we demonstrate that while HIV sequence clone sizes wax and wane over time, they do so under a characteristic distribution. We devise a stochastic mathematical model to simulate cell proliferation under different levels of competition for antigenic stimuli. We discuss how these mechanisms can shape clone-size distributions and contrast them with empirical distributions observed in the latent reservoir. Our findings have direct implications for HIV cure strategies as homeostatic proliferation and antigen driven proliferation might be targeted by different therapies.

Florencia Tettamanti Boshier
Fred Hutch Cancer Research Center
ftettama@fredhutch.org

Daniel Reeves, Joshua Schiffer
Fred Hutchinson Cancer Research Center
dreeves@fredhutch.org, jschiffe@fredhutch.org

MS97

Dynamic Pricing and Learning for Airline Revenue Management

Many airlines have been actively looking into class-free inventory control approaches, in which the control policy consists of dynamically varying prices over a continuous interval rather than opening and closing fare classes. As evidenced both in literature and in practice, one of the big challenges in this setting is the trade-off between policies that learn the demand parameters quickly and those that maximize expected revenue. Starting in a typical single-leg airline revenue management context, we investigate the applicability of recent advances in the area of optimal control with learning. We consider a parametric demand model and consider reinforcement learning based pricing approach for revenue management in the finite inventory setting. We show the effectiveness of these methods via simulated examples.

Ravi Kumar
PROS
rkumar04@pros.com

MS97

Studying and Predicting Customer Churn at Scale

At Sysco, customer service is part of our daily mission to be our customers most valued and trusted business partner. Delivering exceptional customer service is an integrated dynamic process ranging from supply chain, sales, and logistics business functions. The work presented here is tasked with sales forecasting at a customer level, which is useful for identifying customer churn. We first investigated our customer attribute database to generate clusters of similar customers. Next, we leveraged our historical sales data and item master data using Exploratory Data Analysis methods to describe a customers sensitivity to common customer service issues likes fulfillment, pricing, and delivery delays for relevant items. The combination of customer, item, and sales data were used in a Long Short Term Memory Recurrent Neural Network to predict sales and then churn for every customer. Finally, we discuss the implantation and infrastructure required to deploy the churn model in production at scale for all US customers.

Majid Latif
Sysco
Latif.Majid@corp.sysco.com

MS97

Amazon Locker Capacity Management

Amazon has installed a large number of delivery lockers in the US, UK and EU. During checkout, customers have the option of getting packages delivered to a locker of their choice. Amazon lockers provide unique advantages, such as not having to wait for leasing offices to be open for package pickup, and allowing a customer to pick up at the time and location of their choice. Since the program's launch in 2012, lockers have gained immense popularity due the conveniences they offer. With increased demand for locker deliveries, efficient capacity management becomes critical to offer the best possible customer experience across an increasing number of available lockers. Orders come in the form of different shipping options (3-5 day, two day, next and same day). Typically, orders for faster shipping options are placed later than slower shipping options. To ensure good customer experience for all customers, locker space needs to be reserved for higher value faster shipping option packages. Furthermore, to guarantee timely

delivery, we cannot afford to overbook lockers resulting in a rejected delivery. To accommodate all shipping options and prevent overbooking, Amazon Planning Research and Optimization Science has designed a comprehensive locker capacity management algorithm to determine locker reservation levels for each shipping option and, to determine if lockers have capacity available for a customers order. Our presentation describes this algorithm and its application.

Samyukta Sethuraman
Amazon
samyukts@amazon.com

MS97

Forecasting Airline Purchases under Endogeneity

As Airline Revenue Management shifts from a fare class based framework to class-free, airlines are looking to offer revenue maximal prices from a continuous demand curve rather than the discrete fare ladder used today. Such price recommendations require a forecast of the entire demand curve, and oftentimes the only data available are historical time series of bookings and price. To address endogeneity concerns arising from higher historical prices likely correlated with higher booking conditions, a variety of approaches can be considered such as instrumental variables, deviance from expectations, and inclusion of competitor prices as part of a consumer choice model.

Ross A. Winegar
PROS
rwinegar@pros.com

MS98

Spectral Properties of the Neumann-Poincaré Opertor of a Bowtie Antenna

The Neumann-Poincaré operator is an integral operator that naturally stems from the representation with layer potentials of the solutions to elliptic PDE's with piecewise constant coefficients. Its spectral properties are of interest in particular in the study of plasmonic resonances of metallic particles. We study the Neumann-Poincaré operator of a domain shaped as a bowtie, where the presence of two touching or close to touching corners may enhance the concentration of the fields. When the wings of the bowtie touch, the essential spectrum occupies the whole interval $[-1/2, 1/2]$, while when they are any positive distant apart, the essential spectrum is completely determined by the angles of their corner, and thus is strictly embedded in $[-1/2, 1/2]$. We show how eigenvalues fill the gap between the spectra as the distance between the wings of the bowtie tends to 0.

Eric Bonnetier
Université Grenoble-Alpes
Institut Fourier
eric.bonnetier@univ-grenoble-alpes.fr

Charles Dapogny, Faouzi Triki
Laboratoire Jean Kuntzmann
Université Grenoble Alpes
charles.dapogny@univ-grenoble-alpes.fr,
faouzi.triki@univ-grenoble-alpes.fr

Hai Zhang
Hong Kong University of Science and Technology
haizhang@ust.hk

MS98

Temporal control of graphene plasmons

Electrostatic gating and optical pumping schemes enable efficient time modulation of graphene's free carrier density, or Drude weight. We develop a theory for plasmon propagation in graphene under temporal modulation. When the modulation is on the timescale of the plasmonic period, we show that it is possible to create a backwards-propagating or standing plasmon wave and to amplify plasmons. The theoretical models show very good agreement with direct Maxwell simulations.

Fadil Santosa
School of Mathematics
University of Minnesota
santosa@math.umn.edu

Tony Low
Department of Electrical and Computer Engineering
University of Minnesota
tlow@umn.edu

Josh Wilson
School of Mathematics
University of Minnesota
wil00108@umn.edu

MiSun Min
Argonne National Laboratory
Mathematics and Computer Science Division
mmin@mcs.anl.gov

MS98

On Scattering Resonances of Open Sub-wavelength Metallic Cavities

In the talk we present a recent study aimed at understanding the mechanism of localization and confinement of electromagnetic fields in open sub-wavelength metallic cavities. The local amplification of the fields near the aperture of these cavities can be strikingly high, sometimes up to a factor 10^6. In mathematical terms, the localization and enhancement of the fields is the mark of a resonance phenomenon. We derive a rigorous asymptotic of the scattering resonances associated to the Helmholtz operator when the width of the cavities tends to zero. The approach is based on a generalized Rouché Theorem on operator-valued functions and integral equations techniques.

Faouzi Triki
Laboratoire Jean Kuntzmann
Université Grenoble Alpes
faouzi.triki@univ-grenoble-alpes.fr

Abdelfettah Gtet
Université Grenoble-Alpes
abdelfettah.gtet@univ-grenoble-alpes.fr

Eric Bonnetier
Université Grenoble-Alpes
Institut Fourier

eric.bonnetier@univ-grenoble-alpes.fr

MS98

Field Concentration in Plasmonics and Elasticity

When two inclusions are close to touching, the physical field such as the stress or the electric field may be arbitrarily large in the narrow region between the inclusions. In this talk, we will present the recent developments on the qunatitative understanding of the field concentrations. This problem requires to analyze the Neumann-Poincare operator on two nearly touching domains. We will consider 3D plasmonic spheres systems and 2D particles with general convex shapes. We then show how the plasmonic resonant fields (or the spectral properties of the NP operator) behave when the particles get closer. The plasmonic sensing by strong interaction between the particles will also be discussed. We will also consider the stress concentration, which is a similar problem in the linear elasticity. We find singular functions which characterize the stress blow-up in the narrow region. As an application of our singular functions, we are able to justify the asymptotic formulas for the effective properties of a denesely packed elastic composite.

Sanghyeon Yu
ETH
sanghyeon.yu@sam.math.ethz.ch

Habib Ammari
ETH Zurich
habib.ammari@math.ethz.ch

MS99

Hedging Non-tradable Risks with Transaction Costs and Price Impact

An agent hedges exposure to a non-tradable risk factor U using a correlated traded asset S and accounts for the impact of trades on both factors. We obtain in closed-form the optimal strategy when the agent holds a linear position in U. With non-linear exposure to U, we provide an approximation to the optimal strategy in closed-form, and prove that the value function is correctly approximated when cross-impact and risk-aversion are small. With non-linear exposure, the approximate optimal strategy can be written in terms of the optimal strategy for linear exposure with the size of the position changing dynamically according to the exposure's "Delta" under a particular probability measure.

Ryan Donnelly
Applied Mathematics
University of Washington
rdon@uw.edu

Sebastian Jaimungal
University of Toronto, Canada
sebastian.jaimungal@utoronto.ca

Alvaro Cartea
School of Economics and Math.
University College of London
alvaro.cartea@gmail.com

MS99

A Technical Analysis of Technical Analysis

We study trading strategies based on exponential moving averages (ExpMA), an important indicator in technical analysis. We seek optimal ExpMA strategies when the drift of the underlying is modeled by an Ornstein-Uhlenbeck process or a two-state continuous-time Markov chain. Closed-form solutions are obtained under the logarithm utility maximization and the long-term growth rate maximization.

Matthew Lorig
University of Washington
Applied Mathematics
mattlorig@gmail.com

Zhou Zhou
School of Mathematics and Statistics
zhouzhou@umich.edu
zhouzhou@umich.edu

Bin Zou
Department of Mathematics
University of Connecticut
bin.zou@uconn.edu

MS99

Investor Concentration, Flows, and Cash Holdings: Evidence from Hedge Fund Regulatory Findings

We show that when only a few investors own a substantial portion of a hedge fund's net asset value, the possibility of more volatile flows to a fund increases because investors' exogenous, idiosyncratic liquidity shocks are not diversified away. By using data from hedge fund regulatory lings, we confirm that high investor concentration hedge funds experience more volatile flows. We also find that these hedge funds hold more cash and invest in more liquid assets, which help absorb large and unexpected out flows. To hold more precautionary cash and invest in more liquid assets, the hedge funds would have to pay a liquidity premium. Consistent with this prediction, we find that hedge funds with a high investor concentration generate significantly lower risk-adjusted returns. These results are robust to a variety of controls, including redemption and lock-up periods, investment strategy, and manager ownership. Our data shows that a hedge fund's investor concentration does not affect its flow-performance sensitivity.

Phillip Monin
Office of Financial Research
phillip.monin@ofr.treasury.gov

Mathias Kruttli
Federal Reserve
mathias.s.kruttli@frb.gov

Sumudu Watugala
Cornell University
sumudu@cornell.edu

MS99

Stochastic Modelling of Limit Order Books

We present a new approach associated with stochas-

tic modelling (namely, semi-Markov modelling) of price changes in the evolution of limit order books associated with high-frequency and algorithmic trading. Our approach is justified and illustrated by using real data such as Lobster, Deutsche Boerse Group and Cisco data. Well also talk about the recent stock market crash (Monday, February 5, 2018-another Black Monday?), what was the cause of it and what was driving the big global sell-off.

Anatoliy Swishchuk
University of Calgary
aswish@ucalgary.ca

MS100

Probabilistic Learning for Efficient Optimization under Risk Constraints

In this presentation, we tackle the challenge of mitigating the high cost of accurately estimating the expectations appearing in expressions of the objective and constraint functions. In order to facilitate the optimization task, we introduce two complementary perspectives. First, we consider jointly the decision variables and the quantities of interest (QoI) whose expectations form the constraints and objective functions. The second perspective recognizes that the mode input and outputs, as well as decision variables, are all related by the same physics (or black-box) constraints. The locus of these samples is a manifold. We then rely on diffusion manifold theory concepts to construct an algebraic basis for this manifold, following which a projected Ito equation is constructed that samples on this manifold without any further recourse to the (expensive) function evaluator. This Ito equation is constructed with an invariant measure specified by the distribution of the initial sample, thus controlling the probability measure on the manifold. With the sampling challenge thus addressed, optimization under uncertainty, with various types of probabilistic constraints, can be pursued without sacrificing accuracy or the form of of the constraints (eg replacing a probability requirement by a standard deviation requirement). Demonstrations on a number of mathematical and physics problems will be shown.

Roger Ghanem
University of Southern California
Aerospace and Mechanical Engineering and Civil Engineering
ghanem@usc.edu

Christian Soize
University of Paris-Est
MSME UMR 8208 CNRS
christian.soize@univ-paris-est.fr

MS100

Design Optimization under Uncertainty using Polynomial Chaos Expansion

Recent work by Keshavarzzadeh, Meidani, and Tortorelli, and by Keshavarzzadeh, Fernandez, and Tortorelli, illustrates the computational efficiency of polynomial chaos expansions in representing uncertainty in stochastic topology optimization as compared to Monte Carlo approaches. In this polynomial chaos approach, sparse quadrature methods are used to compute coefficients of a series expansion in uncertainty space. However, in many cases, these same quadrature methods could be used to compute objective functions and/or constraints directly, without passing through a polynomial chaos expansion. We contrast the relative efficiency of these two approaches, tradeoffs, and algorithmic specializations necessary to expose parallelism and improve performance while maintaining numerical stability.

Geoffrey M. Oxberry
Lawrence Livermore National Laboratory
oxberry1@llnl.gov

MS100

Optimization under Uncertainty: Modeling and Algorithms

Standard deviation, mean-squared error, and regression are integral parts of even the most rudimentary data analysis. Decision making based on utility theory and risk, in the Markowitzian sense of mean-plus-standard deviation, is equally widely adopted. In this presentation, we review far-reaching extensions of these concepts that enable alternative approaches to risk mitigation and preference-driven data analysis. We give fundamental connections between regression and decision making, which lead to the construction of measures of residual risk. These measures quantify the improved situation faced by a hedging investor compared to that of a single-asset investor, but the notion reaches further with relations to forecasting, learning, and regression. Relying on convex analysis, we establish properties of broad classes of measures of error, deviation, regret, risk, and residual risk. These measures can play central roles in the development of risk-tuned approximations of random variables, in tracking of statistics, and in estimation of the risk of conditional random variables. We illustrate the framework by develop a risk-based sparsity-inducing approach to surrogate models in high-dimensional dynamical systems as well as by learning of computationally costly simulation output from inexpensive simulations in the context of an ultra-high speed navy vessel.

Johannes O. Royset
Operations Research Department
Naval Postgraduate School
joroyset@nps.edu

MS100

Optimal Allocation of Retirement Portfolios

This presentation develops methodology for optimizing retirement portfolios. The distinct feature of this method is that it uses mortality tables to select the best combination of assets given that a portfolio holder wishes to maximize the terminal wealth. The developed model estimates continuous nonlinear functions that control the re-balancing of the invested amounts at the end of each period. These functions are estimated using kernel methods. The developed model also incorporates CVaR constraints on the amount of available funds that can be withdrawn from a portfolio at a given time.

Stan Uryasev
University of Florida
uryasev@ufl.edu

MS101

Inverse Problem for the Microstructure of a Heterogeneous Material

Microstructural analysis problem is formulated as an inverse multiscale problem in which subscale information

about the micro- or nanostructure of a heterogeneous material is recovered from coarse scale data.

Elena Cherkaev
University of Utah
Department of Mathematics
elena@math.utah.edu

MS101

Multiple Scattering and Cross-sections

In time-harmonic scattering theory, one quantity of interest is the scattering cross-section (SCS): it gives a measure of how much energy is radiated to infinity. For an incident plane wave, it is well known that the SCS can be related to the far-field pattern in the forward direction: this is the famous optical theorem. It turns out that textbook proofs of this theorem are defective: we show how to fix the proof. Then, we discuss the SCS for multiple scattering by a cluster of objects. Recent literature is aimed at decomposing the cluster SCS into contributions from individual scatterers. We show when this can be done, and when it cannot be done.

Paul A. Martin
Department of Applied Mathematics and Statistics
Colorado School of Mines
pamartin@mines.edu

MS101

Traveling Waves in FitzHugh-Nagumo Systems with Rapidly Oscillating Coefficients

This talk is devoted to pulse solutions in FitzHugh–Nagumo systems that are coupled parabolic equations with rapidly periodically oscillating coefficients. In the limit of vanishing periods, there arises a two-scale FitzHugh–Nagumo system, which qualitatively and quantitatively captures the dynamics of the original system. We prove existence and stability of pulses in the limit system and show their proximity on any finite time interval to pulse-like solutions of the original system.

Sina Reichelt
Weierstraß-Institut für Angewandte Analysis und Stochastik
sina.reichelt@wias-berlin.de

Pavel Gurevich
Free University Berlin
gurevich@math.fu-berlin.de

MS101

A Multiscale Approximation of a Cahn-Larch System with Phase Separation on the Microscale

We consider the process of phase separation of a binary system under the influence of mechanical deformation and we derive a mathematical multiscale model, which describes the evolving microstructure taking into account the elastic properties of the involved materials. Motivated by phase-separation processes observed in lipid monolayers in film-balance experiments, the starting point of the model is the Cahn–Hilliard equation coupled with the equations of linear elasticity, the so-called Cahn–Larché system. Owing to the fact that the mechanical deformation takes place on a macrosopic scale whereas the phase separation happens on a microscopic level, a multiscale approach is imperative. We assume the pattern of the evolving microstructure to have an intrinsic length scale associated with it, which, after nondimensionalisation, leads to a scaled model involving a small parameter $\epsilon > 0$, which is suitable for periodic-homogenisation techniques. For the full nonlinear problem the so-called homogenised problem is then obtained by letting ϵ tend to zero using the method of asymptotic expansion. Furthermore, we present a linearised Cahn–Larché system and use the method of two-scale convergence to obtain the associated limit problem, which turns out to have the same structure as in the nonlinear case, in a mathematically rigorous way. Properties of the limit model will be discussed.

Lisa Reischmann
department of mathematics, University of Augsburg
lisa.reischmann@math.uni-augsburg.de

Malte A. Peter
University of Augsburg
malte.peter@math.uni-augsburg.de

MS102

Nonlinear Stability of Source Defects in Oscillatory Media

We prove the nonlinear stability under localized perturbations of spectrally stable time-periodic source defects of reaction-diffusion systems. Consisting of a core that emits periodic wave trains to each side, source defects are important as organizing centers of more complicated flows. Our analysis uses spatial dynamics combined with a phase-tracking technique to obtain detailed pointwise estimates, which allow us to describe in detail the leading order behavior of perturbations as the perturbed solution converges to a space-time translate of the original source pattern.

Margaret Beck
Boston University
mabeck@bu.edu

Toan Nguyen
Pennsylvania State University
nguyen@math.psu.edu

Bjorn Sandstede
Division of Applied Mathematics
Brown University
bjorn_sandstede@brown.edu

Kevin Zumbrun
Indiana University
USA
kzumbrun@indiana.edu

MS102

Defect Formation Dynamics in Curved Elastic Surface Crystals

Topological defects shape the material and transport properties of physical systems. Examples range from vortex lines in quantum superfluids, defect-mediated buckling of graphene, and grain boundaries in ferromagnets and colloidal crystals, to domain structures formed in the early universe. The Kibble-Zurek (KZ) mechanism describes the topological defect formation in continuous non-equilibrium phase transitions with a constant finite quench rate. Universal KZ scaling laws have been verified experimentally

and numerically for second-order transitions in planar Euclidean geometries, but their validity for non-thermal transitions in curved and topologically nontrivial systems still poses open questions. Here, we use recent experimentally confirmed theory to investigate topological defect formation in curved elastic surface crystals formed by stress-quenching a bilayer material. Studying both spherical and toroidal crystals, we find that the defect densities follow KZ-type power laws independent of surface geometry and topology. Moreover, the nucleation sequences agree with recent experimental observations for spherical colloidal crystals. Our results suggest that curved elastic bilayers could provide an experimentally accessible macroscopic system to study universal properties of non-thermal phase transitions in non-planar geometries.

Joern Dunkel, Norbert Stoop
MIT
dunkel@math.mit.edu, stoopn@mit.edu

MS102

Multi-dimensional Patterns from Directional Quenching

In this talk I will discuss some multi-D patterns and their interfaces in an Allen-Cahn equation on the plane. We will focus on a directional quenching regime, considered as an externally triggered change in system parameters, changing the system from monostable to bistable across an interface (known as the quenching front). We are then interested in patterns forming in the bistable region, in particular as the trigger progresses with small speed and increases this bistable region. After introducing the construction of these patterns, I will discuss some selection mechanisms that can be seen in a perturbative setting in a vicinity of a symmetric situation: in this case, the growth of the region of bistability selects the angle of contact between an inner layer and the quenching front. Time allowing, I shall mention more recent work, where inner layers form contact angles "at infinity". Joint work with Arnd Scheel (Univ. of Minnesota, USA).

Rafael Monteiro da Silva
School of Mathematics
University of Minnesota
rmonteir@umn.edu

MS102

Phase Fields, Defects, and Patterns in Finite Domains

The Cross-Newell phase diffusion equation is a reduced equation describing the fully nonlinear (far from threshold) behavior of stripe patterns in terms of a slowly varying phase. This equation is usually obtained by a formal argument as the solvability condition in applying the method of multiple scales to a "microscopic" model for stripe patterns, e.g. the Swift-Hohenberg equation. It is of significant interest to rigorously derive the Cross-Newell equation from an underlying microscopic model. I will discuss some of the impediments as well as some recent algorithmic and analytical advances that allow us to formulate rigorous conjectures in this direction. I will also present some numerical evidence for the validity of these conjectures.

Shankar C. Venkataramani
University of Arizona
Department of Mathematics
shankar@math.arizona.edu

Jinjin Liang
Department of Mathematics
University of Arizona
jliang@math.arizona.edu

Guanying Peng
Department of Mathematics
The University of Arizona
gypeng@math.arizona.edu

Alan Newell
University of Arizona
Department of Mathematics
anewell@math.arizona.edu

MS103

Forecasting the Gulf of Mexico Loop Current: A Machine Learning Approach

The Loop Current is the dominant circulation feature in the Gulf of Mexico (GOM). It is a warm current that enters through the Yucatan Channel, proceeds north and then loops east and then south to exit through the Florida Straits. On a semi-annual cycle the Loop Current will extend into the northern and central Gulf, and shed large anti-cyclonic eddies, referred to as Loop Current Eddies (LCEs). The Loop Current and its associated LCEs can have significant impacts on oil and gas operations in the deep water GOM. When these features overlap a site, they bring strong currents that penetrate deep into the water column, posing significant design and operating hazards. These currents can be a major source of downtime for deep water drilling and installation activities. Ocean physics-based numerical models are used to forecast the evolution of the Loop and LCEs over periods up to two weeks. Ensemble run schemes of these models are used to project the statistics of encounters at time horizons up to eight weeks, with mixed success. For long-lead projects, forecasts in excess of two months would be of great value. This presentation documents an investigation of machine learning approaches to the problem of very long range (2+ month) Loop Current/LCE forecasting. Early results suggest that this approach may result in a forecasting capability skillful enough to provide significant benefits to major capital project and drilling campaign planning in the deep water GOM.

Cole Harris
Chevron
coleharris@chevron.com

James Stear
Chevron Energy Technology Company
james.stear@chevron.com

MS103

Big Data at its Best - Emerging Machine Learning Approaches in Seismic Imaging and Interpretation

Abstract not available at time of publication.

Detlef Hohl
Shell Global Solutions (US)
detlef.hohl@shell.com

MS103

Machine Learning in Nuclear Magnetic Resonance

Applications for Fluid Typing

Different fluids such as bound and free hydrocarbon, bitumen, free and clay bound water have different nuclear magnetic resonance signatures. These signatures are often unknown. Downhole drilling and wireline tools measure different linear combinations of the signatures of these fluids. It is desirable to estimate the individual fluid signatures and their volumes. This problem is posed in a machine learning framework, where unsupervised learning is proposed to derive the fluid signatures and corresponding volumes.

Lalitha Venkataramanan
Schlumberger
lvenkataramanan@slb.com

MS103

On the Promise of Machine Learning for Interpretation and Multi-Physics Integration of Subsurface Measurements

The current advances in machine learning are creating opportunities to revisit and enhance the inversion and interpretation of subsurface measurement data. Traditional deterministic approaches that rely on physical models describing the interaction of the measurement with the rock formation have been successful for a wide array of applications but have shown their limitations when the physics is not well understood, in the context of large parametric uncertainty or data incompleteness, when there is need to render an answer in real time, or when delivered by an operator lacking training in the domain. We are learning how to apply machine learning to help address these challenges. We use supervised learning on labelled data to develop learned models for inference in required timeframes and in ways that augment the capabilities of an operator through automation of some parts of the workflow. We use unsupervised learning to learn the structure in the data and provide plausible interpretation by leveraging domain knowledge and physical models, devising interpretation workflows for problems difficult to tackle deterministically. We also use probabilistic graphical modeling as a framework to integrate multi-modality data to provide answers with more robustness vis--vis uncertainties and non-uniqueness. We will share our experience in solving real applications related to the interpretation of borehole logging data emphasizing acoustic measurements for well integrity.

Smaine Zeroug
Schlumberger-Doll Research Center
zeroug1@slb.com

Sandip Bose
Schlumberger-Doll Research
bose1@slb.com

Peter Tilke
Schlumberger-Doll Research
Cambridge, MA 02139, USA
tilke@slb.com

MS104

Mathematical and Physical Sciences for the Developing World

Developing countries have by definition a systemic difficulty to achieve their goal for large scale, high-quality education. This challenge is even more important for mathematical and physical sciences. In this communication, we will discuss some recent international cooperation and outreach initiatives that have been proposed to strengthen scientific education and research in these countries.

Yanne Chembo
Optics department, FEMTO-ST Institute, Besancon, France
yanne.chembo@femto-st.fr

MS104

Pathways to Inclusion : Mathematics Education at Bryn Mawr College

Bryn Mawr College has produced a number of successful women mathematicians and is also the birthplace of the renowned Enhancing Diversity in Graduate Education program for women in the mathematical sciences. The Mathematics Department is home to roughly ten percent of each graduating class. In reviewing the accomplishments of the mathematics program and its role in educating women, we discuss the successes and challenges of mathematics education and inclusion at multiple levels.

Erica J. Graham
Bryn Mawr College
ejgraham@brynmawr.edu

MS104

Young, Mathematically Gifted, and Black

In February 2017, inspired by the award-winning film Hidden Figures, Erica Graham, Raegan Higgins, Shelby Wilson, and I created the website "Mathematically Gifted and Black" to highlight the contributions and service of Black Mathematicians to academia, education, government, industry, and society. This website hit on the importance of representation, knowing OUR history and knowing OUR impact. In this presentation, I will reflect on the journey of creating such a website and the impact that www.mathematicallygiftedandblack.com has on the academic community.

Candice Price
University of San Diego
cprice@sandiego.edu

MS104

Morehouse College : A Mathematics Program that Makes a Difference

In 2016, the American Mathematical Society named the mathematics program at Morehouse College its "Program That Makes a Difference." In this talk, we will discuss the success of this program and how the Mathematics Department at Morehouse College fosters a welcoming and caring environment that encourages students to meet high expectations. We will touch on how the department reaches students who are often underserved in the area of mathematics and fosters their development to the point of pursuing graduate studies the mathematical sciences. We will present both the historical and recent perspectives of the department that can be replicated at other institutions.

Shelby Wilson
Morehouse College

shelby.wilson@morehouse.edu

MS105

Isogeometric Analysis on 2D and 3D Trimmed Domains

In this work we propose a new methodology for performing isogeometric analysis on volumetric geometries (V-reps), constructed using the IRIT modeler through boolean operations and trimming. It allows to use isogeometric discretizations for 2D and 3D spline trimmed domains in a fully automatic way. When trying to assemble element by element the operators of a discrete variational problem, it is immediately clear that integrals for the Bzier elements affected by boolean operations are not easily computable: only the part of the element inside the computational must be integrated. We present two different strategies for creating suitable quadrature formulas for trimmed elements: a first approach (only for 2D currently) re-parametrizes trimmed elements by splitting them into spline patches (tiles); a second methodology consists in meshing la finite elements every trimmed element, using high-order finite elements (tiles). Thus, suitable quadrature formulas are created by gathering a set of quadratures, one for every tile of the re-parametrization. The method presents optimal approximation properties for any degree when the same polynomial order is used for the tiles description and the discretization of the unknowns. Numerical results that support this theoretical result are presented, as well as examples involving complex geometries that illustrate the potential of the method.

Pablo Antolin
Institute of Mathematics,
École polytechnique fédérale de Lausanne, Switzerland
pablo.antolin@epfl.ch

Annalisa Buffa
Institute of Mathematics
École polytechnique fédérale de Lausanne, Switzerland.
annalisa.buffa@epfl.ch

MS105

3-Variate Spline Representation for IGA and Additive Manufacturing

The challenges of geometric representation for Additive Manufacturing (AM) are many. Material properties can vary through the object, lattice structure and internal voids are used for improving performance. State-of-the-art CAD-tools are not well suited for AM as they are b-rep based: An object is represented by its inner and outer hulls. b-rep representation was developed more than 3 decades ago targeting design for subtractive/abrasive manufacturing. IsoGeometric Analysis (IGA) [Hughes 2005] bridge the gap between CAD and Finite Element Analysis. The shape functions in FEM are replaced by B-splines, allowing higher order continuity between elements and accurate shape representation. However, going from b-rep CAD models to 3-variate B-spline based IGA models is as complex as meshing CAD-models. Thus, research started addressing 3-variate spline based CAD-models that can be used directly in IGA [EC FoF project www.caxman.eu]. Continuously varying properties inside an object can be represented by additional spline functions connected to the geometry through a shared parametrization. For objects to be built from multi materials, is easy to see that such fields can be used for specifying the material mixture imitating RGB in colour representation. However, these fields also have a potential to be used as parameters for procedural generation of lattice structures: Required density; required geometry or property anisotropy, etc.

Tor Dokken
SINTEF ICT, Department of Applied Mathematics
Oslo, Norway
tor.dokken@sintef.no

MS105

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Thomas A. Grandine
Applied Mathematics
The Boeing Company
thomas.a.grandine@boeing.com

MS105

Solving PDEs on Manifolds using Splines

Functions on manifolds can be approximated with optimal accuracy by restricting tensor product splines defined on ambient space to the manifold. The process becomes stable if data of the given function are extended suitably. We review the underlying theory and then develop a framework for approximating solutions of elliptic PDEs on manifolds which is based on similar ideas. In particular, we show how to extend the intrinsic PDE to an equally elliptic PDE on ambient space. Restricting a spline approximation of the latter one to the manifold yields a smooth and accurate solution with relatively few coefficients.

Ulrich Reif
Darmstadt University of Technology, Germany
reif@mathematik.tu-darmstadt.de

MS106

Online Data Analysis and Reduction

A growing disparity between supercomputer computation speeds and I/O rates makes it increasingly infeasible for applications to save all results for offline analysis. Instead, applications must analyze and reduce data online so as to output only those results needed to answer target scientific question(s). This change in focus complicates application and experiment design and introduces algorithmic, implementation, and programming model challenges that are unfamiliar to many scientists and that have major implications for the design of various elements of supercomputer systems. We review these challenges and describe methods and tools that we are developing to enable experimental exploration of algorithmic, software, and system design alternatives.

Ian Foster
Argonne National Laboratory
Data Science and Learning Division
foster@anl.gov

Scott Klasky
Oak Ridge National Laboratory
Oak Ridge, TN
klasky@ornl.gov

Kerstin Kleese Van Dam
Brookhaven National Laboratory

kleese@bnl.gov

Todd Munson
Argonne National Laboratory
Mathematics and Computer Science Division
tmunson@mcs.anl.gov

MS106

Data Compression

In many of today's simulations, over trillions of cells are generated producing over terabytes of scientific data per simulation step. Moving large amounts of data between simulations to disk introduces many I/O and storage bottlenecks. These limitations are contantly making compression techniques a viable choice for data reduction. While lossless techniques are able to compress large simulations with no loss of information, they do not produce a large-enough reduction compared to recent lossy methods. By using the latest multi-resolution lossy compressors, simulations can be reduced significantly while preserving coherent features and statistics required for post-analysis routines. In this work, we examine both lossy and lossless compression methods for data reduction and data analysis.

Jesus Pulido
Los Alamos National Laboratory
pulido@lanl.gov

MS106

Splitting Methods for Reconstructing Jointly Sparse Data

We consider the problem of reconstructing multiple sets of sparse data sharing a common sparsity pattern from limited measurements. To take account of the joint sparsity and promote the coupling of nonvanishing components, we employ a convex relaxation approach with mixed norm penalty $\ell_{2,1}$. This talk discusses recent advances in forward-backward and Douglas-Rachford splitting methods for the solutions of linear inverse problems with such relaxation. New convergence results of the algorithms are proved, and we illustrate the efficiency of the proposed methods in exploiting the joint-sparse structure with several high-dimentional parameterized applications.

Hoang A. Tran
Oak Ridge National Laboratory
Computer Science and Mathematics Division
tranha@ornl.gov

Nick Dexter
University of Tennessee
ndexter@utk.edu

Clayton G. Webster
Oak Ridge National Laboratory
webstercg@ornl.gov

MS106

Hierarchical Splitting and Adaptive Reduction of Data

We develop a technique for multigrid adaptive reduction of data (MGARD). Special attention is given to the case of tensor product grids, where our approach permits the use of nonuniformly spaced grids in each direction, which can prove problematic for many types of data reduction methods. An important feature of our approach is the provision of guaranteed, computable bounds on the loss incurred by the reduction of the data. Many users are leery of lossy algorithms, and will only consider using them provided that numerical bounds on the pointwise difference between the original and the reduced datasets are given. Accordingly, we develop techniques for bounding the loss measured in the $L^\infty(\Omega)$ norm, and we show that these bounds are realistic in the sense that they do not significantly overestimate the actual loss. The resulting loss indicators are used to guide the adaptive reduction of the data so that the reduced dataset meets a user-prescribed tolerance or memory constraint. Illustrative numerical examples, including the reduction of data arising from the simulation of a nonlinear reaction–diffusion problem, a turbulent channel flow, and a climate simulation, are provided.

Mark Ainsworth, Ben Whitney
Division of Applied Mathematics
Brown University
Mark_Ainsworth@brown.edu, ben_whitney@brown.edu

Ozan Tugluk
Department of Astronautical Engineering
University of Turkish Aeronautical Association
ozan_tugluk1@brown.edu

Scott Klasky
Oak Ridge National Laboratory
Oak Ridge, TN
klasky@ornl.gov

MS107

The Numerical Range and Stability of Reduced-order Models

Projection methods provide a convenient way to construct reduced order models for the linear dynamical system $\dot{x}(t) = Ax(t) + bu(t)$. When this projection is performed onto a Krylov subspace, the reduced model matches moments of the original model's transfer function, suggesting an accurate approximation. However, even when the original model is stable, the reduced model need not be. For orthogonal projection methods, where the reduced model has the form V^*AV for V with orthonormal columns, the eigenvalues of V^*AV must fall with the numerical range of A, denoted $W(A)$. How many unstable modes can the reduced model have? To investigate this issue, we apply results from Russell Carden that bound how the eigenvalues of V^*AV can be distributed within $W(A)$. Furthermore, we argue that unstable modes should not simply be suppressed: they hint at interesting transient dynamics in the original model.

Mark Embree
Department of Mathematics
Virginia Tech
embree@vt.edu

MS107

Applications of the Numerical Range and K-spectral Sets

Let A be an n by n matrix. A closed set Ω in the complex plane is said to be a K-spectral set for A if Ω contains the spectrum of A and if, for every rational function f with poles outside of Ω, we have

$$\|f(A)\| \leq K\|f\|_\Omega,$$

where $\|\cdot\|$ on the left is the matrix 2-norm and $\|\cdot\|_\Omega$ on the right is the ∞-norm on Ω. It was recently shown [Crouzeix and Palencia, SIAM J. Matrix Anal. Appl. 38 (2017), pp. 649-655] that the numerical range, $W(A) := \{\langle Aq, q\rangle : \|q\| = 1\}$, is a $(1+\sqrt{2})$-spectral set for A, and Crouzeix has conjectured that it is a 2-spectral set. In many applications, functions of A such as powers A^j, $j = 1, 2, \ldots$, and exponentials e^{tA}, $t > 0$ are of interest. Eigenvalues determine asymptotic behavior as $j \to \infty$ or $t \to \infty$, but eigenvalues alone do not determine the norm behavior of these functions of A for j or t in a given range of interest. Instead, one can say that if a disk of radius r is a K-spectral set for A, then $\|A^j\| \le Kr^j$, and if the half-plane $\{z : \mathrm{Re}(z) \le -r\}$ is a K-spectral set, then $\|e^{tA}\| \le Ke^{-tr}$. In this talk we describe some examples in which estimates of this sort are important and in which too much reliance on eigenvalues can lead to disaster.

Anne Greenbaum
University of Washington
greenbau@uw.edu

MS107

The Generalized Numerical Range of a Set of Matrices

For a given set of $n \times n$ matrices $\mathcal{F}$, we study the union of the C-numerical ranges of the matrices in the set $\mathcal{F}$, denoted by $W_C(\mathcal{F})$. We obtain basic algebraic and topological properties of $W_C(\mathcal{F})$, and show that there are connections between the geometric properties of $W_C(\mathcal{F})$ and the algebraic properties of C and the matrices in $\mathcal{F}$. Furthermore, we consider the starshapedness and convexity of the set $W_C(\mathcal{F})$. In particular, we show that if $\mathcal{F}$ is the convex hull of two matrices such that $W_C(A)$ and $W_C(B)$ are convex, then the set $W_C(\mathcal{F})$ is star-shaped. We also investigate the extensions of the results to the joint C-numerical range of an m-tuple of matrices.

Pan-Shun Lau
Hong Kong Polytechnic University
panlau@connect.hku.hk

Chi-Kwong Li
College of William & Mary
Department of Mathematics
ckli@math.wm.edu

Yiu-Tung Poon
Iowa State University
ytpoon@iastate,edu

Nung-Sing Sze
Hong Kong Polytechnic University
raymond.sze@inet.polyu.edu.hk

MS107

Star-shapedness and Convexity of (p,q)-Matricial Range

Let $A = (A_1, \ldots, A_m)$ be an m-tuple of bounded linear operators acting on a Hilbert space H. Their joint (p,q)-matricial range $\Lambda_{p,q}(A)$ is the collection of $(B_1, \ldots, B_m) \in M_q^m$, where $I_p \otimes B_j$ is a compression of A_j on a pq-dimensional subspace. This definition covers various kinds of generalized numerical ranges for different values of p, q, m. We showed that $\Lambda_{p,q}(A)$ is star-shaped if the dimension of H is sufficiently large. When H is infinite dimensional, we consider the joint essential (p,q)-matricial range

$$\Lambda_{p,q}^{ess}(A) = \bigcap \{cl(\Lambda_{p,q}(A_1+F_1, \ldots, A_m+F_m)) : F_1, \ldots, F_m \text{ are compact}\}.$$

The above set is shown to be non-empty, compact and convex.

Pan-Shun Lau
Hong Kong Polytechnic University
panlau@connect.hku.hk

Chi-Kwong Li
College of William & Mary
Department of Mathematics
ckli@math.wm.edu

Yiu-Tung Poon
Iowa State University
ytpoon@iastate,edu

Raymond N.S. Sze
Hong Kong Polytechnic University
raymond.sze@polyu.edu.hk

MS108

Fluctuating Hydrodynamics Approach Toward Realistic Simulation of Reactive Microfluids

One of the key components needed for realistic simulation of microfluids is the incorporation of thermal fluctuations. Fluctuating hydrodynamics (FHD) provides a framework incorporating thermal fluctuations into hydrodynamic description of a fluid in a manner consistent with statistical physics description. However, systematic development of grid-based numerical schemes solving FHD equations has been put into practice only recently. I present a general framework for developing efficient and accurate FHD simulation methods and address how these methods can be combined with a mesoscopic stochastic reaction model based on the chemical master equation description.

Changho Kim, Andy Nonaka
Lawrence Berkeley National Laboratory
changhokim@lbl.gov, ajnonaka@lbl.gov

John B. Bell
CCSE
Lawrence Berkeley Laboratory
jbbell@lbl.gov

Alejandro Garcia
San Jose State University
algarcia@algarcia.org

Aleksandar Donev
Courant Institute of Mathematical Sciences
New York University
donev@courant.nyu.edu

MS108

A Monolithic Constraint-based Approach for Handling Fluid-solid Interaction Problems via Smoothed Particle Hydrodynamics

We present a meshless discretization of Navier-Stokes equations that draws on a differential-algebraic equation (DAE) formulation and results in a monolithic coupling between

the fluid and solid phases. The methodology is particularly attractive when dealing with Fluid-Solid Interaction (FSI) problems containing a large number of bodies whose dynamics are governed by kinematic constraints, friction, and contact. In this approach, the dynamics of the fluid phase is resolved by Smoothed Particle Hydrodynamics (SPH) and is formulated as a set of DAEs. Particularly, the mass conservation is satisfied by enforcing bilateral constraints on the density of SPH markers at the velocity level. Overall, the solution to the fluid-solid interaction problem is posed as a quadratic optimization problem with conic constraints. We present numerical results demonstrating the scalability and accuracy of the current approach for three test studies. Furthermore, we demonstrate the capability of the current method when dealing with real world problems such as tracked-vehicle fording simulation. In conclusion, the resulting FSI solution is both fast and scalable. It is fast owing to the semi-implicit and monolithic nature of the approach that results in two-orders of magnitude larger time steps compared to an explicit SPH approach. It is scalable owing to its reliance on a matrix-free iterative solver for the solution of the underlying optimization problem.

Milad Rakhsha
University of Wisconsin-Madison
rakhsha@wisc.edu

Arman Pazouki
California State University
apazouk@calstatel

Radu Serban
University of Wisconsin- Madison
serban@wisc.edu

Dan Negrut
University of Wisconsin Madison
Department of Mechanical Engineering
negrut@cae.wisc.edu

MS108

General Finite Difference Flow Simulations on Moving Nonuniform Meshfree Grids

We present incompressible flow simulations on moving meshfree grids. The incompressible Navier-Stokes equations are discretized directly on the meshfree grid using General Finite Differences (GFD). The fully discretized system is solved using an approximate block LU factorization which introduces a splitting error in the momentum and continuity equation. The splitting error is controlled by solving for a pressure increment rather than the pressure itself. The meshfree grid is then evolved with field variables appropriately updated. The spatial distribution of grid nodes is controlled by introducing an explicit shift. The shift relaxes the compressed pseudosprings that connect a particular node to its cloud of neighbors. By varying the spring stiffness, nonuniform moving grids are generated. We present several numerical test cases on moving uniform grids to verify the spatial and temporal convergence order of the scheme and compare results to moving nonuniform grids.

Yaroslav Vasyliv, Alexander Alexeev
George W. Woodruff School of Mechanical Engineering
Georgia Institute of Technology
yvasyliv3@gatech.edu, alexander.alexeev@me.gatech.edu

MS108

Coarse-grained Dynamics of Molecules in Solvent using the Generalized Langevin Equation

In this talk, we present the dynamics of molecules immersed in solvent can be accurately captured in coarse-grained models via the generalized Langevin equation (GLE). GLE can effectively capture the non-Markovian dynamics with the memory effects introduced during coarse-graining. The memory kernel and random noise in GLE were determined from molecular dynamics simulations using Mori-Zwanzig (MZ) formalism. In evaluation of the memory kernel, auxiliary variables were introduced to replace the non-Markovian dynamics with a higher-dimensional Markovian dynamics, which significantly reduced the computational complexity and cost. This approximation converges with more auxiliary variables introduced in the computation. This GLE approach was previously employed for coarse-graining pure systems like polymer melts. In this work, we extend it in the coarse-graining of mixtures of polymers and solvent.

Shu Wang
University of Wisconsin-Madison
swang597@wisc.edu

Zhen Li
Division of Applied Mathematics
Brown University
Zhen_Li@brown.edu

Wenxiao Pan
University of Wisconsin Madison
wpan9@wisc.edu

MS110

Two-Field Finite Element Solvers for Poroelasticity

In this talk, we examine finite element solvers for linear poroelasticity based on the displacement-pressure two-filed model. Specifically we investigate such solvers on quadrilateral meshes, since this type of meshes accommodate complicated geometry and involve less degrees of freedom. We use weak Galerkin elements for Darcy flow discretization and weak Galerkin or Bernardi-Raugel elements for discretization of elasticity. The elements are combined through the implicit Euler temporal discretization. These new solvers do not use any penalty factor and are free of nonphysical pressure oscillations, as demonstrated by numerical simulations.

James Liu
Department of Mathematics
Colorado State University
liu@math.colostate.edu

MS110

Robust Preconditioners for a New Stabilized Discretization of the Poroelastic Equations

In this talk, we present block preconditioners for a stabilized discretization of the poroelastic equations developed recently. The discretization is proved to be well-posed with respect to the physical and discretization parameters, and thus provides a framework to develop preconditioners that are robust with respect to such parameters as well. We

construct these preconditioners for both the stabilized discretization and a perturbation of the stabilized discretization that leads to a sparser overall problem. Numerical tests confirm the robustness of the block preconditioners with respect to the physical and discretization parameters.

James H. Adler
Tufts University
james.adler@tufts.edu

Francisco José Gaspar
University of Zaragoza
fjgaspar@unizar.es

Xiaozhe Hu, Peter Ohm
Tufts University
xiaozhe.hu@tufts.edu, mailto:peter.ohm@tufts.edu

Carmen Rodrigo
University of Zaragoza
carmenr@unizar.es

Ludmil Zikatanov
Pennsylvania State University
ludmil@psu.edu

MS110

A Finite Element Method for Surface Navier-stokes Flows

Multiphase problems that arise in modeling of emulsions, foams, biological membranes and some other areas feature two-phase flows of bulk fluids coupled with a two-dimensional flow of matter along the curved interface between the phases. The later can be modeled by fluid systems posed on manifolds. In this talk we present a trace finite element method for solving the Navier-Stokes equations posed on a smooth closed surface. TraceFEM builds on finite element spaces defined on a fixed, surface-independent background mesh which consists of shape-regular tetrahedra. We use stabilized P_1-P_1 pair for velocity and pressure and P_2 level-set functions for geometric approximation. Tangentiality of the velocity vector field is enforced by a penalty term. Altogether this results in a second order method for solving the surface fluid problem. Theoretical and numerical results are presented to illustrate the properties of the method.

Maxim A. Olshanskii
Department of Mathematics
University of Houston
molshan@math.uh.edu

Vladimir Yushutin
University of Houston
yushutin@math.uh.edu

MS110

An Adaptive Immersed Finite Element Method for Interface Problems

The immersed finite element method (IFEM) is a class of numerical methods for solving interface problems with unfitted meshes. In this talk, we introduce a posteriori error estimation for IFEM. The error estimators can provide accurate assessment of approximation error and can also be used as a guidance for adaptive mesh refinement. Numerical results are provided to demonstrate the features of the adaptive IFEM.

Xu Zhang
Mississippi State University
xuzhang@math.msstate.edu

MS111

Enabling Large-scale Computational Biology Applications by Parallelizing and Scaling Graph and String Algorithms

Methods for processing and analyzing DNA and genome data are built upon combinatorial graph and string algorithms. The advent of high-throughput DNA sequencing is enabling the generation of billions of short reads per experiment. Classical and sequential algorithms can no longer deal with these growing data sizes - which for the last 10 years have greatly out-paced advances in processor speeds. To process and analyze state-of-the-art genomic data sets requires the design of scalable and efficient parallel algorithms and the use of large computing clusters. In this talk, we will discuss (1) distributed-memory algorithms for clustering de-bruijn graphs and its application to solving a grand challenge metagenomic dataset, and (2) distributed-memory algorithms for indexing large genomic datasets via suffix arrays and trees.

Patrick Flick
Georgia Tech
patrick.flick@gatech.edu

MS111

Scalable Parallel Algorithms for Metagenome Assembly

Metagenomics is the leading technology in studying uncultured microbial communities. Effective microbiome analysis depends on metagenome assembly: the transformation of short, randomly sampled sequences called reads, into the contiguous and accurate reconstruction of the underlying microbial genomes. In addition to the challenges due to the high error rates or short read lengths, metagenome assembly is further complicated by repeated sequences across genomes, polymorphisms within species and variable frequency of the genomes within the sample. Modern assemblers have been unable to keep pace with the flood of data, due to the dramatic increases in sequencer capabilities, combined with the computational requirements and the algorithmic complexity of assembling large scale metagenomes. Here we present metaHipMer, the first high-quality, distributed memory metagenome assembler. MetaHipMer is end-to-end parallelized and employs specialized graph algorithms that leverage the one-sided communication capabilities of UPC to facilitate the requisite fine-grained, irregular parallelism. MetaHipMer produces assemblies that are competitive or better in quality than those of other assemblers, but it is orders of magnitude faster since it scales efficiently to distributed memory systems. Most importantly, metaHipMer is not limited by the concurrency and memory of a single node and thus it handles multi-terabyte datasets that other shared-memory tools are incapable of dealing with.

Evangelos Georganas
Intel Labs
evangelos.georganas@intel.com

Steven Hofmeyr, Rob Egan
Lawrence Berkeley National Laboratory

shofmeyr@lbl.gov, rsegan@lbl.gov

Eugene Goltsman
Joint Genome Institute
egoltsman@lbl.gov

Aydin Buluc, Leonid Oliker
Lawrence Berkeley National Laboratory
abuluc@lbl.gov, loliker@lbl.gov

Daniel Rokhsar
Joint Genome Institute
dsrokhsar@lbl.gov

Katherine Yelick
UC Berkeley
Lawrence Berkeley National Laboratory
kayelick@lbl.gov

MS111

Mining for Communities in Large-scale Graphs

Community detection in a graph computes partitions of the vertex set into clusters of vertices that are well connected within their cluster and loosely connected to the rest of the graph. We present our recent work on heuristics for scaling community detection on massive scale graphs on shared-memory and distributed-memory architectures. Our MPI+OpenMP implementation yields about 7x speedup (on 4K processes) for soc-friendster network (1.8B edges) over a state-of-the-art shared memory multicore implementation (on 64 threads), and processed a large graph (uk-2007; 3.3B edges) in 32 seconds on 1K cores (64 nodes) of NERSC Cori system.

Mahantesh Halappanavar
Pacific Northwest National Laboratory
mahantesh.halappanavar@pnnl.gov

Sayan Ghosh
Washington State University
sghosh1@eecs.wsu.edu

Ananth Kalyanaraman
Boeing Centennial Chair, Associate Professor
School of EECS, Washington State University
ananth@eecs.wsu.edu

Arif Khan
Pacific Northwest National Lab
ariful.khan@pnnl.gov

MS111

Rapid Construction and Analysis of Large Graphs for Protein Function Determination Based on Sequence N-grams

Determination of protein function based on sequence is an important area for characterization of novel infectious disease agents and microbiome analysis. Traditional methods for functional determination depend on sequence alignment based on regions of sequence similarity between novel proteins and proteins with known functions. However, convergent evolution results in proteins with similar functions but highly distinct sequences. In fact, a large portion of proteins from novel organisms cannot be mapped to any function. We have developed an approach which makes use of degenerate n-grams from protein sequence to represent that sequence in a high-dimensional space. We first applied this approach to classification of proteins into single specific functional classes using machine learning. We next used a very fast similarity method (the Blazing Signature Filter) to construct graphs from large sequence collections and analyze these large graphs using a rapid community detection algorithm. Communities are assessed for ability to specifically encapsulate known functional groups that may or may not be related by traditional sequence similarity.

Jason McDermott, Mahantesh Halappanavar, Ariful Khan, William Nelson, Samuel Payne, Joshua Adkins
Pacific Northwest National Laboratory
jason.mcdermott@pnnl.gov, mahantesh.halappanavar@pnnl.gov, ariful.khan@pnnl.gov, william.nelson@pnnl.gov, samuel.payne@pnnl.gov, joshua.adkins@pnnl.gov

MS112

Numerical Methods for Wave Scattering from Layered Media

In this talk, several recent developments of Green's function based numerical methods for wave scattering from layered media will be discussed. First, for the periodically patterned layered media, instead of using well-known quasi-periodic Green's function, the free-space Green's function with a periodizing algorithm is applied to overcome slow convergence and Wood anomaly issues of the quasi-periodic Green's function. Then, the large linear system from multi-layered media is efficiently solved using Schur complement and the block tri-diagonal matrix solver. Numerical results for both 2-D and 3-D will be presented. Secondly, for the planar-layered media, layered media Green's function method is used. The layered media Green's function has some advantage as it includes all the jump interface conditions at the cost of computing Greens function itself. Therefore, the free-space numerical methods works for layered media with a minimal modification. The heterogeneous fast multipole method is used to accelerate computation of layered media Green's function in the half-space as a numerical example.

Min Hyung Cho
Department of Mathematical Sciences
University of Massachusetts Lowell
minhyung_cho@uml.edu

MS112

A Fast Algorithms Framework for Dense Rigid Body Suspensions in Stokes Flow

A considerable number of complex natural and engineered systems may be modeled as suspensions of rigid spherical particles in Stokes flow. Often, we are interested in observing the onset of large-scale dynamical behavior, such as collective motion of bacterial suspensions, pattern formation in magneto-rheological fluids and material self-assembly. For this purpose, we must be able to accurately and robustly simulate dense and potentially confined suspensions, and to correctly account for the effects of long-range hydrodynamic forces and short-range contact dynamics. We present a general fast algorithms simulation framework based on second-kind integral equation formulations. This approach involves (I) a fast singular and near-singular integration scheme based on vector spherical harmonic expansions, (II) Fast Multipole Method for smooth integral evaluation in far-field interactions, (III) Preconditioned iterative solve of BIEs and (IV) a distributed memory im-

plementation of contact detection and resolution, modeled as a linear complementarity optimization problem.

Eduardo Corona
Department of Mathematics
University of Michigan
coronae@umich.edu

MS112

Fast Multipole Matrix Factorization

We present a new "FMM factorization" for structured matrices that achieves linear scaling by compressing only far-field interactions in the recursive skeletonization factorization framework. The algorithm is simple and direct, especially when compared with other linear-complexity methods, and produces an efficient representation of the matrix as a multilevel generalized LU decomposition that facilitates fast multiplication, inversion, and determinant computation, among others. From the general framework, it also inherits an explicit tree-local structure that further enables a high degree of parallelism while supporting extremely efficient sublinear-time algorithms for certain sparse or local operations such as local updating. We believe that this factorization provides the proper translation of the FMM to the direct solver context and conclude by offering some directions for future research.

Kenneth L. Ho
TSMC Technology Inc.
klho@alumni.caltech.edu

Victor Minden
Stanford University
vminden@stanford.edu

Anil Damle
Cornell University
Department of Computer Science
asd239@cornell.edu

Lexing Ying
Stanford University
Department of Mathematics
lexing@stanford.edu

MS112

Quantum Mechanical Simulations of Nanoscale Optoelectronic Devices

An efficient quantum mechanical approach is formulated to model electron-photon interactions in nanoscale devices. Based on nonequilibrium Green's function formalism, electron-photon interactions and open boundaries in the nanoscale systems are taken into account in terms of self-energies. By separating different components in the electron-photon interactions, optical absorption and emission processes in the devices can be analyzed, and the method allows studies of different optoelectronic devices. In conjunction with density-functional tight-binding method, photo-induced current and other optical properties of nanoscale devices can be simulated without relying on empirical parameters. To demonstrate our approach, numerical studies of nanoscale solar cells and light-emitting diodes of realistic sizes are presented.

Rulin Wang, Chi-Yung Yam
Beijing Computational Science Research Center
rulin@csrc.ac.cn, yamcy@csrc.ac.cn

MS114

Optimal Convection Cooling Flows in Channels and General 2D Geometries

We generalize a recent method for computing optimal 2D convection cooling flows in a horizontal layer to a wide range of geometries, including those relevant for technological applications. We write the problem in a conformal pair of coordinates which are the pure conduction temperature and its harmonic conjugate. We find optimal flows for cooling a cylinder in an annular domain, a hot plate embedded in a cold surface, and a channel with hot interior and cold exterior. With a kinetic energy constraint, the optimal flows consist of vortices ranging in size from the length of the hot surface to a small cutoff length at the interface of the hot and cold surfaces. With a constraint on input power (fixed rate of viscous dissipation), the optimal flows are dominated by large-scale vortices, with the same size as the flow domain. We also adapt the method to the special case of channel cooling by incorporating inflow and outflow boundary conditions. For an energy budget given by Pe squared, the optimal flows give heat transfer that scales as Pe to the power 2/5, larger than that of Poiseuille flow, which scales as Pe to power 1/3.

Silas Alben
University of Michigan, USA
alben@umich.edu

MS114

Diffusion-limited Mixing by Incompressible Flows

Incompressible flows can be effective mixers by appropriately spreading and shearing a passive tracer. In addition, diffusion is generally perceived as beneficial to mixing due to its ability to homogenize a passive tracer. However we provided numerical evidence that, in the case where advection and diffusion are both actively present, diffusion produces nearly neutral or even negative effects by limiting the mixing effectiveness of incompressible optimal flows. This limitation appears to be due to the presence of a limiting length scale given by a generalized Batchelor length. This length scale limitation in turn affects long-term mixing rates. More specifically, we consider local-in-time flow optimization under energy and enstrophy flow constraints with the objective of maximizing mixing rate performance. We observe that, for enstrophy-bounded optimal flows, the strength of diffusion has a weak impact on the long-term mixing rate performance. For energy-constrained optimal flows, however an increase in the strength of diffusion decreases the mixing rate. We provide analytical lower bounds on mixing rates and length scales achievable under related constraints (pointwise bounded speed and rate-of-strain) by extending the work of Z. Lin et al. (Journal of Fluid Mech., 2011) and C.-C. Poon (Comm. in Partial Differential Equations, 1996).

Christopher J. Miles
University of Michigan
chrisjohnmiles@gmail.com

MS114

Signature of Optimal Solutions in Turbulent Rayleigh-Benard Convection

Optimal solutions in two-dimensional Rayleigh-Bénard

convection (RBC) are obtained for a variety of Rayleigh (Ra) and Prandtl (Pr) numbers. These optimal solutions maximize vertical heat transport as measured by the Nusselt number (Nu) and are solutions to the Boussinesq equations with no-slip boundary conditions. A power law behavior $Nu \sim Ra^{\gamma}$ is observed with $\gamma \approx 0.31$ up to $Ra = 10^9$, which is in agreement with simulations of three-dimensional RBC. Any dependence on Pr for $1 \leq Pr \leq 100$ is very weak, also in agreement with existing data. Additionally, we consider the scaling of the horizontal wavenumber (α) of the optimal solutions with Ra. This analysis indicates the emergence of two structures that maximize Nu for a given Ra leading to two possible candidate structures for optimizing heat transport. Optimal solutions for fluids with $Pr \leq 7$ have a smaller horizontal wavenumber whereas optimal solutions for fluids with $Pr > 7$ have a larger horizontal wavenumber. The role that these optimal solutions play in turbulent RBC is also discussed.

David Sondak
Institute for Applied Computational Science
Harvard University
dsondak@seas.harvard.edu

Parvathi Madthil Kooloth
University of Wisconsin-Madison
Department of Mathematics
madathilkool@wisc.edu

Leslie Smith
Mathematics and Engineering Physics
University of Wisconsin, Madison
lsmith@math.wisc.edu

MS114

Convection in Porous Media with Dispersion

Convection in porous media is a classic example of pattern formation. The mass flux and geometry of the convective pattern are thought to be controlled by the molecular Rayleigh number Ra_m, the ratio of the buoyant driving force over diffusive dissipation. The dimensionless mass flux F is expected to increase with Ra_m linearly and the dimensionless spacing of the convective plumes δ is expected to decrease approximately as $\delta \sim {Ra_m}^{-1/2}$. Here we show that these scaling laws do not hold for experiments of solutal convection in porous media comprised of glass beads. Instead, we observe that the flux levels off as Ra_m becomes large and that the finger spacing increases with Ra_m. The scaling breaks down because it does not consider mechanical dispersion, which is captured by a dispersive Rayleigh number, $Ra_d = H/\alpha_t$, where H is the domain height and α_t is the transverse dispersivity. In experiments, the convective pattern is controlled by Ra_d. Increasing the bead size of the porous medium increases Ra_m but decreases Ra_d and hence coarsens the pattern. In contrast, flux is predominantly controlled by Ra_m. To understand the physics observed in the experiments, we perform direct numerical simulations (DNS) in a 2D Rayleigh-Darcy domain. Our DNS results reveal that the inherent anisotropy of mechanical dispersion leads to an asymmetry in the pattern that eventually limits the flux as the bead size increases.

Baole Wen
University of New Hampshire
wenbaole@gmail.com

Yu Liang
University of Texas at Austin
liangyu@utexas.edu

Marc A. Hesse
University of Texas
Department of Geological Sciences
mhesse@jsg.utexas.edu

David DiCarlo
University of Texas at Austin
dicarlo@mail.utexas.edu

MS115

Numerical Algebraic Geometry and Semidefinite Programming

Traditional interior point methods for solving SDPs track along a central path, which arises as a solution curve to a system of polynomial equations from first-order optimality conditions. By viewing this through the lens of numerical algebraic geometry, this talk will present new approaches for both feasibility testing and solving. Several examples will be presented to demonstrate the effectiveness of the new techniques.

Jonathan Hauenstein
University of Notre Dame
Dept. of App. Comp. Math. & Stats.
hauenstein@nd.edu

Yi Zhang
UNC Greensboro
y_zhang7@uncg.edu

Alan Liddell
Vidrio Technologies
alan.c.liddell@gmail.com

MS115

On Positive Duality Gaps in Semidefinite Programming

We study semidefinite programs (SDPs) whose optimal value differs from the optimal value of their dual. Such SDPs are said to have a *positive duality gap*, they are often seen as extremely pathological and are very difficult to solve. They also serve as models of more general pathological convex programs. We characterize the existence of positive duality gaps in several classes of SDPs. We also present a library of SDPs with positive duality gaps, which cannot be solved by current SDP solvers.

Gabor Pataki
University of North Carolina, at Chapel Hill
gabor@unc.edu

MS115

On the Complexity of Testing Attainment of the Optimal Value in Nonlinear Optimization

We prove that unless P=NP, there exists no polynomial time (or even pseudo-polynomial time) algorithm that can test whether the optimal value of a nonlinear optimization problem where the objective and constraints are given by low-degree polynomials is attained. If the degrees of these polynomials are fixed, our results along with previously-known "Frank-Wolfe type' theorems imply that exactly one of two cases can occur: either the optimal value is attained

on every instance, or it is strongly NP-hard to distinguish attainment from non-attainment. We also show that testing for some well-known sufficient conditions for attainment of the optimal value, such as coercivity of the objective function and closedness and boundedness of the feasible set, is strongly NP-hard. As a byproduct, our proofs imply that testing the Archimedean property of a quadratic module is strongly NP-hard, a property that is of independent interest to the convergence of the Lasserre hierarchy. Finally, we give semidefinite programming (SDP)-based sufficient conditions for attainment of the optimal value, in particular a new characterization of coercive polynomials that lends itself to an SDP hierarchy.

Jeff Zhang, Amir Ali Ahmadi
Princeton University
jeffz@princeton.edu, a_a_a@princeton.edu

MS115

Optimization over the Boolean Hypercube via Sums of Nonnegative Circuit Polynomials

Various key problems from theoretical computer science can be expressed as polynomial optimization problems over the boolean hypercube $\mathcal{H}$. One particularly successful way to prove complexity bounds for these types of problems are based on sums of squares (SOS) as nonnegativity certificates. We initiate optimization over $\mathcal{H}$ via a recent, alternative certificate called sums of nonnegative circuit polynomials (SONC). We show that key results for SOS based certificates remain valid: First, for polynomials, which are nonnegative over the n-variate boolean hypercube $\mathcal{H}$ with constraints of degree at most d there exists a SONC certificate of degree at most $n + d$. Second, if there exists a degree d SONC certificate for nonnegativity of a polynomial over $\mathcal{H}$, then there also exists a short degree d SONC certificate, that includes at most $n^{O(d)}$ nonnegative circuit polynomials.

Timo de Wolff
Texas A&M University
dewolff@math.tu-berlin.de

MS116

Looking to the Future: Ongoing and Potential Activities of the Board on Mathematical Sciences and Analytics

Abstract not available at time of publication.

James Curry
University of Colorado
James.H.Curry@colorado.edu

MS116

Impacts of Recent Board on Mathematical Sciences and Analytics Activities

Abstract not available at time of publication.

Stephen M. Robinson
University of Wisconsin-Madison
smrobins@wisc.edu

MS116

Engaging Mathematical Communities in the Work of the National Academies Board on Mathematical Sciences and Analytics

Abstract not available at time of publication.

Michelle K. Schwalbe
Board on Mathematical Sciecnes and Analytics
National Academies of Sciences, Engineering, and Medicine
mschwalbe@nas.edu

MS117

Optimal Cash-and-Carry Trading and Roll Forward of Futures Contracts

Futures prices are known to deviate from their theoretical no-arbitrage counterparts because of various market frictions and inefficiencies. Indeed, a future price may not even converge to the spot price at maturity, as in the case of the US grain markets for most of 2005-2010 where futures contracts regularly expired up to 35% above the spot price. We propose a new model for future and spot prices that allow for such deviations, and then use it to formulate two common problems faced by futures traders. The first one is Cash-and-Carry trading, where a trader takes opposite positions in a futures contract and its underlying in order to exploit temporary mispricings. The second problem is roll forward of futures contract where a trader maintains investment position beyond the maturity of a futures contract by closing the position and opening a new longer-term contract with the same underlying asset. For each problem, we derive the optimal trading strategy and discuss its properties.

Bahman Angoshtari, Tim Leung
University of Washington
bahmang@uw.edu, timleung@uw.edu

MS117

Optimal Portfolio under Fractional Stochastic Environments

Rough stochastic volatility models have attracted a lot of attention recently, in particular for the linear option pricing problem. In this paper, starting with power utilities, we propose to use a martingale distortion representation of the optimal value function for the nonlinear asset allocation problem in a (non-Markovian) fractional stochastic environment (for all Hurst index $H \in (0, 1)$). We rigorously establish a first order approximation of the optimal value, where the return and volatility of the underlying asset are functions of a stationary slowly varying fractional Ornstein-Uhlenbeck process. We prove that this approximation can be also generated by a fixed zeroth order trading strategy providing an explicit strategy which is asymptotically optimal in all admissible controls. Similar results are also obtained under fast mean-reverting fractional stochastic environment. Furthermore, we extend the discussion to general utility functions, and obtain the asymptotic optimality of this fixed strategy in a specific family of admissible strategies.

Jean-Pierre Fouque, Ruimeng Hu
UC Santa Barbara
fouque@pstat.ucsb.edu, hu@pstat.ucsb.edu

MS117

Optimal Portfolio Choice under Mean Reversion

We study the problem of trading when asset or derivatives

prices individually or collectively exhibit stochastic mean-reverting price behaviors. We present the construction of optimal portfolios in detail, examine their resulting path behaviors using both simulated and real price data, and discuss their financial interpretations.

Tim Leung
University of Washington
timleung@uw.edu

MS117

High-water Mark Fees with Stochastic Benchmark

A hedge fund manager invests the fund in a constant investment opportunity, and receives high-water mark fees when the fund reaches a new maximum relative to a stochastic benchmark, aiming to maximize the expected power utility from fees in the long run. The manager's optimal portfolio includes a Merton component with the risk aversion parameter shifted towards one, and a hedging component against the risk in the benchmark, both of which depend on how the fund investment opportunity compares to the benchmark. A stochastic benchmark in the calculation of high-water mark fees introduces the moral hazard of risky fund investment with hedging motives, but also provides a possibility of regulating the manager's risk taking with a carefully chosen benchmark.

Gu Wang
Worcester Polytechnic Institute
gwang2@wpi.edu

MS118

Unstructured-grid Algorithms for a Many-core HPC Landscape

In the field of computational fluid dynamics (CFD), the Navier-Stokes equations are often solved using an unstructured-grid approach to accommodate geometric complexity. Furthermore, turbulent flows encountered in aerospace applications generally require highly anisotropic meshes, driving the need for implicit solution methodologies to efficiently solve the discrete equations. Time-dependent simulations demand strong scaling and, in the coming exascale era, this will mean an order of magnitude increase in concurrency at the node level, which may overburden domain-decomposed MPI codes. We explore the transition of an unstructured-grid CFD code from a dense MPI model to a shared-memory model suitable for a many-core landscape. Included are node-level studies of computationally intensive CFD kernels on the Intel Xeon Phi Knights Landing, NVIDIA Pascal P100, and NVIDIA Volta V100 architectures. We also perform strong scaling studies on several supercomputing systems of a hybrid MPI+OpenMP model and compare results to our conventional MPI code.

Eric Nielsen
NASA Langley
eric.j.nielsen@nasa.gov

Aaron Walden
NASA
aaron.walden@nasa.gov

M Zubair
Department of Computer Science
Old Dominion University
zubair@cs.odu.edu

Justin Luitjens
NVIDIA Corporation
juitjens@nvidia.com

MS118

Advances in HPC Technology and their Applications to NASA Missions

The evolution of high performance computing (HPC) has seen several paradigm shifts since the introduction of supercomputing in the 1960s. Original supercomputers were driven by the total floating point operations per second (FLOPS) a machine could deliver, and carried a large operational cost. By the 1970s and 1980s, the number of processors in supercomputers increased which shifted HPC from symmetric multiprocessing systems to low cost compute clusters. HPC has since continued to evolve moving from systems with a relatively low number of fast processing cores (multi-core) to ones with a vast number of cores and an increased level of parallelism (many-core). Todays leadership class machines are expected to deliver petascale (10e15 FLOPS) performance, with the potential of reaching exascale (10e18 FLOPS) performance by the 2020s. The objective of this presentation is to generate important discussions necessary for advancing HPC technologies within the applied mathematics community. Key concepts that will be discussed include (but are not limited to) the: differences between parallel architectures and programming models including both shared memory (OpenMP, OpenACC) and distributed memory (MPI); scalability of programming models; different capabilities of compute performance and algorithm acceleration available through CPU, GPU, Xeon Phi, and FPGA hardware interfaces; and applications to NASA Missions.

Michelle Pizzo
NASA Langley Research Center
Comprehensive Digital Transformation Group (HPC)
michelle.e.pizzo@nasa.gov

MS118

Rapid Development and Certification of Novel Materials and Aerospace Structures using HPC

The future of aerospace design will be defined by a technology shift towards a reliance on novel materials and structural concepts. Emerging vehicles will see an incorporation of composite materials and additively manufactured components in addition to, or instead of, traditional aluminum alloys. New structural concepts such as the truss-braced wing, blended wing body, and distributed propulsion will represent a significant departure from the standard tube and wing design that has been in use for decades. It is imperative that this shift away from traditional materials and designs does not adversely impact safely and reliability. In the absence of extensive empirical datasets that exist for traditional designs, certification of novel materials and aerospace structures will require that experimentation be heavily supplemented with modeling and simulation. To this end, this talk describes efforts to develop new algorithms that leverage high performance computing (HPC) to ensure the reliability of materials and structures. With the acknowledgement that rigorously quantifying uncertainty is critical to predicting safety and reliability, the focus will be on scalable algorithms for large-scale probabilistic simulation of structural performance. Results from applications including structural health management and

stochastic topology optimization will be presented.

James Warner
Nasa Langley Research Center
james.e.warner@nasa.gov

MS118

Parallel Trajectory Reconstruction of Spacecraft Entering Mars Atmosphere

Parallelizing software to execute on multi-core central processing units (CPUs) and graphics processing units (GPUs) can prove to be very challenging, and for some fields outside of Computer Science, this transition comes with new issues. For example, memory limitations can require modifications to code not initially developed to run on GPUs. The parallel programming techniques implemented on a Monte Carlo based approached on trajectory reconstruction in this work include OpenMP and OpenACC, which are used to run software on multi-core CPUs and GPUs, respectively. Large matrix operations are the most common use of GPUs, which are not present in this algorithm; however, the natural parallelism of independent trajectories in Monte Carlo simulations is exploited. Benchmarking data are presented comparing execution times of the software for single-thread CPUs, multi-thread CPUs with OpenMP, and multi-thread GPUs using OpenACC. These data were collected using CPU and GPU compute nodes on the Pleiades Supercomputer cluster at the National Aeronautics and Space Administration (NASA) Ames Research Center (ARC) and a local Intel© Xeon Phi™ 7210 CPU node.

Anthony Williams
Department of Mathematics and Statistics
Old Dominion University
robert.a.williams@nasa.gov

Justin Green
NASA Langley Research Center
justin.s.green@nasa.gov

MS119

Particle Filter for Hidden Non-Markov Models

Particle filters estimate the states of a stochastic process from (partial) noisy observations. It quantifies the uncertainty by approximating the posterior distributions of the states. Most particle filters assume that the process is Markov. However, non-Markovian processes appear in many applications with memory effect. We will discuss the extensions and developments of particle filters for non-Markovian models, based on the general framework of sequential Monte-Carlo.

Fei Lu
Johns Hopkins University
feilu@math.jhu.edu

MS119

Localization for MCMC

We investigate how ideas from covariance localization in numerical weather prediction can be used to construct effective Markov chain Monte Carlo (MCMC) methods for sampling high-dimensional distributions with banded covariance and precision matrices. The main idea is to exploit banded structure during problem formulation and numerical solution. In particular, we propose to solve high-dimensional Bayesian inverse problems with nearly banded structure (i.e., small off-diagonal elements) by first replacing the problem with a banded version, and then solving the modified problem using a Metropolis-within-Gibbs sampler that exploits this banded structure. We discuss conditions under which posterior moments of the modified problem are close to those of the original problem. Under the same conditions, the convergence rate of an associated sampler is independent of dimension. We present our ideas in the context of Gaussian problems, where mathematical formulations are precise and for which convergence analysis can be made rigorous.

Matthias Morzfeld
University of Arizona
Department of Mathematics
mmo@math.arizona.edu

Xin T. Tong
National University of Singapore
Department of Mathematics
mattxin@nus.edu.sg

Youssef M. Marzouk
Massachusetts Institute of Technology
ymarz@mit.edu

MS119

Interacting Particle Filters for High-dimensional Nonlinear Filtering Problems

Nonlinear filtering, in particular in a high-dimensional setting, still poses a big challenge. Out of necessity practitioners have developed very robust methodologies, e.g., the popular Ensemble Kalman Filter (EnKF), to tackle nonlinear and high-dimensional filtering problems with the currently available computational resources. Although such techniques perform surprisingly well in a general setting they are often tied to very restricting assumption, e.g., in case of the EnKF Gaussianity assumptions, and from a theoretical point of view the accuracy and the properties of such filters are not well understood yet. Recently conducted studies with respect to this issue will be presented and discussed. The curse of dimensionality often permits the usage of classical particle filters, which do not require restricting assumption, to address nonlinear filtering in high dimensions. Three promising approaches to maneuver around this obstacle are: localization, hybrid formulations and improved proposal densities. Here will discuss the first two advances and present corresponding novel interacting particle filters.

Jana de Wiljes
University of Potsdam
wiljes@uni-potsdam.de

Sebastian Reich
Universität Potsdam
sereich@rz.uni-potsdam.de

Sahani Pathiraja
University of New South Wales
s.pathiraja@student.unsw.edu.au

Wilhelm Stannat
TU Darmstadt

stannat@math.tu-berlin.de

MS119

Kernel Embedding of Maps for Bayesian Inference: The Variational Mapping Particle Filter

Abstract not available at time of publication.

Peter Jan van Leeuwen
University of Reading
p.j.vanleeuwen@reading.ac.uk

MS120

A Many-body Adiabatic Theorem

I will present an adiabatic theorem for the driven dynamics of ground state projections of a smooth family of many-body gapped quantum systems. The diabatic error is uniformly bounded in the volume of the interacting system. This is joint work with Martin Fraas and Wojciech De Roeck.

Sven Bachmann
Dept. of Mathematics
University of British Columbia
sbach@math.ubc.ca

MS120

Hawking Radiation from Rotating Acoustic Black Hole

We are studying the Hawking radiation from rotating acoustic black hole. In the previous works of S. Hawking, T. Jacobson, W. Unruh and others the case of one space variable or a spherically symmetric case was considered. Our emphasis is on the case of two space variables allowing to treat the rotating acoustic black holes with variable radial and angular velocities.

Gregory Eskin
Mathematics
UCLA
eskin@math.ucla.edu

MS120

The Effective Equations for Polaron, Derivation and Dynamics

Polaron theory is a model of an electron in a crystal lattice. It is studied in the framework of nonequilibrium statistic mechanics. There are two different mathematical models: H. Frohlich proposed a quantum model in 1937; L. Landau and S. I. Pekar proposed a system of nonlinear PDEs in 1948. In this talk I will present a proof that these two models are equivalent to certain orders, and the dynamics of the equation. These are joint works with Rupert Frank.

Zhou Gang
Dept of Mathematical Sciences
Binghamton University (SUNY)
gangzhou@binghamton.edu

Rupert Frank
California Institute of technology
rlfrank@caltech.edu

MS120

Quantum Resonances: Unusual Properties

We consider the large L limit of the resonances of $H_L = -d^2/dx^2+V_1(x)+\mu(L)V_2(x-L)$ where the V_j have compact support and either $\mu(L) = 1$ or $\mu(L)$ decreases to zero as $L \to \infty$. Most of the resonances of H_L do not converge to those of $H = -d^2/dx^2 + V_1(x)$ unless $\mu(L)$ decays at least exponentially fast and even then there are some surprises which we will discuss in this talk. This is joint work with Richard Froese.

Ira Herbst
Dept. of Mathematics
University of Virginia
iwh@virginia.edu

MS121

Computation of the Evans Function in Large Systems

We discuss recent results that are aimed at enabling the numerical computation of the Evans function for large systems. These new methods are particularly helpful for computing the Evans function for multi-dimensional planar traveling waves. Specifically, we discuss the use of "pseudo-Lagrangian" coordinates rather than Lagrangian coordinates, the use of the balanced flux formulation of the Evans function, and computing the Evans function via solving a boundary value problem.

Blake Barker, Jeffrey Humpherys
Brigham Young University
blake@math.byu.edu, jeffh@math.byu.edu

Greg Lyng
Department of Mathematics
University of Wyoming
glyng@uwyo.edu

Rose Nguyen
University of Washington
rnguyenx@uw.edu

Bjorn Sandstede
Division of Applied Mathematics
Brown University
bjorn_sandstede@brown.edu

Nathaniel Ventura
Binghampton University
nventur1@binghamton.edu

Colin Wahl
University of California, Berkeley
colin_wahl@berkeley.edu

Kevin Zumbrun
Indiana University
USA
kzumbrun@indiana.edu

MS121

Nodal Deficiency, Spectral Flow, and the Dirichlet-

to-Neumann Map

Courant's nodal domain theorem provides a natural generalization of Sturm–Liouville theory to higher dimensions; however, the result is in general not sharp. It was recently shown that the nodal deficiency of an eigenfunction is encoded in the spectrum of the Dirichlet-to-Neumann operators for the eigenfunction's positive and negative nodal domains. While originally derived using symplectic methods, this result can also be understood through the spectral flow for a family of boundary conditions imposed on the nodal set. In this talk I will describe this flow for a Schrödinger operator with separable potential on a rectangular domain, and describe a mechanism by which lower energy eigenfunctions do or do not contribute to the nodal deficiency. Operators on non-rectangular domains and quantum graphs will also be considered. This talk represents joint work with Gregory Berkolaiko (Texas A&M) and Jeremy Marzuola (UNC Chapel Hill).

Graham Cox
Memorial University of Newfoundland
Department of Mathematics and Statistics
gcox@mun.ca

MS121

Pattern Formation in the Wake of Growth Mechanisms

Externally mediated, or triggered, spatial patterns have become a topic of recent interest in many fields, such as directional quenching in alloy melts, growing interfaces in biological systems, and traveling reaction fronts. Mathematically, they can be encoded in a step-like parameter dependence that allows patterns in a half plane, and suppresses them in the complement, while the boundary of the pattern-forming region propagates with fixed normal velocity. In this talk, I will show how techniques from dynamical systems, functional analysis, and numerical continuation, can be used to study the effect of these traveling in-homogeneities on patterns left in the wake; finding for example how the speed of the parameter interface affects orientation and deformation of striped patterns. I will explain this approach in the context of the Swift-Hohenberg PDE, a prototypical model for many pattern forming systems, posed in one and two spatial dimensions. I will also discuss recent work studying the stability of these structures and their dynamics via a modulational approach.

Ryan Goh
Boston University
Dept. of Mathematics and Statistics
rgoh@bu.edu

Arnd Scheel
University of Minnesota - Twin Cities
scheel

MS121

Spectral Stability of Roll Waves in Inclined Shallow Water Flow

We carry out a systematic analytical and numerical study of spectral stability of discontinuous roll wave solutions of the inviscid Saint Venant equations, based on a periodic Evans-Lopatinski determinant analogous to the periodic Evans function of Gardner in the (smooth) viscous case, obtaining a complete spectral stability diagram useful in hydraulic engineering and related applications. In particular, we obtain an explicit low-frequency stability boundary, which, moreover, matches closely with its (numerically-determined) counterpart in the viscous case. This is seen to be related to but not implied by the associated formal first-order Whitham modulation equations.

Mat Johnson
University of Kansas
matjohn@math.ku.edu

Pascal Noble
University of Toulouse
pascal.noble@math.univ-toulouse.fr

Miguel Rodrigues
Université de Rennes 1
luis-miguel.rodrigues@univ-rennes1.fr

Zhao Yang
Indiana University Bloomington
yangzha@indiana.edu

Kevin Kevin Zumbrun
Indiana University
USA
kzumbrun@indiana.edu

MS122

Comparisons between Experimental Measurements and Predictions from Bidirectional Whitham Equations

In 1978, Hammack & Segur performed a series of tightly-controlled laboratory water-wave experiments. The experiments were conducted in a long, narrow tank with relatively shallow undisturbed water and a wave maker at one end. Among many other things, they showed that analytic and asymptotic results obtained from the KdV equation compared favorably with measurements from the experiments. In 2016, Trillo *et al.* conducted new experiments and demonstrated that the Whitham equation models those experiments more accurately than does the KdV equation. In this talk, we will compare measurements from

the Hammack & Segur experiments with numerical simulations of the St. Venant, KdV, Serre, and Whitham equations. We will focus on various forms of the Whitham equation including the Whitham equation with surface tension and three different bidirectional Whitham equation.

John Carter
Seattle University
Mathematics Department
carterj1@seattleu.edu

MS122

Stability of Long Water Waves

Surface water waves and their stability have been the topic of investigation for well over 200 yrs. I will provide a partial overview of stability results for long waves, and I will discuss how they related to the stability results in the context of the asymptotic models that are supposed to mimic them.

Bernard Deconinck
University of Washington

deconinc@uw.edu

MS122

On Shoaling of Solitary Waves

One of the classic analytical predictions of shoaling wave amplification is Green's law – the wave amplitude grows proportional to $h^{-\frac{1}{4}}$ where h is the local water depth. Green's law is valid for linear shallow-water waves unidirectionally propagating in a gradually varying water depth. On the other hand, conservation of mechanical energy shows that the shoaling wave amplitude of a solitary wave grows like $a \propto h^{-1}$, if the waveform maintains its solitary wave identity, i.e. the adiabatic shoaling process. None the less, some recent laboratory measurements (as well as the recent tsunami measurements in the ocean) indicate that wave growth during shoaling is slower than what is predicted by Green's law. We hypothesize that the discrepancy in the analytical predictions must be attributed to the factors overlooked in the theories. Obvious missing factors in Green's law are the nonlinearity and frequency-dispersion effects as well as wave reflection from the beach, whereas the adiabatic shoaling process does not recognize the transformation of the waveform on a beach of finite slope and length. Here we first examine this problem analytically based on the variable-coefficient perturbed KdV (vKdV) equation. Then, we implement a fifth-order pseudo-spectral numerical model for the full-water-wave Euler theory adapted to a varying bottom bathymetry. The numerical results are compared with laboratory experiments.

Jeff Knowles, Harry Yeh
Oregon State University
knowleje@oregonstate.edu, harry@oregonstate.edu

MS122

General Overview of Geophysical Flows and Extreme Hazards

Predicting and simulating natural hazards caused by earth-surface flows is challenging due to the need for suitable yet tractable mathematical models, computational difficulties presented by those models, and uncertainty or availability of input data. For instance, hazards caused by long waves (e.g. tsunamis and storm surges) are not sufficiently understood due mainly to the lack of data and the complexity owing to the influence of bathymetry. Flows that involve interactions of fluids and granular materials (e.g. tsunami inundation, landslides, and outburst floods) are complex due their two-phase nature. These problems are also multiscale (e.g. an ocean-scale tsunami interacts with meter-scale topographic/structural features) and require efficient and accurate numerical schemes. Here we introduce several important long-wave behaviors that are relevant to long-wave propagation and transformation. Granular-fluid modeling difficulties are briefly introduced. Then, the state-of-the-art computational techniques are discussed providing some examples. Our talk is considered as a prelude to the subsequent presentations.

Harry Yeh
Oregon State University
harry@oregonstate.edu

David George
U.S. Geological Survey
Cascades Volcano Observatory
dave.jorge@gmail.com

MS123

A Mathematical Analysis of Aerobic Glycolysis Triggered By Glucose Uptake in Cones

The degenerative disease Retinitis Pigmentosa (RP) is typically categorized by loss of night vision due to rod degeneration and eventually progressing to daylight-blindness and cone death. Those afflicted with RP rely on aerobic glycolysis to supply the metabolites necessary for renewal and maintenance of the photoreceptors. In this work we mathematically model and investigate the biochemical processes in the retina triggered by glucose catabolism in cones. We develop a system of nonlinear ordinary differential equations that describe the experimental work of Leveillard et al. with Nxnl1 -/- mice and the rod-derived cone viability factor (RdCVF). We utilize our mathematical model and resulting simulations to confirm the reliance of cones on rods. We investigate which processes contribute the most to the renewal of the cone photoreceptors by using Latin Hypercube Sampling and global sensitivity analysis. Through a series of simulations we are able to validate the model and confirm the laboratory results.

Danielle Brager
Arizona State University
dbrager@asu.edu

MS123

A 3D Mass-spring Mesh Model of Eye Deformation

Blunt force trauma to the eye can inflict long-term damage, which can even cause a loss of vision. During sports, like handball, the eye is highly susceptible to injuries resulting from blunt trauma. A recent study at Pacific University found the traditional protective eyewear used by handball athletes does not adequately prevent impact injuries to the eye. Computational models of eye deformation can support the development of more effective eye protection by providing a virtual environment in which to analyze the forces accompanying eye impacts. Eyes are complex three-dimensional solids, and their deformations can be modeled using partial differential equations. However, solving such a PDE model is computationally expensive. This work modifies an existing two-dimensional model of elastic membranes utilizing a damped mass-spring system approximation. This system consists of a tetrahedral mesh of point masses connected by springs, whose motion is modeled by a system of coupled ordinary differential equations. This model aims to provide a physiologically-realistic venue to support testing the effects of various blunt force trauma on the eye and support related projects focused on evaluating and improving protective eyewear in sports.

Kory Melton, Ian Besse
Pacific University
melt6457@pacificu.edu, besse.ian@pacificu.edu

MS123

A Novel Framework to Study Task Allocation in Multi-agent Systems

Task allocation in multi-agent systems is a topical subject of research in many fields, from biology to computer science and economics. One question that is commonly studied is whether agents using simple learning rules can produce collective patterns that are decidedly functional (or effi-

cient) for a given environment. Here, I introduce a mathematical framework to analyze this problem for the case of reinforcement-learning systems (i.e., ones where individuals attempt to maximize personal rewards gained from trying different actions in an unknown environment). I present a set of results for N agents and M tasks, including asymptotic conditions that favor the emergence of task specialists (vs. generalists) at equilibrium. Simulations of a model where agents hold similar task preferences but vary in their work rates across tasks reveals evidence of multiple co-existing attractors. This result demonstrates a likely influence of initial conditions in the organization of systems where individuals must balance the costs of performing different activities.

Oyita Udiani
Applied Mathematics for the Life & Social Sciences
College of Liberal Arts and Sciences ASU
oyita.udiani@asu.edu

MS123

A Mathematical Model of the Transmission of Rat Lungworm Disease

Angiostrongylus cantonensis (AC) is a parasitic nematode with a complex lifecycle. Adult worms reproduce in the lungs and pulmonary artery of rats (Rattus sp.). Larvae exit rats through feces which may be eaten by gastropods such as snails. Gastropods become infected by eating rat feces, and support the development of the larvae until the stage that can infect a rat. Rats consume these snails and support the late-stage development of the larval worms in their brain. During the final larval stage, worms leave the rats brain, and mature in the cardiopulmonary region, completing the lifecycle. Humans become infected by accidentally eating infectious snails or produce contaminated by infectious snails. AC infection in humans causes rat lungworm disease (also known as angiostrongyliasis) that may manifest with severe eosinophilic meningitis leading to chronic neurological abnormality. Although rat lungworm disease is an emerging public health problem across tropical and subtropical regions of Asia, the Americas, and the Pacific, environmental and ecological drivers of AC transmission are poorly described. In this paper, we develop a mathematical model to represent the transmission of AC through its life cycle. Numerical simulations are conducted to determine the factors that have the most impact on the transmission of AC. The results have important implications for understanding AC transmission and informing mitigation strategies to suppress infection rates in human populations.

Kamuela Yong
University of Hawaii - West Oahu
kamuela.yong@hawaii.edu

Matthew Medeiros
University of Hawaii
mcmedeir@hawaii.edu

MS124

Uniqueness and Computation of Block Term Decompositions of Tensors

Let $\mathcal{T}$ be an $I_1 \times I_2 \times I_3$ tensor. A mode-n fiber of $\mathcal{T}$ is a column vector obtained by fixing indices $\{1,2,3\} \setminus \{n\}$. An $I_n \times I_1 I_2 I_3 / I_n$ matrix $\mathbf{T}_{(n)}$ formed by all mode-n fibers is called a mode-n matrix unfolding of $\mathcal{T}$. By definition, $\mathcal{T}$ is MultiLinear (ML) rank-(L,M,N) (resp. ML rank-$(L,M,\cdot)$) if $rank(T_{(1)}) = L$, $rank(T_{(2)}) = M$, and $rank(T_{(3)}) = N$ (resp. $rank(T_{(3)})$ is not specified). In the first part of our talk we consider a decomposition of $\mathcal{T}$ into a sum of ML rank-$(L_r, M_r, \cdot)$ terms. (This decomposition can be reformulated as the joint block diagonalization problem of the frontal slices of $\mathcal{T}$ in which the diagonal blocks have dimensions $L_r \times M_r$, i.e., are not necessarily square.) We find conditions on the terms which guarantee that the decomposition is unique and can be computed by means of the eigenvalue decomposition of a matrix. In particular, we show that if the terms are generic, then the conditions are satisfied if

$$I_1 \geq \sum L_r, \;\; I_2 \geq \sum M_r, \;\; I_3 \geq \max\left(\max\left\lceil \frac{L_r}{M_r} \right\rceil + \max\left\lceil \frac{M_r}{L_r} \right\rceil, 3\right).$$

In the second and third part of our talk we study similar questions for a decomposition of $\mathcal{T}$ into a sum of ML rank-$(L_r, L_r, 1)$ and ML rank-$(L, L, 2)$ terms, respectively.

Ignat Domanov
Faculty of Science
KU Leuven, Campus Kulak
ignat.domanov@kuleuven.be

Nico Vervliet
Department of Electrical Engineering (ESAT)
KU Leuven
nico.vervliet@esat.kuleuven.be

Lieven De Lathauwer
KU Leuven - KULAK
lieven.delathauwer@kuleuven.be

MS124

Causes of Swamps in Tensor Approximations

Optimization algorithms attempting to approximate tensors with short sums of separable tensors regularly encounter periods of slow progress, informally know as swamps. Slow progress near a local minimum is caused by ill-conditioning in the Hessian at the minimum and is amenable to conventional analysis. Slow progress during the transient phase occurs more regularly and much more severely than in other optimization problems. Such transient swamps are the bane of users and their cause has been a great mystery for decades. I will describe some of the causes of swamps and address this great mystery.

Martin J. Mohlenkamp
Ohio University
mohlenka@ohio.edu

MS125

Analysis of Weak Graph Signals via the Random Matrix Theory Lens

Inference problems on graphs often involve the detection of weak signals (or subgraphs) distributed and buried in noisy edge measurements. Random Matrix Theory has provided a fresh perspective for understanding limits of detectability of such signals as well as for designing algorithms that boost detection. We discuss several case studies inspired by realistic settings (multi-source, temporal, noisy graph measurements) and characterize their limiting spectral properties. DISTRIBUTION STATEMENT A. Approved for public release: distribution unlimited. This material is based upon work supported by the Assistant Secretary of Defense for Research and Engineering under Air Force Contract No.

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Rajmonda Caceres
Lincoln Laboratory
Massachusetts Institute of Technology
rajmonda.caceres@ll.mit.edu

Benjamin A. Miller
MIT Lincoln Laboratory
bamiller@ll.mit.edu

MS125

Low Rank Equivalent Networks

Many methods for studying and describing complex networks rely on low rank approximations of associated linear operators. Examples include centrality measures, spectral decompositions for clustering, and inferential processes for generative models among others. In this talk I will discuss the related inverse problem of determining the properties of networks that have equivalent low rank representations and some of the interesting pure and applied questions that arise in this setting.

Daryl R. Deford
Dartmouth College
Department of Mathematics
daryl.r.deford.gr@dartmouth.edu

MS125

Minimizing Dissemination on Large Social Networks

I will discuss the problem of minimizing the dissemination of pathogens on large social networks by removing k edges. To minimize dissemination, we need to reduce the networks connectivity, which is determined by the leading eigenvalue of its adjacency matrix λ_1. Thus, reducing λ_1 can minimize the dissemination. However, in social networks the small gaps between the largest eigenvalues create a challenge for minimizing λ_1. I will describe a scalable algorithm called *MET* (short for Multiple Eigenvalues Tracking), which minimizes λ_1. MET performs well even if the gaps between the largest eigenvalues are small. Time-permitting, I will also describe two other approaches: (1) a machine learning approach which is useful when the exact structure of network is not available; and (2) an approach that minimizes dissemination on a network while maintaining its community structure.

Tina Eliassi-Rad
Northeastern University
t.eliassirad@northeastern.edu

MS125

Our Friends Are Cooler than Us

In 1991 the Friendship Paradox was identified by Scott Feld in the American Journal of Sociology. His title says it all: "Why your friends have more friends than you do." This mathematical result, which is a direct consequence of the Cauchy-Schwarz inequality, is also described very clearly by Steven Strogatz in a New York Times article of September 2012. From a network science perspective, counting friendships corresponds to measuring the degrees of the nodes. Several authors have subsequently made empirical observations about generalized versions of the paradox involving other types of nodal measures. In this talk I will give some new results concerning these Generalized Friendship Paradoxes. In doing so I will exploit connections with classical work in combinatorial graph theory.

Des Higham
University of Strathclyde
Univ of Strathclyde
d.j.higham@strath.ac.uk

MS126

Numerical and Analytical Study of K-spectral Sets: Part I

In this talk, we discuss analytical and numerical approaches to deriving bounds on norms of matrix functions using K-spectral sets. In particular, we extend the arguments used by Crouzeix and Palencia, who recently showed that the numerical range $W(A)$ of a square matrix (or linear operator) A is a $(1+\sqrt{2})$-spectral set for A. This extension allows us to consider regions in the complex plane which do not necessarily contain the numerical range, generalizing some of their results to other sets of interest, such as the unit disk or left half-plane. We will demonstrate how to use these techniques to derive analytical bounds in simple cases, as well as show the results of some numerical experiments. We detail our approach for optimizing the ratio $\|f(A)\|/\|f\|_\Omega$ numerically for a fixed matrix A and domain Ω, which primarily involves numerical conformal mapping and optimization over certain Blaschke products. In particular, the conformal maps from smooth domains Ω to the unit disk can be quickly computed in Chebfun to an accuracy near the limits of machine precision and the conditioning of the problem.

Trevor Caldwell, Anne Greenbaum, Kenan Li
University of Washington
tcal42@u.washington.edu, greenbau@uw.edu, lknan@uw.edu

MS126

Numerical and Analytical Study of K-spectral Sets: Part II

In the second part of the lecture, 2 classes of one-parameter matrices are shown to satisfy the Crouzeix's Conjecture. The upper bound which depends on the parameter is not greater than 2. In the first class, the optimal Blaschke product is not unique, and a 'turning point' is given when the Blaschke product degenerates to a lower degree.

Kenan Li, Anne Greenbaum, Trevor Caldwell
University of Washington
lknan@uw.edu, greenbau@uw.edu, tcal42@u.washington.edu

MS126

Partial Smoothness of the Numerical Radius at Matrices Whose Fields of Values are Disks

Solutions to optimization problems involving the numerical radius often belong to a special class: the set of matrices whose numerical range is a disk centered at the origin. We illuminate this phenomenon by studying matrices around which this set is a manifold M with respect to which the numerical radius is partly smooth. At such matrices, the

numerical radius varies smoothly w.r.t. changes to the matrix contained in or tangent to M, and nonsmoothly w.r.t changes normal to M. Examples include Jordan blocks, and the Crabb-Choi-Crouzeix matrix related to a well-known conjecture of Crouzeix.

Michael L. Overton
New York University
Courant Instit. of Math. Sci.
mo1@nyu.edu

Adrian Lewis
Cornell University
Oper. Res. and Indust. Eng.
aslewis@orie.cornell.edu

MS126

Generalized Numerical Ranges, Lie Groups, and Lie Algebras

The celebrated Toeplitz-Hausdorff theorem asserts that the classical numerical range of a square complex matrix is a convex set. Schur-Horn Theorem asserts that the set of the diagonals of Hermitian matrices of prescribed eigenvalues is the convex hull of the orbit of the eigenvalues under the action of the symmetric groups. These results are about the unitary orbit of a matrix. Among interesting generalizations, we will focus our discussion on those in the context of Lie structure, more precisely, compact connected Lie groups and semisimple Lie algebras. Some results on convexity and star-shapedness will be presented.

Tin-Yau Tam
Auburn University
tamtiny@auburn.edu

MS127

Pressure Control in Dissipative Particle Dynamics and Applications in Microbubble and Droplet Simulation

Pressure control is of extensive interest in meso-scopic simulation and particle-based numerical methods. In dissipative particle dynamics (DPD) and many-body DPD (MDPD), a natural thermostat has been already incorporated. Therefore, the barostat for pressure control could be an important part for the (M)DPD application. In current work, the Berendsen barostat from molecular dynamics simulation is applied in both DPD and MDPD simulations. The original Berendsen barostat works well in (M)DPD simulation of single-component system under constant pressure condition. The novel partial Berendsen barostat is proposed for multi-component system simulation with (M)DPD. The displacement rescaling process of Berendsen barostat is only applied on the particles outside the center region, acting as a pressure 'boundary condition'. The center part forms the free zone, in which the interface shape, non-equilibrium dynamic behavior between different phases can be captured properly. Immiscible bubble/droplet in the second fluid under outside pressure condition is studied. A microbubble/droplet model with liquid to gas density ratio up to 10 is created in (M)DPD simulation, and the oscillation of bubble radius is captured and compared with classical Rayleigh–Plesset equation. Bubble oscillation under harmonic pressure wave are also reported in current simulation which may have potential application in the studies on sonoporation and ultrasound bubble dynamics.

Yuqing Lin, Dingyi Pan, Xueming Shao
Zhejiang University
linyuqing@zju.edu.cn, dpan@zju.edu.cn, mecsxm@zju.edu.cn

MS127

A Molecular Fingerprint Algorithm for Learning Force Fields from Ab Initio Calculations

Molecular fingerprints, i.e. feature vectors describing atomistic neighborhood configurations, is an important abstraction and a key ingredient for data-driven modeling of potential energy surface and interatomic force. In this talk, we present the Density-Encoded Canonically Aligned Fingerprint (DECAF) fingerprint algorithm, which is robust and efficient, for fitting per-atom scalar and vector quantities. The fingerprint is essentially a continuous density field formed through the superimposition of smoothing kernels centered on the atoms. Rotational invariance of the fingerprint is achieved by aligning, for each fingerprint instance, the neighboring atoms onto a local canonical coordinate frame computed from a kernel minisum optimization procedure. We show that this approach is superior over PCA-based methods especially when the atomistic neighborhood is sparse and/or contains symmetry. We propose that the 'distance' between the density fields be measured using a volume integral of their pointwise difference. This can be efficiently computed using optimal quadrature rules, which only require discrete sampling at a small number of grid points. We also experiment on the choice of weight functions for constructing the density fields, and characterize their performance for fitting interatomic potentials. The applicability of the fingerprint is demonstrated through a set of benchmark problems.

Yu-Hang Tang
Lawrence Berkeley National Laboratory
tang@lbl.gov

Dongkun Zhang
Division of Applied Mathematics
Brown University
dongkun_zhang@brown.edu

George Em Karniadakis
Brown University
george_karniadakis@brown.edu

MS127

Many-body Dissipative Particle Dynamics Simulation of Multi-fluid/Phase Flow in Nano- to Microporous Heterogeneous Shale Pore Networks

The quest of a numerical model for simulating flow and transport phenomena in oil/gas shale rocks is challenging, because of the multiscale nature of pore networks in shale where pore sizes range from a few nanometers to a few micrometers, and because of the complex interactions between the fluids and pore surfaces which are physically and chemically heterogeneous. A many-body dissipative particle dynamics (mDPD) model has been found particularly attractive for modeling multi-fluid/phase flow in nano- to micro-scale pore networks, for its capability to model some key characteristics of fluid dynamics at both those scales. The present work will introduce a virtual rock analysis approach based on an integration of high-resolution microscopy & digital imaging and mDPD multiphase pore-

network flow simulation, in which the former is used to inform the construction of shale pore surface walls with mDPD particles. Simulations for permeability-fluid dependence study will be conducted in a region of interest from a Vaca Muerta shale micro core sample. Simulation results as well as the parallel computing performance will be reported and discussed. Though not sophisticated enough to account for all physics of interest, the present mDPD approach will be continuously improved toward a more capable multiscale flow modeling solution for bridging the gap between the molecular dynamics models and the continuum flow models.

Yidong Xia
Idaho National Laboratory
yidong.xia@inl.gov

Zhen Li
Division of Applied Mathematics
Brown University
Zhen_Li@brown.edu

Matthew Andrew
Carl Zeiss X-Ray Microscopy
matthew.andrew@zeiss.com

Joshua Kane
Idaho National Laboratory
joshua.kane@inl.gov

Jan Goral
University of Utah
jgoral@egi.utah.edu

Lixiang Luo
IBM
lixiang.luo@ibm.com

Hai Huang
Idaho National Laboratory
Idaho National Laboratory
hai.huang@inl.gov

MS127

Non-Markovian Dissipative Particle Dynamics Models Based on the Mori-Zwanzig Formalism and Iterative Boltzmann Inversion

We propose a non-Markovian dissipative particle dynamics (NMDPD) method, which takes advantage of the Mori-Zwanzig (MZ) formalism for extracting memory kernels together with the iterative Boltzmann inversion (IBI) for improving a representation of static properties. We demonstrate that the MZ-guided NMDPD model exploiting auxiliary variables, which allow for the replacement of a non-Markovian equation with a Markovian one in a higher dimensional space, can successfully reproduce dynamic properties such as a velocity autocorrelation function and mean square displacement of a reference Lennard-Jones system, as long as the pairwise memory kernels are appropriately evaluated. More specifically, we find that the memory kernels should be constructed based on the Volterra integral equation using force-velocity and velocity-velocity correlations, rather than based on the time-correlations of instantaneous force deviations from the mean force, which correspond to a zeroth order approximation of the exact memory kernels. Furthermore, the IBI correction of a pair potential ensures an accurate representation of a radial distribution function and pressure, while it has little influence on the dynamic properties that depend primarily on the memory kernels. Our findings suggest that combining the advantages of both the MZ formalism and IBI leads to a faithful representation of both the static and dynamic properties of microscopic systems that exhibit non-Markovian behavior.

Yuta Yoshimoto
University of Tokyo
yyoshimoto@fel.t.u-tokyo.ac.jp

Zhen Li
Division of Applied Mathematics
Brown University
Zhen_Li@brown.edu

Ikuya Kinefuchi
University of Tokyo
kine@fel.t.u-tokyo.ac.jp

George E. Karniadakis
Brown University
Division of Applied Mathematics
george_karniadakis@brown.edu

MS129

Network Analysis in Spatio-temporal Data

The complex network paradigm is increasingly being pursued in the analysis of spatio-temporal data that is collected in both neuroscience and climate science. These domains provide rich opportunities for exploring novel ways of defining nodes and edges in spatio-temporal data. In this talk, I will present some research directions we pursued in defining new types of relationships in spatio-temporal data.

Gowtham Atluri
University of Cincinnati
atlurigm@ucmail.uc.edu

Saurabh Agrawal
Dept. of Computer Science
University of Minnesota
agraw066@umn.edu

Vipin Kumar
University of Minnesota
kumar001@umn.edu

MS129

Communication-avoiding Algorithms for Large-scale Graph and Machine Learning Problems

Machine learning and graph analysis are two of the most commonly used methods to extract information from data. These methods either already heavily rely on linear algebra, as in the case of machine learning, or the computations can be cast into linear algebra for performance reasons, as in the case of graph analysis. In many interesting scenarios, the data is sparse; hence the underlying computation is based on sparse linear-algebraic operations. The performance of these sparse matrix operations become easily communication bound, severely limiting scalability. Communication-avoiding sparse-matrix algorithms offer a theoretically sound remedy to this scalability problem. In this short talk, I will give a broad overview of communication-avoiding sparse matrix algorithms and

their novel applications in the areas of machine learning and graph analysis.

Aydin Buluc
Lawrence Berkeley National Laboratory
abuluc@lbl.gov

MS129

New Approximation Algorithms for Edge Cover

An edge cover in a graph is a subset of edges such that at least one edge in the cover is incident on every vertex in the graph. This problem is rich in approximation algorithms which run in near-linear time in the size of the graph. We describe several 3/2- and 2-approximation algorithms for the Minimum Weighted Edge Cover Problem. The techniques used to design these algorithms include lazy greedy evaluation, dual fitting and transformation to matching. Almost all these algorithms can be easily extended to the more general b-Edge Cover problem. We describe a few real-world applications of Edge Cover problem including Adaptive Anonymity, graph sparsification and k-nearest neighbor graph construction.

S M Ferdous
Purdue University
sferdou@purdue.edu

Alex Pothen
Purdue University
Department of Computer Science
apothen@purdue.edu

MS129

Kokkoskernels: Graph and Linear Algebra Kernels on Modern Architectures

Kokkoskernels is part of the Kokkos C++ Performance Portability Programming EcoSystem, specifically providing Math and Graph Kernels such as BLAS, sparse and dense linear algebra, and graph kernels implementation for a number of architectures. KokkosKernels implements local computational kernels for linear algebra and graph operations, using the Kokkos shared-memory parallel programming model. KokkosKernels can be the building block of a parallel linear algebra library for thread parallelism, or it can be used stand-alone in your application. This talk describes the Kokkoskernels project, capabilities in the current version of Kokkoskernels library, most recent performance results for graph algorithmic kernels in the library.

Siva Rajamanickam, Mehmet Deveci, Kyungjoo Kim, Christian Trott, Michael Wolf
Sandia National Laboratories
srajama@sandia.gov, mndevec@sandia.gov, kyukim@sandia.gov, crtrott@sandia.gov, mmwolf@sandia.gov

MS130

Reconstruction of a Sound Profile in the Presence of a Background Stochastic Random Medium

We present different methods to reconstruct an unknown compact sound profile embedded in a random noisy background medium, given measurements of the scattered field and information about the probability distribution of the background medium and the sound profile. In the methods presented, we apply the Gauss-Newton method with the recursive linearization algorithm. A fast direct solver is used to speed-up the solution of the forward model, which allowed simulations with thousands of samples.

Carlos Borges
Institute for Computational Engineering and Sciences
University of Texas at Austin
borges@ices.utexas.edu

George Biros
The Institute for Computational Engineering and Sciences
The University of Texas at Austin
biros@ices.utexas.edu

MS130

Integral Equation Methods for Unsteady Stokes Flow using Heat and Laplace Potentials

We propose a new integral equation formulation for unsteady Stokes flow. Unlike existing integral formulation that uses unsteady Stokeslets, the new formulation uses only the heat and Laplace potentials to treat the source term, the initial data, and the boundary conditions. The main advantage of the new formulation is that all existing fast algorithm tools for the heat and Laplace potentials can be directly applied to solve the unsteady Stokes flow. The spectrum of the integral equation system is analyzed in detail when the boundary is a circle. We also develop an alternating marching scheme for solving the resulting boundary integral equation system at each time step, which solves the system in two stages where a well-conditioned second kind integral equation is solved at each stage. Numerical experiments indicates that both the second order and the third order alternating schemes are stable. Finally, we apply spectral deferred correction scheme to obtain arbitrary high-order schemes in time for solving unsteady Stokes flow. The performance of the scheme is illustrated via several numerical examples.

Shidong Jiang
Department of Mathematical Sciences
New Jersey Institute of Technology
shidong.jiang@njit.edu

Leslie Greengard
Simons Foundation and Courant Institute
New York University
greengar@cims.nyu.edu

MS130

Fast Algorithms for Electromagnetic Scattering of Axis-symmetric Objects

Fast algorithm for the electromagnetic scattering of dielectric objects is of great importance in optics, biomedical imaging and inverse scattering. In this talk, we apply a second kind integral formulation to the three dimensional scattering problem of axis-symmetric objects. The resulted surface integral equation is reduced to a sequence of line integral equations by Fourier transform along the azimuthal direction. These equations are decoupled from each other and a high order kernel splitting technique is applied to the evaluation of singular integrals. The algorithm is efficient and high order even for the scattering of non-smooth objects by using generalized Gaussian quadrature. Numerical experiments are presented to demonstrate the efficiency of

the algorithm.

Jun Lai
Zhejiang University
School of Mathematical Sciences
laijun6@zju.edu.cn

MS130

Efficient Algorithms for Cryo-electron Microscopy Image Denoising

Scientific breakthroughs often build upon successful visualization of objects invisible to the human eye. The 2017 Nobel Prize in Chemistry was awarded for the development of cryo-electron microscopy (cryo-EM) that allows us to image biomolecules in their native functional states at high resolution, which has moved biochemistry into a new era. Despite the recent progress, there still remain a lot of challenges for the current computational framework of cryo-EM single particle reconstruction (SPR). In this talk, we introduce a set of new algorithms to improve the efficiency and accuracy of cryo-EM 2D image classification and denoising.

Zhizhen Zhao
University of Illinois
zhizhenz@illinois.edu

MS131

Learning to Match Kernels for Deformable Shape Correspondence

In this talk, I will describe Kernel Matching - a promising novel framework for efficient matching of deformable shapes via matching positive definite kernels. I will provide a theoretical and empirical overview, ranging from the basic construction which uses heat kernels to learnable kernels obtained via a convolutional neural network on the product manifold. In particular, I will address the problem of learning discrete distributions on manifolds, which poses a main challenge in learning based schemes for matching.

Amit Boyarski
Computer Science
Technion Israel Institute of Technology, Israel
amitboy@cs.technion.ac.il

MS131

Geometric Deep Learning for 3D Data

The past decade in computer vision research has witnessed the emergence of deep learning, allowing to automatically learn powerful feature representations from large collections of examples. Deep neural networks achieved a breakthrough in performance in a wide range of applications such as image classification, segmentation, detection and annotation. When attempting to apply deep learning to 3D geometric data, one has to face fundamental differences between images and geometric objects. One of the key differences is that in the geometry processing and computer graphics communities, shapes are modeled as manifolds, and one requires to generalize deep neural networks using intrinsic constructions. Intrinsic deep neural networks have recently been used to learn invariant shape features and correspondence, allowing to achieve state-of-the-art performance in several shape analysis tasks, while at the same time allowing for different shape representations, e.g. meshes, point clouds, or graphs. I this talk, I will overview the foundations and the current state of the art in learning techniques for 3D shape analysis, including the tasks of shape classification, recognition, retrieval and correspondence. I will present in a new light the problems of shape analysis, emphasizing the analogies and differences with the classical 2D setting, and showing how to adapt popular learning schemes in order to deal with deformable objects.

Michael M. Bronstein
Institute of Computational Science Faculty of Informatics
Università della Svizzera italiana, USI, Switzerland
michael.bronstein@usi.ch

MS131

Fast Point Cloud Distances and Multi-sample Testing

We consider the question of estimating the total variation between two distributions in high dimensional space, given only a finite number of samples drawn iid from each distribution. We construct a new anisotropic kernel-based Maximum Mean Discrepancy (MMD) statistic for estimating such a distance, which builds upon the Reproducing Kernel Hilbert Space MMD proposed by Gretton, et al. The new anisotropic kernel scales linearly in the number of points by establishing landmarks throughout the space that approximate the local geometry of the union of the two datasets by constructing principle components of local covariance matrices. These landmarks can be interpreted as points that, under the action of a heat kernel on the data, diffuse to the entire space as quickly as possible. When the distributions are locally low-dimensional, the proposed test can be made more powerful to distinguish certain alternatives. We establish error bounds on the approximation by landmark points. We also consider the k-sample setting in which we measure pairwise distances between the k different point clouds. This test has complexity by $O(\binom{k}{2}|R| + kN|R|d)$ for N points per cloud with $|R|$ landmarks in d dimensions. This is opposed to complexity $\mathbb{O}(\binom{k}{2}N^2d)$ of the naive algorithm of directly computing the MMD between any two distributions.

Alexander Cloninger
University of California, San Diego, USA
acloninger@ucsd.edu

MS131

Learning Invariants and Representation Spaces of Shapes and Forms

We study the power of the Laplace Beltrami Operator (LBO) in processing and analyzing geometric information. The decomposition of the LBO at one end, and the heat operator at the other end provide us with efficient tools for dealing with images and shapes. Denoising, segmenting, filtering, exaggerating are just few of the problems for which the LBO provides an efficient solution. We review the optimality of a truncated basis provided by the LBO, and a selection of relevant metrics by which such optimal bases are constructed. In contrast to geometry understanding there is the emerging field of deep learning. Learning systems are rapidly dominating the areas of audio, textual, and visual analysis. Recent efforts to convert these successes over to geometry processing indicate that encoding geometric intuition into modeling, training, and testing is a non-trivial task. It appears as if approaches based on geometric understanding are orthogonal to those of data-heavy computational learning. We propose to unify these two methodologies by computationally learning geometric representations and invariants and thereby take

a small step towards a new perspective on geometry processing. If time permits I will present examples of shape matching, facial surface reconstruction from a single image, reading facial expressions, shape representation, and finally definition and computation of invariant operators and signatures.

Ron Kimmel
Technion, Haifa, Israel
ron@cs.technion.ac.il

MS132

A Lagrangian Approach to Turbulent Rayleigh-Benard Convection

We obtain new exact results for turbulent Rayleigh-Benard convection, exploiting a general Lagrangian fluctuation-dissipation relation. Applied to convection, the relation shows that the ratio of the Kraichnan-Spiegel dimensional prediction for Nusselt number with the true Nusselt number is precisely equal to the ratio of a near-wall scalar mixing time with the free-fall-time. Thus, Kraichnan-Spiegel scaling can fail only if the mixing time becomes much longer than the free-fall time and also much longer than the time to mix by pure diffusion across the thermal and kinetic boundary layers. This implies the existence of a Lagrangian mixing zone wider than the traditional boundary layers, with transition to an ultimate regime plausibly connected with development of turbulence in this zone. We discuss how to measure empirically the near-wall mixing time, which should shed light on the Lagrangian mechanisms of turbulent convection. This is joint work with Gregory Eyink.

Theodore D. Drivas
Princeton University
tdrivas@princeton.edu

MS132

New Perspectives on Wall-to-Wall Transport

The maximal transport of heat by incompressible flows is formulated as an unconstrained non-convex variational problem leading to new insights on the development of algorithms as well as the connection to existing upper bound techniques. We show how to convert the original constrained optimization problem into an unconstrained one and highlight how this approach connects research spanning over half a century. Numerical computations for 2D time-independent incompressible flow fields are shown to illustrate the method in practice.

Andre N. Souza
Georgia Institute of Technology
andre.souza@math.gatech.edu

MS132

Heat Exchange and Exit Times

A heat exchanger can be modeled as a closed domain containing an incompressible fluid. The moving fluid has a temperature distribution obeying the advection-diffusion equation, with zero temperature boundary conditions at the walls. Starting from a positive initial temperature distribution in the interior, the goal is to flux the heat through the walls as efficiently as possible. Here we consider a distinct but closely related problem, that of the integrated mean exit time of Brownian particles starting inside the domain. Since flows favorable to rapid heat exchange should lower exit times, we minimize a norm of the exit time. This is a time-independent optimization problem that we solve analytically in some limits, and numerically otherwise. We find an (at least locally) optimal velocity field that cools the domain on a mechanical time scale, in the sense that the integrated mean exit time is independent on molecular diffusivity in the limit of large-energy flows.

Jean-Luc Thiffeault
Dept. of Mathematics
University of Wisconsin - Madison
jeanluc@math.wisc.edu

Florence Marcotte
ENS
florence.marcotte@dalembert.upmc.fr

Charles Doering
University of Michigan
doering@mich.edu

William Young
SIO
UCSD
wryoung@ucsd.edu

MS132

On the Optimal Design of Wall-bounded Heat Transport

We consider the variational problem of achieving optimal transport of heat through an incompressible fluid layer. Modeling passive scalar transport by the advection-diffusion equation, we maximize the mean rate of total transport achieved by a divergence-free velocity vector field. Subject to various boundary conditions and intensity constraints, we prove that the maximal rate of transport scales linearly in the r.m.s. kinetic energy and, up to possible logarithmic corrections, as the 1/3rd power of the mean enstrophy in the advection-dominated limit. While convection rolls are optimal for energy-constrained transport, optimizers for the enstrophy-constrained problem are significantly harder to describe. Motivated by connections to materials science, we introduce a self-similar "branching" construction with an unbounded number of degrees of freedom. We prove that such designs come within a logarithm of achieving optimal transport in the infinite enstrophy limit. Though the talk will focus initially on the analysis of optimal transport in a planar fluid layer, our approach can be applied in much greater generality. Time permitting, we will discuss extensions to optimal transport in general domains, as well as to problems of internal heating.

Charles R. Doering
University of Michigan
Mathematics, Physics and Complex Systems
doering@umich.edu

Ian Tobasco
Courant Institute of Mathematical Sciences
New York University
itobasco@umich.edu

MS133

Symmetirc Sums of Squares in Optimization

I will present results on using symmetric sums of squares

in optimization, in particular some elementary results on proving graph density inequalities.

Greg Blekherman
Georgia Tech
greg@math.gatech.edu

MS133

Using SDP Relaxations in Spatial Branch-and-Cut

We explore the use of semidefinite programming (SDP) in a spatial branch-and-cut implementation to solve polynomial optimization problems. Spatial branching tends to produce SDP instances with near-infeasibility (or near-feasibility). Furthermore in a major application (power flow in an electric grid), these relaxations can be very large and incorporating sparsity is paramount to practical solution times. One alternative to SDP relaxations is polyhedral approximation (of rank-one constrained SDP), and thus solve linear programming relaxations instead. We discuss both theoretical and methodological issues associated with this linear programming strategy, and how SDP might be used to bolster this approach.

Daniel Bienstock
Columbia University
dano@ieor.columbia.edu

Chen Chen
Ohio State University
chen.8018@osu.edu

Gonzalo Munoz
Ecole Polytechnique de Montreal
gonzalo.munoz@polymtl.ca

MS133

Fast Fourier Linear Programming with Application to the Turans Conjecture

Since the winter of 2016, when Maryna Viazovska published her remarkable proof of the optimal sphere packing in eight dimensions, there has been an increasing interest in using infinite dimensional linear programming to problems involving Fourier Transforms, including the densest packing of convex bodies problem. Many important instances of this family of problems have intuitive conjectured solutions, however they remain unsolved. Also numerical efforts so far, have made no significant progress in approximating the solutions, because the computational cost grows exponentially with the geometric dimension. We believe that the important underlying factors to making tractable approximations are: (1) a clever application of Fourier transformation to provide a sparse constraint matrix, (2) the choice of discretization, and (3) dimension reduction. The latter issue has been addressed by adopting specialized admissible functions, and SOS polynomials to obtain the density upper-bounds with constrained solutions. It has also been successfully explored with direct construction of the packings for the density lower-bounds. In addition to exploring the possible approaches for (1) and (2), we are exploiting the possibility of using Turan's conjecture on the exact solution of a similar problem for a universal approach to compute the density upper bounds for packing of the convex bodies in n dimensional Euclidean space.

Elahesadat Naghib
Princeton University
enaghib@princeton.edu

Robert J. Vanderbei
Princeton University
Department of Operations Research and Management Science
rvdb@princeton.edu

MS133

Maximum Likelihood Estimation under Total Positivity

Nonparametric density estimation is a challenging problem in theoretical statistics—in general the maximum likelihood estimate (MLE) does not even exist! Introducing shape constraints allows a path forward. This talk offers an invitation to non-parametric density estimation under total positivity (i.e. log-supermodularity) and log-concavity. Totally positive random variables are ubiquitous in real world data and possess appealing mathematical properties. Given i.i.d. samples from such a distribution, we prove that the maximum likelihood estimator under these shape constraints exists with probability one. We characterize the domain of the MLE and show that it is in general larger than the convex hull of the observations. If the observations are 2-dimensional or binary, we show that the logarithm of the MLE is a tent function (i.e. a piecewise linear function) with "poles" at the observations, and we show that a certain convex program can find it. In the general case the MLE is more complicated. We give necessary and sufficient conditions for a tent function to be concave and supermodular, which characterizes all the possible candidates for the MLE in the general case.

Elina Robeva
Massachusetts Institute of Technology
erobeva@mit.edu

MS134

Identification of Hybrid Dynamical Systems via Clustering and Sparse Regression

Inferring the structure and dynamical interactions of complex systems is critical to understanding and controlling their behavior. Hybrid systems are challenging to identify because the parameters and equation structure may vary across multiple dynamical regimes. Key examples include varying transmission rates in epidemiological problems and legged locomotion. Many current methods focus on inferring a model for the system and detecting switching points in a time-centric framework. We reframe the problem by clustering in data-driven coordinates, such that similar dynamical behavior is close together, and then use the sparse identification of nonlinear dynamics (SINDy) method to identify different dynamical regimes. We demonstrate the success of the method hybrid-SINDy on a spring-mass model and a simple infectious disease model with time-dependent transmission rates. We also investigate robustness to noise and cluster-size.

Niall M. Mangan
Department of Applied Mathematics
University of Washington, Seattle
niall.mangan@northwestern.edu

Travis Askham
University of Washington
askham@uw.edu

J. Nathan Kutz
University of Washington, Seattle
Dept of Applied Mathematics
kutz@uw.edu

Steven Brunton
University of Washington
sbrunton@uw.edu

Joshua L. Proctor
Institute for Disease Modeling
JoshLProctor@gmail.com

MS134

Using Dynamic Mode Decomposition to Analyze Data and Plan Interventions for Human African Trypanosomiasis

Dynamic Mode Decomposition (DMD) is a matrix decomposition technique that extracts low dimensional dynamics from high dimensional data. DMD can create a dynamical picture from data coming from a system that may not have parsimonious mathematical model on which to do traditional analyses. Human African Trypanosomiasis (HAT) is a disease endemic to rural parts of Sub-Saharan Africa, and has many partially understood dynamics including: Transmission routes, importation, spatial effects, and even the impact of interventions. Hence, there is a significant appeal to use DMD for analysis of HAT data. In this talk, we will discuss how DMD can be applied to the available data for HAT, and the challenges associated with its operational interpretation and use. In particular, we will use DMD alongside modeling to zero in on two particular issues in HAT control in the Democratic Republic of the Congo: Finding areas of higher prevalence, and identifying villages where the coverage of screening interventions has been below expected levels. We will also address the limitations of this method, and how additional data and better models could be used to increase its efficacy.

Cody Palmer, Joshua L. Proctor, Caitlin Bever
Institute for Disease Modeling
cpalmer@idmod.org, JoshLProctor@gmail.com, cbever@intven.com

MS134

Diffusion Network Approaches to Quantifying Malaria Transmission in Near-elimination Settings

Increasingly disease surveillance data capture a wealth of information which can improve the control and elimination of infectious diseases. However challenges exist in making use of these diverse data sources. Robust methods to make the most of these data to are required in order best support decision making. Diffusion network approaches address the general problem of reconstructing information transmission using known or inferred times of infection by a contagion. They provide an adaptable framework to integrate multiple data types, identify likely unobserved cases/external infection sources, and have been evaluated using real and simulated transmission processes at multiple scales and network structures. We adapt these approaches to quantify likely chains of transmission and spatio-temporal heterogeneities in transmission of malaria in near elimination settings, where malaria transmission often takes on epidemic-like dynamics. We also introduce recent work to incorporate spatial as well as temporal information into our inference. We carry out model selection and fitting to explore the relationship between spatio-temporal distance between two cases and the likelihood of transmission occurring between them and identify which models best explain the observed times and locations of cases. Finally, we discuss the wider applicability of such methods, both within epidemiology and more generally in the modelling and analysis of Hawkes (self-exciting temporal point) processes.

Isobel Routledge
Routledge, Imperial College
i.routledge15@imperial.ac.uk

Kyle B. Gustafson
US Navy
gustafsonkyle@gmail.com

Joshua L. Proctor
Institute for Disease Modeling
JoshLProctor@gmail.com

Samir Bhatt
Imperial College
s.bhatt@imperial.ac.uk

MS134

Advances in the Development of Decision-making Support Tools to Predict Epidemic Years in Dengue Endemic Regions

Focusing on the important but not-fully-understood relationship between (a) climate indicators (e.g. temperature, rainfall) and (b) the empirically observed 3-4 year cyclical disease burden, and dengue incidence, we propose a data-driven, machine learning approach capable of identifying weather patterns and population's susceptibility variations to predict dengue fever epidemics in Brazilian municipalities. These predictions are produced months ahead of the historically-observed seasonal onset of dengue epidemics. Specifically, we designed ensemble learning approaches that generate city-level dynamic models that leverage a globally-available meteorological data source and local historical patterns of dengue burden. The out-of-sample prediction retrospective results of this approach show very promising performances and have motivated us to develop a real-time version that may prove to be useful to public health decision makers. This work has been conducted in collaboration with Sarah McGough (Harvard) and Nathan Kutz (University of Washington).

Mauricio Santillana
Harvard University, School of Engineering and Applied Scienc
msantill@fas.harvard.edu

J. Nathan Kutz
University of Washington, Seattle
Dept of Applied Mathematics
kutz@uw.edu

Sarah McGough
Harvard University
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MS135

On Mean Field Games Models of Exhaustible Resource Production

We study mean field games systems of partial differential equations of the type introduced by Gueant, Lasry, and

Lions as well as Chan and Sircar. We study the problem of epsilon Nash equilibria and provide a rigorous justification of the mean field limit.

Jameson Graber
Baylor University
jameson_graber@baylor.edu

Charafeddine Mouzouni
Ecole Centrale de Lyon
charafeddine.mouzouni@ec-lyon.fr

MS135
Mean Field Games with Latent Factors

Financial markets are often driven by latent factors which traders cannot observe. Here, we address an algorithmic trading problem with collections of heterogeneous agents who aim to perform statistical arbitrage. All agents filter the latent states of the world, while their trading actions exhibit both permanent and temporary price impact. This leads to a large stochastic game with heterogeneous agents. We solve the stochastic game by investigating its mean-field game limit (which contains sub-populations of heterogenous agents) and, using a novel convex analysis approach, we show that the solution is characterized by a vector-valued forward-backward stochastic differential equation (FBSDE). We demonstrate that the FBSDE admits a unique solution, obtain it in closed-form, and characterize the optimal behaviour of the agents in the MFG equilibrium. Moreover, we prove that the MFG equilibrium provides an ϵ-Nash equilibrium property in the finite player game. We conclude by illustrating the behaviour of agents using the optimal MFG strategy through simulated examples.

Philippe Casgrain
University of Toronto
p.casgrain@mail.utoronto.ca

Sebastian Jaimungal
University of Toronto, Canada
sebastian.jaimungal@utoronto.ca

MS135
Energy Prices, Dynamic Mean Field Games and Stochastic Demand

We discuss oligopoly games with a continuum of players that have mean field structure. These may be of Bertrand (price setting) or Cournot (quantity setting) type and may apply to analysis of consumer goods or energy markets respectively. Key advantages over finite player nonzero sum differential games are analytical and numerical tractability. Models for energy markets with competition between producers with heterogeneous costs (fossils vs. renewables) are presented as motivation. The dramatic decline in oil prices, from around \$110 per barrel in June 2014 to below \$30 in January 2016 (and in early 2018 up to about \$65) highlights the importance of competition between different energy sources. Indeed, the price drop has been primarily attributed to OPEC's strategic decision, until recently, not to curb its oil production in the face of increased supply of shale gas and oil in the US. We also discuss how declining and uncertain demand from China and India may be a major factor driving oil price volatility.

Ronnie Sircar
Princeton University
sircar@princeton.edu

MS135
Large Tournament Games

We consider a stochastic tournament game in which each player works toward accomplishing her goal and is rewarded based on her rank in terms of the time to completion. We prove existence, uniqueness and stability of the game with infinitely many players, and existence of approximate equilibrium with finitely many players. When players are homogeneous, the equilibrium has an explicit characterization. We find that the welfare may be increasing in cost of effort in its low range, as the cost reduces players eagerness to work too hard. The reward function that minimizes the expected time until a given fraction α of the population has reached the target, as well as the aggregate welfare, only depends on whether the rank is above or below α. However, that is no longer true when maximizing a function of the completion time.

Yuchong Zhang
Columbia University
Statistics
yz2915@columbia.edu

Erhan Bayraktar
University of Michigan
Department of Mathematics
erhan@umich.edu

Jakša Cvitanic
Caltech
cvitanic@hss.caltech.edu

MS136
Optimal Sensor Placement for Estimation and Control

Optimal sensor and actuator placement is one of the foremost challenges in the estimation and control of high-dimensional complex systems. For high-dimensional systems it is impractical to monitor or actuate every state, or perform brute-force combinatorial searches among all possible placements. Hence, practitioners must often find an optimal placement of a fixed budget of sensors and actuators with respect to some objective function. Our work leverages dimensionality reduction and balanced model reduction to determine which placements best characterize the balanced (direct and adjoint) modes of a system. These modes quantify the observability and controllability of a system, as well as the uncertainty associated with a given sensor and actuator placement. We propose a greedy, scalable sensor & actuator placement method based on the pivoted matrix QR factorization of the direct and adjoint balanced modes of a system. Our method surpasses the performance of competing convex optimization methods for sensor placement, and is demonstrated on a variety of examples including fluid flows and the linearized Ginzburg-Landau equation with stochastic disturbances.

Krithika Manohar
University of Washington
Dept of Applied Mathematics
kmanohar@uw.edu

J. Nathan Kutz
University of Washington, Seattle
Dept of Applied Mathematics

kutz@uw.edu

Steven Brunton
University of Washington
sbrunton@uw.edu

MS136

Graph-based Bayesian Learning: Continuum Limits and Algorithms

The principled learning of functions from data is at the core of statistics, machine learning and artificial intelligence. The aim of this talk is to present some new theoretical and methodological developments concerning the graph-based Bayesian approach to semi-supervised learning. I will show suitable scalings of graph parameters that provably lead to robust Bayesian solutions in the limit of large number of unlabeled data. The analysis relies on a careful choice of topology and in the study of the the spectrum of graph Laplacians. Besides guaranteeing the consistency of graph-based methods, our theory explains the robustness of discretized function space MCMC methods in semi-supervised learning settings.

Daniel Sanz-Alonso
Brown University
daniel_sanz-alonso1@brown.edu

MS136

Bayesian Point Set Registration for High Entropy Alloys

Point set registration involves identifying a smooth invertible transformation and correspondences between points in two point sets, one of which may be smaller than the other and possibly corrupted by observation noise. This problem is typically decomposed into two separate optimization problems: (i) correspondence and (ii) optimal transformation between the ordered point sets. In this talk, we propose an approach to solving both problems simultaneously via a Bayesian perspective. Our formulation of the problem results in a marginal posterior distribution on the transformation, which is explored within a Markov chain Monte Carlo scheme, posing the solution as not just a point, but as a distribution. Motivated by Atomic Probe Tomography (APT), in the context of structure inference for high entropy alloys (HEA), we focus on the registration of noisy sparse observations of rigid transformations of a known reference configuration. We will present examples on both synthetic and real data sets.

Adam Spannaus
The University of Tennessee, Knoxville
spannaus@utk.edu

MS136

Compressive Sensing Adaptation for Polynomial Chaos Expansions

Basis adaptation in Homogeneous Chaos spaces rely on a suitable rotation of the underlying Gaussian germ. Several rotations have been proposed in the literature resulting in adaptations with different convergence properties. In this paper we present a new adaptation mechanism that builds on compressive sensing algorithms, resulting in a reduced polynomial chaos approximation with optimal sparsity. The developed adaptation algorithm consists of a two-step optimization procedure that computes the optimal coefficients and the input projection matrix of a low dimensional chaos expansion with respect to an optimally rotated basis. We demonstrate the attractive features of our algorithm through several numerical examples including the application on Large-Eddy Simulation (LES) calculations of turbulent combustion in a HiFIRE scramjet engine.

Panagiotis Tsilifis
University of Southern California
pantsili@gmail.com

Roger Ghanem
University of Southern California
Aerospace and Mechanical Engineering and Civil Engineering
ghanem@usc.edu

MS137

Traveling Multi-pulses in the FitzHugh–Nagumo Equation

The FitzHugh–Nagumo system is a simplified model of nerve impulse propagation, which is known to admit stable traveling pulse solutions. I will present existence and stability results for (multi)pulse solutions, and I will describe a phenomenon whereby a single pulse can be continuously deformed into a double pulse by parameter continuation. Along this transition, eigenvalues accumulate on the positive real axis due to the fact that the pulse solutions spend long times near a slow manifold which exhibits absolute spectrum.

Paul Carter
Department of Mathematics
University of Arizona
pacarter@math.arizona.edu

MS137

On the Moduli Spaces of 2-Dimensional Non-linear Sigma Models

Non-linear (gauged) sigma models can be viewed as generalizations of the Ginzburg-Landau equations with non-linear targets. When the physical space is 2-dimensional (and possibly curved) and the target is the round 2-sphere, a novel feature of the theory is that there are solutions with both vortex and anti-vortex regions. This is in contrast to the linear case, when the target space is complex plane. In this work we analyse the behavior of the above mentioned solutions when a vortex and an anti-vortex are close to each other. We find that outside of the center of mass of the pair, the solutions limit to the solution with one less vortex and one less anti-vortex, and furthermore that the canonical metric on the corresponding moduli space is incomplete, but a natural metric compactification exists. This is a joint work with Nuno Romão (University of Augsburg).

kos Nagy
Dept. of Mathematics
Duke University
akos@math.duke.edu

MS137

On Density Functional Theory

In this talk I will review some recent results in the density

functional theory including the time-dependent one and the one coupled to the electro-magnetic field. I will also formulate some open problems. The talk is based on the joint results with Ilias Chenn.

Israel Michael Sigal
Department of Mathematics
University of Toronto
im.sigal@utoronto.ca

MS137

On the Construction of Large Global Solutions for Super-critical Nonlinear Dispersive Equations

Abstract I will review the problem of Global existence for dispersive equations, in particular, supercritical equations. These equations which play a fundamental role in science, have been , and remain a major challenge in the field of Partial Differential Equations. They come in various forms, derived from Geometry, General Relativity, Fluid Dynamics , Field Theory. I present a new approach to study the asymptotic behavior of wave equations, supercritical and others, and construct global solutions with large initial data. I will then describe current extensions to Nonlinear Schrödinger Equations.

Avraham Soffer
Departemnt of Mathematics
Rutgers University
soffer@math.rutgers.edu

MS138

Low Regularity Global Existence for the Periodic Zakharov System

In this talk, we present a low-regularity global existence result for the periodic Zakharov system. This is a dispersive model for the motion of ionized plasma. Its dynamics have been extensively studied, and existence of solutions is in known for data in the Sobolev space $H^{\frac{1}{2}} \times L^2$. In this talk, we present a global existence result which holds for even rougher data, in a class of Fourier Lebesgue spaces. It is obtained by combining the high-low decomposition method of Bourgain with an almost-conserved energy result of Kishimoto. Combining these two tools allows us to obtain a low-regularity result which was out of reach of either method alone.

Erin L. Compaan
Massachusetts Institute of Technology
compaan@mit.edu

MS138

Spiral Waves and Alternans in Models of Cardiac Tissue

Ventricular fibrillation in the heart is often caused by the formation and breakup of spiral waves in cardiac tissue. Clinically, spiral wave breakup has been linked to the formation of alternans, an oscillation in the action potential duration. We seek to understand how and why alternans develop, and if stable alternans patterns exist. To investigate these questions, we analyze spectral properties of spirals on bounded disks formed in reaction-diffusion systems. Moreover, I will address difficulties that arise if the reaction-diffusion system has one or more variables without diffusion: in this situation, the eigenvalues exhibit unexpected accumulation points, far from the asymptotically predicted absolute spectrum curves.

Stephanie Dodson
Division of Applied Mathematics
Brown University
Stephanie_Dodson@Brown.edu

Stephanie Dodson
Brown University
Stephanie_Dodson@Brown.edu

Bjorn Sandstede
Division of Applied Mathematics
Brown University
bjorn_sandstede@brown.edu

MS138

Metastable Traveling Fronts Arising in Nanoscale Pattern Formation

We study an equation that models ripple formation when a flat surface is bombarded by an ion beam. The experimentally observed ripples consist of parts with a certain positive slope, parts with a certain negative slope, and transitions between the two slopes. The transitions admit a solitary wave solution with stable point spectrum but unstable essential spectrum. At first glance this may be written off as unstable. However numerical results suggest that the instability has two parts; a convecting part that saturates to some value and an exponentially decaying part that slightly modulates the underlying transition. We define an exponential weight that decays in the direction the first part of the instability travels in, allowing us to focus on the second part of the instability. In this exponentially weighted space we obtain a linear stability result. Inspired by the repeating part of the experimental results, we also consider gluing together solitary waves in an ad hoc periodic pattern. For some specific methods of gluing the entire spectrum is stable, with the implication that while an individual transition is unstable, the instability is benign enough that it can be stabilized by repeating the transition.

Connor Y. Smith, Mathew Johnson
University of Kansas
c406s460@ku.edu, matjohn@ku.edu

Gregory Lyng
Department of Mathematics
University of Wyoming
glyng@uwyo.edu

MS138

Traveling Vegetation Bands from Advection and Autocatalysis

We motivate and analyze a simple model for the formation of banded vegetation patterns. The model incorporates a minimal number of ingredients for vegetation growth in semi-arid landscapes. It allows for comprehensive analysis and sheds new light onto phenomena such as the migration of vegetation bands, their alignment with contour lines, and the interplay between their upper and lower edges.

Jasper Weinburd, Arnd Scheel
University of Minnesota - Twin Cities

weinburd@umn.edu, scheel@umn.edu

MS139

Asteroid-generated Tsunamis

In 2013, an uncharted asteroid exploded in the atmosphere over Chelyabinsk, causing damage for a radius of 20 kilometers. We examine the question of what would happen if an asteroid burst over water instead of land. Could it generate a tsunami that would cause widespread damage far away? We present numerical simulations using the GeoClaw software and the shallow water equations in a variety of settings.We have a model problem with an explicit solution that explains the phenomena found in the computations. Finally, we discuss whether compressibility and dispersion are important effects that should be included, and show results using the linearized Euler equations that begin to address this.

Marsha Berger
Courant Institute of Mathematical Sciences
New York University
berger@cims.nyu.edu

MS139

Conservative Schemes for Variable Coefficient Transport Equations

We discuss four different methods for formulating the wave propagation algorithm used in Clawpack (R. J. LeVeque) for the variable coefficient conservative advection equation on a finite volume mesh. Both cell-centered and face-centered velocities are considered, and first and second order schemes. Of special interest is the treatment of sonic points where converging or diverging flows can lead to loss of hyperbolicity. We demonstrate the approaches on volcanic ash transport simulations, and if time permits, we discuss the correction terms needed to maintain conservation on mapped, adaptive quadtree meshes, including surface meshes.

Donna Calhoun
Boise State University
donnacalhoun@boisestate.edu

MS139

Embedding Sea-walls into Grids (h-box Style)

Abstract not available at time of publication.

Jiao Li
Columbia University
Applied Physics and Applied Mathematics
jl4170@columbia.edu

MS139

A Theoretical Study on Tsunami Propagation and Run-up in Convergent Bays

Two-dimensional tsunami evolution in convergent bays is theoretically investigated. The wave behavior for particular bay types can be described by one-dimensional dispersive wave equations on the assumption of weak transverse flows. The analytical solutions for monochromatic incident waves are characterized as the leading-order plane-wave solutions with higher-order corrections for two-dimensionality due to wave refraction. The perturbation analysis of very high-order wave celerity suggests that the derived solutions are valid only when the ratio of the bay width to the wavelength is smaller than a certain limit. Beyond the limit, the higher-order effect is no longer a minor correction, implying that wave behaviors become highly two-dimensional and possibly cause total reflection. Tsunami propagation and run-up characteristics for various bay geometries are discussed based on the derived model.

Takenori Shimozono
University of Tokyo
shimozono@coastal.t.u-tokyo.ac.jp

MS140

A Parasite for Sore Eyes: Living Together in a Social Network

Individuals who live in close, collaborate groups are susceptible to infections diseases such as pathogens and parasites through their social network. Ectoparasites, external parasites that may be spread through social grooming, differ from pathogens in that the number of parasites impacts an individual's fitness. In this talk, we will discuss two approaches to understanding the effects of ectoparasites on social groups. The first is a system of differential equations that shows the importance of a hub-like structure in a social network, and the second is an agent-based model that shows parasite spread based on individual behavior in a dynamic network. We will also briefly talk about my experience at the Women Advancing Mathematical Biology (WAMB) Workshop at the Mathematical Biosciences Institute (MBI) including our group's development and successes.

Maryann Hohn
University of California, Santa Barbara
hohn@pstat.ucsb.edu

MS140

Clots Or Not? Mathematics Making the Invisible Visible

Mathematical modeling is the art of representing real-world processes in mathematical terms. These abstractions can be used to understand the behavior of devices, to predict outcomes, or to test hypotheses. In this talk I will describe current work whose goal is to understand how traditional in vitro coagulation tests compare to what is actually going on in vivo. Since these in vitro tests are used to prescribe anti-coagulants, it is crucial to know whether they are indeed a measure of how quickly a clot will form. I will show how differential equations can be used to "see what is happening inside the blood vessel. I will discuss the mathematical challenges inherent in this type of research, as well as the potential for discovery. No expertise in mathematical modeling OR anti-coagulants is assumed. Please come join the discussion! This is joint work with the WhAM! clotbusters research group.

Ami Radunskaya
Pomona College
Mathematics Department
ami_radunskaya@pomona.edu

Erica J. Graham
Bryn Mawr College
ejgraham@brynmawr.edu

Lisette de Pillis

Harvey Mudd College
depillis@g.hmc.edu

Kaitlyn Hood
University of California, Los Angeles
kthood @ mit.edu

Yan Ping Ma
Loyola Marymount University
yanping.ma@lmu.edu

Julie Simons
California Maritime Academy
jsimons@csum.edu

MS140

Modeling Tumor Immune Dynamics in Multiple Myeloma

We propose a mathematical model that describes the dynamics of multiple myeloma and three distinct populations of the innate and adaptive immune system: cytotoxic T cells, natural killer cells, and regulatory T cells. The model includes significant biologically- and therapeutically-relevant pathways for inhibitory and stimulatory interactions between these populations. We focus on five main aspects: 1) obtaining and justifying parameter ranges and point estimates; 2) determining which parameters the model is most sensitive to; 3) determining which of the sensitive parameters could be uniquely estimated given various types of data; 4) exploring the model and updated parameter estimates numerically; and 5) analytically exploring the equilibria and stability of a reduced model. Using multiple sensitivity analysis techniques, we found that the model is generally most sensitive to parameters directly associated with M protein levels. Consistent with dynamical systems analysis of the reduced model, numerical results revealed parameter regimes for which bistability exits. The two stable states in these cases may correspond to long-term disease control or a higher level of disease burden. This analysis provides the foundation for a future ultimate application of the model: prediction of optimal combination regimens in patients with multiple myeloma.

Marissa Renardy
The Ohio State University
renardy.1@osu.edu

Diana White
Clarkson University
dtwhite@clarkson.edu

Nessy Tania
Smith College
Mathematics and Statistics Department
ntania@smith.edu

Blerta Shtylla
Pomona College
shtyllab@pomona.edu

Jill Gallaher
H. Lee Moffitt Cancer Center and Research Institute
Integrated Mathematical Oncology Department
jill.gallaher@moffitt.org

Helen Moore
AstraZeneca
dr.helen.moore@gmail.com

Karen E Wood
University of California, Irvine
math.kwood@gmail.com

Kamila Larripa
Humboldt State University
kamila.larripa@gmail.com

Urszula Ledzewicz
Southern Illinois University, USA
uledzew@siue.edu

MS140

Explaining Autism Spectrum Disorder with Placenta via Machine Learning

The placenta is the essential organ of maternal-fetal interactions, where nutrient, oxygen, and waste exchange take place. In recent studies, differences in the morphology of the placental chorionic surface vascular network (PCSVN) have been associated with developmental disorders such as autism. This suggests that PCSVN could potentially serve as a biomarker for early diagnosis and treatment of autism. Studying PCSVN features in large cohorts requires a reliable and automated mechanism to extract the vascular networks. In this talk, we present two distinct methods for PCSVN extraction. Our first algorithm builds upon a directional multiscale mathematical framework based on a combination of shearlets and Laplacian eigenmaps and is able to isolate vessels with high success in high-contrast images such as those produced in CT scans. Our second algorithm applies a conditional generative adversarial neural network (cGAN) and was trained to simulate a human-traced PCSVN given a digital photograph of the placental chorionic surface. This method surpasses any existing automated PCSVN extraction methods reported on digital photographs of placentas.

Karamatou Yacoubou Djima
Amherst College
kyacouboudjima@amherst.edu

Catalina Anghel
University of California Davis
catalina.anghel@alum.utoronto.ca

Kellie Archer
The Ohio State University
archer.43@osu.edu

Jen-Mei Chang
California State University, Long Beach
Department of Mathematics
jen-mei.chang@csulb.edu

Amy Cochran
University of Wisconsin
cochran4@wisc.edu

Anca R. Radulescu
State University of New York at New Paltz
Ms.
radulesa@newpaltz.edu

Carolyn Salafia
Placental Analytics, LLC

car- olyn.salafia@gmail.com

Rebecca Turner
The University of Auckland
rm.turner@auckland.ac.nz

Lan Zhong
University of Delaware
lanzhong@udel.edu

MS141

Comparative Spectral Decompositions for Personalized Cancer Diagnostics, Prognostics, and Therapeutics

I will describe the development of novel, multi-tensor generalizations of the singular value decomposition, and their use in the comparisons of brain, lung, ovarian, and uterine cancer and normal genomes, to uncover patterns of DNA copy-number alterations that predict survival and response to treatment, statistically better than, and independent of, the best indicators in clinical use and existing laboratory tests. Recurring alterations have been recognized as a hallmark of cancer for over a century, and observed in these cancers genomes for decades; however, copy-number subtypes predictive of patients outcomes were not identified before. The data had been publicly available, but the patterns remained unknown until the data were modeled by using the multi-tensor decompositions, illustrating the universal ability of these decompositions generalizations of the frameworks that underlie the theoretical description of the physical world to find what other methods miss.

Orly Alter
Scientific Computing and Imaging Institute
University of Utah
orly@sci.utah.edu

MS141

Decompositions in Sum of Low-rank Block Terms: Can Block Size be Considered as a Type of Diversity

In order to achieve a unique and interpretable decomposition, models make use of the different types of diversity in the data. For example, in certain cases, data that contains diversity in time, space, and frequency, can be formulated as a three-way tensor, and be uniquely factorized in a sum of rank-1 terms under mild constraints. However, the assumption that data can be modeled as a sum of rank-1 contributions is sometimes inaccurate, for various physical reasons. Therefore, models that factorize the data in a sum of terms whose rank is larger than one have been proposed. Such models are sometimes referred to as decompositions in a sum of low-rank block terms. In this talk, we raise the question whether the size of the block, or the value of the rank of each low-rank term in a decomposition, can be regarded as a diversity. To address this matter, we present cases in which a different block size guarantees uniqueness, as well as other situations in which the presence of terms with a different rank sometimes prevents uniqueness.

Dana Lahat, Christian Jutten
GIPSA-Lab
Dana.Lahat@gipsa-lab.grenoble-inp.fr,
christian.jutten@gipsa-lab.grenoble-inp.fr

MS141

Mathematics of Neural Nets

A plethora of exciting mathematics questions have gotten raised in trying to explain the resurgence of neural networks in being able to execute complex artificial intelligence tasks. In this talk I will give a brief overview of some of the questions that me and Amitabh Basu (with other collaborators) have been exploring. We will start from the basic definition of neural networks and will describe various results that we have gotten about the space of functions that these "architectures" represent. We will particularly focus on (1) our recent results [A. Mukherjee and A. Basu, "Lower bounds over Boolean inputs for deep neural networks with ReLU gates," Electronic Colloquium on Computational Complexity, Report No. 190 (2017)] proving a first of its kind lower bounds on the size of high depth neural circuits representing certain Boolean functions and (2) our results trying to formalized the connection between autoencoders and sparse coding [A. Rangamani, A. Mukherjee, A. Basu, T. Ganapathy, A. Arora, S. Chin and T. Tran, "Sparse coding and autoencoders," (arxiv.org/abs/1708.03735)].

Anirbit Mukherjee
Johns Hopkins University
amukhe14@jhu.edu

Amitabh Basu
Dept. of Mathematics
Universiity of California, Davis
abasu@math.ucdavis.edu

MS141

Tensor Decompositions in Deep Learning

First, we discuss several applications of tensor decomposition in deep learning networks. Then, we propose a novel method using tensor decomposition to increase parameter efficiency within a deep neural networks. We demonstrate the performance of our algorithm for several layers of network.

Carmeliza Navasca
Department of Mathematics
University of Alabama at Birmingham
cnavasca@gmail.com

MS142

Perspective Duality in three Liftings

Many modern applications rely on convex optimization, which offers a rich modeling paradigm as well as strong theoretical guarantees and computational advantages. Convex duality often plays a central role. I will describe the geometry behind a simple form of convex duality based on polarity of convex cones, and show how it can be used to develop a computationally efficient algorithm for the phase-retrieval problem in x-ray crystallography.

Michael P. Friedlander
Dept of Computer Science
University of British Columbia

mpf@cs.ubc.ca

MS142

Imaging from the Inside Out - Inverse Scattering in Fluorescence Microscopy

We propose a method to reconstruct the optical properties of a scattering medium with subwavelength resolution. The method is based on the solution to the inverse scattering problem with photoactivated internal sources used in fluorescence microscopy. Numerical simulations of three-dimensional structures demonstrate that a resolution of approximately $\lambda/25$ is achievable. Relation to the source localization problem in fluorescence microscopy will be discussed.

Howard Levinson
University of Michigan - Ann Arbor
Dept. of Mathematics
levh@umich.edu

Anna Gilbert
Department of Mathematics
University of Michigan
annacg@umich.edu

John Schotland
University of Michigan
schotland@umich.edu

MS142

Signal Recovery from Phaseless Correlation Measurements via Wigner Distribution Deconvolution

We will discuss phase retrieval from short-time Fourier transfrom magnitude measurements of a vector x based on a two step approach: First, a modified Wigner distribution deconvolution approach is used to solve for a portion of the lifted rank-one signal xx^*. Second, an angular synchronization approach is used to recover x from the known portion of xx^*. In addition to being computationally efficient the proposed method also gives insight into the design of good window/probe functions.

Sami Merhi, Michael Perlmutter, Mark Iwen
Michigan State University
merhisam@math.msu.edu, perlmut6@mail.msu.edu, markiwen@math.msu.edu

MS142

3D Image Reconstruction from Diffused Light

This talk will describe a new imaging system that uses computational imaging the joint design of optical systems and inverse algorithms - to enable 3D imaging from a single-shot with a lensless camera consisting of only a scattering element (a diffuser) placed in front of a 2D image sensor. We use simple calibration methods and optical models to define computationally efficient forward models for our optical system. Then, reconstruction algorithms based on large-scale nonlinear non-convex optimization are combined with sparsity-based regularizers similar to compressed sensing in order to solve the inverse problem.

Laura Waller
Berkeley
waller@berkeley.edu

MS143

Asynchronous Iterative Methods: Models and Implementations

Asynchronous fixed-point iterations for solving linear and nonlinear equations is an example of a non-bulk synchronous parallel algorithm that allows processors to continue processing without waiting for other processors at synchronization points. Such methods also provide a certain type of resilience against communication delays. We will discuss the classical mathematical models of asynchronous iterative methods, how these models differ from realistic implementations, and the consequences of these differences.

Edmond Chow
School of Computational Science and Engineering
Georgia Institute of Technology
echow@cc.gatech.edu

MS143

Recycling Krylov Subspaces and Preconditioners for Iterative Methods

For a sequence of linear systems, we consider preconditioner updates as maps between matrices, typically from new matrices to a base matrix for which a good preconditioner is available. The main idea is that if $M_k A_k \approx A_0$ and $A_0 P_0 \approx I$, then $M_k A_k P_0 \approx I$. If matrices change slowly, such maps may be cheap to compute. We consider additional updates to the maps M_k (preconditioner updates) based on information from the (augmented) Krylov subspace.

Eric De Sturler
Virginia Tech
sturler@vt.edu

MS143

Symmetrizing Nonsymmetric Toeplitz Matrices in Fractional Diffusion Problems

Fractional diffusion equations are increasingly used in applications. Discretising these equations by shifted Grünwald-Letnikov finite difference approximations on uniform meshes lead to Toeplitz, block Toeplitz, and related matrices, all of which may be nonsymmetric. In this talk we will discuss how to symmetrize these nonsymmetric matrices, and the benefits of doing so. We will also propose preconditioning strategies for the symmetrized problems.

Jennifer Pestana
School of Mathematics
The University of Manchester
jennifer.pestana@strath.ac.uk

MS143

Multiple Preconditioned Gmres for Shifted Systems, with Applications to Hydrology and Matrix Functions

GMRES with multiple preconditioners (MPGMRES) is a method that allows for several preconditioners to be used simultaneously. In this manner, the effect of all preconditioners is applied in each iteration. An implementation of MPGMRES is proposed for solving shifted linear systems

with shift-and-invert preconditioners. With this type of preconditioner, the Krylov subspace can be built without requiring the matrix-vector product with the shifted matrix. Furthermore, the multipreconditioned search space is shown to grow only linearly with the number of preconditioners. This allows for a more efficient implementation of the algorithm. The proposed implementation is tested on shifted systems that arise in computational hydrology and the evaluation of different matrix functions. The numerical results indicate the effectiveness of the proposed approach.

Daniel B. Szyld
Temple University
Department of Mathematics
szyld@temple.edu

Tania. Bakhos
BCAM. Bilbao, Spain
tania.bakhos@gmail.com

Peter K. Kitanidis
Dept. of Civil and Environmental Engineering
Stanford University
peterk@stanford.edu

Scott Ladenheim
Next Ocean
scottladenheim@nextocean.nl

Arvind Saibaba
North Carolina State University
asaibab@ncsu.edu

MS144

Accurate Gradient and Force Computation for Elliptic Interface Problems

The matched interface and boundary (MIB) method is a 2nd order numerical method for elliptic interface problems with piecewise variable coefficients, finite jump across a smooth interface, and singular sources. In this talk, we extend the MIB method by developing second order scheme to compute gradient from each side of the interface and on irregular points of the MIB discretization, particularly when singular sources are regularized using Green's function based decomposition. Furthermore, schemes for computing gradient can be conveniently applied to compute the electrostatic solvation force of the elliptic Poisson-Boltzmann model, which is very significant and useful in biophysics and biochemistry. Numerical examples at various level of complexity are provided to validate the schemes for gradient and force computations.

Weihua Geng
Southern Methodist University
wgeng@smu.edu

Shan Zhao
Department of Mathematics
University of Alabama
szhao@ua.edu

MS144

A Consistent Spatially Adaptive Meshless Method for Modeling Fluid-structure Interactions

We seek to accelerate and increase the size of simulations for fluid-structure interactions (FSI) by using adaptive resolutions in the spatial discretization of the equations governing the time evolution of systems displaying two-way fluid-solid coupling. To this end, we propose a consistent adaptive-resolution smoothed particle hydrodynamics (SPH) approach, in which spatial resolutions adaptively vary according to a recovery-based error estimator of velocity gradient as flow evolves. The second-order consistent discretization of spatial differential operators is employed to ensure the accuracy of the proposed method. The convergence, accuracy, and efficiency attributes of the new method are assessed by simulating different flows. In this process, the numerical results are compared to the analytical and finite element solutions. We anticipate that the proposed adaptive-resolution method will enlarge the class of SPH-tractable FSI applications.

Wei Hu, Guannan Guo
University of Wisconsin-Madison
whu59@wisc.edu, gguo7@wisc.edu

Wenxiao Pan
University of Wisconsin Madison
wpan9@wisc.edu

MS144

Cavitation Occurrence Near the Perforation of the Cell Membrane by Shock-wave Induced Nanobubble Collapse

The collapse of the bubble induced by the shock wave is investigated by Martini coarse-grained molecular dynamic (CG-MD) simulations, as well as the resulting nanojet perforating the membrane. Results show that at the nanoscale, the occurrence of cavitation nucleation is observed during the perforating process. The cavitation located near the puncture of the cell membrane and its ultimate evolutionary form presents a ring-like structure. The volume of the cavitation is calculated for different initial bubble size, and it is found that the maximum volume of the cavitation area has a correlation with the initial bubble size. For a deeper understanding of the cavitation phenomenon, the pressure field of the simulation system is obtained by using Irving-Kirkwood-Noll procedure. The consistence between the results of CG-MD and the classical nucleation theory reveals that the average pressure of the local environment plays a crucial role in cavitation occurrence on a non-equilibrium system subjected to strong inertia, e.g., shock wave.

Nan Nan, Guohui Hu
Shanghai University, China
mechanicsnan@163.com, hu_guohui@126.com

MS144

Investigating Pyrolysis Mechanism of Biomass with Large Scale Reactive Molecular Dynamics

This talk overviews the methodology development of large scale reactive molecular dynamics using ReaxFF force field for challenging problems in energy applications. We created two codes, one is GMD-Reax [Mo Zheng et al., Algorithms of GPU-enabled reactive force field (ReaxFF) molecular dynamics. Journal of Molecular Graphics and Modelling 2013, 41, (April), 1-11] that allows for efficient simulations of large models of 10,000 atoms on a single GPU, another is VARxMD [Jian Liu et al. Reaction Analysis and Visualization of ReaxFF Molecular Dynamics Simulations. Journal of Molecular Graphics and Modelling

2014, 53(9)13-22] that is capable for detailed reaction analysis critical for large model simulation. The pyrolysis simulations of lignin reveals the pyrolysis stages, the underlying linkage behaviour and initial reaction pathways [Tingting Zhang et al. Initial Reactivity of Linkages and Monomer Rings in Lignin Pyrolysis Revealed by ReaxFF Molecular Dynamics. Langmuir 2017, 33 (42), 11646-11657]. Large scale simulation of cellulose was found to give closer prediction of evolution tendency of glycolaldehyde and levoglucosan with temperature than that of small scale model [Mo Zheng et al. Initial reaction mechanisms of cellulose pyrolysis revealed by ReaxFF molecular dynamics. Fuel 2016, 177, 130-141]. The comprehensive insight obtained in simulations of biomass pyrolysis is hardly accessible experimentally or by other computational approach.

Xiaoxia Li
Institute of Process Engineering (IPE), CAS, China
University of Chinese Academy of Sciences, China
xxia@ipe.ac.cn

Mo Zheng
IPE, Chinese Academy of Sciences
mzheng@ipe.ac.cn

Tingting Zhang
IPE, Chinese Academy of Sciences
University of Chinese Academy of Sciences
zhangtt@ipe.ac.cn

MS145

SLATE: Software for Linear Algebra Targeting Exascale

The objective of the Software for Linear Algebra Targeting Exascale (SLATE) project is to provide fundamental dense linear algebra capabilities to the US Department of Energy and to the high-performance computing (HPC) community at large. To this end, SLATE will provide basic dense matrix operations (e.g., matrix multiplication, rank-k update, triangular solve), linear systems solvers, least square solvers, singular value and eigenvalue solvers. The ultimate objective of SLATE is to replace the venerable Scalable Linear Algebra PACKage (ScaLAPACK) library, which has become the industry standard for dense linear algebra operations in distributed memory environments. However, after two decades of operation, ScaLAPACK is past the end of its lifecycle and overdue for a replacement, as it can hardly be retrofitted to support hardware accelerators, which are an integral part of today's HPC hardware infrastructure. Primarily, SLATE aims to extract the full performance potential and maximum scalability from modern, many-node HPC machines with large numbers of cores and multiple hardware accelerators per node. For typical dense linear algebra workloads, this means getting close to the theoretical peak performance and scaling to the full size of the machine (i.e., thousands to tens of thousands of nodes). This is to be accomplished in a portable manner by relying on standards like MPI and OpenMP.

Jakub Kurzak
University of Tennessee, Knoxville
kurzak@icl.utk.edu

Mark Gates
Computer Science Department
University of Tennessee
mgates3@icl.utk.edu

Piotr Luszczek
University of Tennessee
luszczek@icl.utk.edu

Jack J. Dongarra
University of Tennessee, Oak Ridge National Laboratory, USA
dongarra@icl.utk.edu

MS145

Factorization Based Sparse Solvers and Preconditioners for Exascale

Factorization based algorithms are often the most robust algorithmic choices for solving linear systems from multiphysics and multiscale simulations, being used as direct solvers, or as coarse-grid solvers in multigrid, or as preconditioners for iterative solvers. Recently we developed a number of techniques to improve scalability: a new 3D sparse factorization algorithm enables strong scaling to 24,000 cores, a new asynchronous broadcast/reduction tree algorithm enables sparse triangular solve to strong scale to over 4000+ cores, and a new adaptive randomized sampling algorithm improves robustness and efficiency of data-sparse HSS low-rank construction. We will demonstrate performance of these techniques as are implemented in the parallel SuperLU and STRUMPACK libraries.

Sherry Li
Lawrence Berkeley National Laboratory
xsli@lbl.gov

MS145

Approaches for Leveraging Emerging Fine-Grained Parallel Computer Architectures in PETSc

As the high-performance computing (HPC) community approaches the exascale horizon, power and heat considerations have driven the increasing importance and prevalence of fine-grained parallelism in new computer architectures. HPC centers have become increasingly reliant on GPGPU accelerators and "manycore" processors such as the Intel Xeon Phi line, and 512-bit SIMD registers have even been introduced in the latest generation of Intel's mainstream Xeon server processors. The high degree of fine-grained parallelism and more complicated memory hierarchy considerations of such "manycore" processors present several challenges to existing scientific software; additionally, the sheer size of supercomputers as we approach the exascale means complications for leveraging inter-node parallelism as well. Here, we consider how the Portable, Extensible Toolkit for Scientific Computation (PETSc) library can best take advantage of these novel architectures. Our approach is based on compact and architecture-specific kernels, which are composed in an architecture-agnostic manner to preserve runtime configurability and maintainability. We will discuss some key features of these architectures and our code optimizations and algorithmic developments targeted at them, and present experiences with benchmark problems drawn from a wide range of applications.

Richard T. Mills
Argonne National Laboratory
rtmills@anl.gov

Mark Adams
Lawrence Berkeley Laboratory
mfadams@lbl.gov

Jed Brown
University of Colorado Boulder
jed.brown@colorado.edu

Matthew G. Knepley
University at Buffalo
Department of Computer Science and Engineering
knepley@gmail.com

Karl Rupp
Freelance Computational Scientist
me@karlrupp.net

Barry Smith, Hong Zhang
Argonne National Laboratory
bsmith@anl.gov, hongzhang@anl.gov

Hong Zhang
MCS, Argonne National Laboratory
hzhang@mcs.anl.gov

Junchao Zhang
Argonne National Laboratory
jczhang@mcs.anl.gov

MS145

Solving Large-scale Eigenvalue Problems in DOE Applications

Eigenvalue problems arise in several DOE applications. In some applications, we need to compute a few eigenpairs of an extremeley large but sparse matrix. In other applications, the number of eigenpairs to be computed can be quite large even though it is still a small fraction of the dimension of the matrix. We will discss efficient algorithms for solving these types of problems and their implementation on massively parallel computers.

Chao Yang
Lawrence Berkeley National Lab
cyang@lbl.gov

MS146

Sparse Harmonic Transforms: A New Class of Sublinear-time Algorithms for Approximating Functions of Many Variables

The development of sublinear-time compressive sensing methods for signals which are sparse in Tensorized Bases of Bounded Orthonormal Functions (TBBOFs) will be discussed. These new methods are obtained from CoSaMP by replacing its usual support identification procedure with a new faster one inspired by fast Sparse Fourier Transform (SFT) techniques. The resulting sublinearized CoSaMP method allows for the rapid approximation of TBBOF-sparse functions of many variables which are too hideously high-dimensional to be learned by other means. Both numerics and theoretical recovery guarantees will be presented.

Mark Iwen, Bosu Choi
Michigan State University
markiwen@math.msu.edu, choibosu@math.msu.edu

Felix Krahmer
TUM
f.krahmer@math.uni-goettingen.de

MS146

Fast Binary Embeddings of Data

We consider distance-preserving fast binary embeddings. Specifically, we propose fast methods to replace points from a set $\mathcal{X} \subset R^N$ with points in a lower-dimensional cube $\{\pm 1\}^m$, which we endow with an appropriate function to approximate Euclidean distances in the original space.Our methods rely on quantizing fast Johnson-Lindenstrauss embeddings based on bounded orthonormal systems and partial circulant ensembles, both of which admit fast transforms. Our quantizationmethods utilize noise-shaping, and include Sigma-Delta schemes and distributed noise-shaping schemes. The resulting approximation errors decay polynomially and exponentially fast inm, dependingon the embedding method. This dramatically outperforms the current decay rates associated with binary embeddings and Hamming distances. Additionally, it is the first such binary embedding result thatapplies to fast Johnson-Lindenstrauss maps while preserving ℓ_2 norms.

Rayan Saab
University of California, San Diego
rsaab@ucsd.edu

MS146

Learning Interaction Rules from Observations of Opinion Dynamics

Abstract not available at time of publication.

Sui Tang
Johns Hopkins University
stang@math.jhu.edu

MS146

Compatibility of the Rth Order Sigma Delta Quantization and the Partial Fourier Measurements

Sigma Delta quantization has been demonstrated to be compatible with random Gaussian and sub-Gaussian compressed sensing matrices, in the sense that the reconstruction error decreases polynomially with respect to the ratio of the actual sampling rate and the intrinsic dimension of the (sparse) signals. Extending this result to the more practical Fourier matrices faces two issues. 1. the high frequency components in the measurements cannot be preserved by Sigma Delta quantization. 2. very little is known about the singular vectors of the finite difference matrix raised to integer powers which plays a key role in the formulation of Sigma Delta quantization. In this talk, we will address both problems and subsequently prove the reconstruction guarantee under partial Fourier measurements and harmonic frames. Specifically, we will solve the first problem by randomizing the measurements, and solve the second problem by proving useful properties of the finite difference matrix raised to any integer power. (This is joint work with Mark Iwen, Rayan Saab, and Wei-husan Yu).

Rongrong Wang
University of British Columbia
wangron6@msu.edu

MS147

Data-driven Parameterization of Generalized

Langevin Equation

Computational model of multiscale dynamic systems is centered around projecting the high-dimensional full system dynamics onto a set of resolved field variables. For hamiltonian system, the projected dynamics is often casted into the generalized Langevin Equation with unparameterized free energy term and memory kernel. We develop a numerical method based on machine-learning algorithm for multi-dimensional density estimation to construct free energy landscape. Also we develop a method to utilize the trajectory information to parameterize the memory kernel which retains fluctuation-dissipation theorem and invariant measure. The proposed methods enable efficient data-driven parameterization of the GLE with broad applications to multiscale dynamics in physics, engineering and biological systems.

Huan Lei
Pacific Northwest National Laboratory
huan.lei@pnnl.gov

Lei Wu
School of Mathematical Sciences
Peking University, China
leiwu@pku.edu.cn

Xiantao Li
PSU
xli@psu.edu

Nathan Baker
Pacific Northwest National Laboratory
nathan.baker@pnnl.gov

MS147

Thermodynamic Formalism and Uncertainty Quantification for Stochastic Processes and Generalized Langevin Equations

We present a number of tools and techniques based on information theory, applied probability, and the thermodynamic formalism which provide computable Uncertainty Quantification bonds for stochastic processes, especially in the long-time (steady state regime). We will discuss both sensitivity analysis (i.e. linearized UQ bounds) as well as more robust bounds to quantify uncertainties beyond the linear regime. We will illustrate our results with various examples including the generalized Langevin equation.

Luc Rey-Bellet
Department of Mathematics & Statistics
University of Massachusetts
luc@math.umass.edu

MS147

The Strong Coupling Limit of the Quasiclassical Generalised Langevin Equation

We present a quasiclassical generalised Langevin equation (GLE) based on the GLE approach introduced in L. Stella et al. Phys. Rev. B 89 134303 (2014). In this way, we simulate the quantum delocalisation of light particles coupled to a large class of non-markovian environments, also in the strong coupling limit. The expected isotopic effect is observed, as well as a quantum-to-classical crossover when the strength of the system-environment interaction is increased. Saturation of the transition rates at low temperature is also retrieved, in qualitative, yet not quantitative, agreement with the quantum transition state theory. The discrepancies and the role of the effective classical potential are discussed to clarify the domain of applicability of this flexible and computationally efficient quasiclassical GLE approach.

Lorenzo Stella
Queen's University Belfast
l.stella@qub.ac.uk

MS147

Renormalized Reduced Order Models for Long Time Prediction

We examine the challenging problem of constructing reduced models for the long time prediction of systems where there is no timescale separation between the resolved and unresolved variables. In previous work we focused on the case where there was only transfer of activity (e.g. energy, mass) from the resolved to the unresolved variables. Here we investigate the much more difficult case where there is two-way transfer of activity between the resolved and unresolved variables. Like in the case of activity drain out of the resolved variables, even if one starts with an exact formalism, like the Mori-Zwanzig (MZ) formalism, the constructed reduced models can become unstable. We show how to remedy this situation by using dynamic information from the full system to renormalize the MZ reduced models. In addition to being stabilized, the renormalized models can be accurate for very long times. We use the Korteweg-de Vries equation to illustrate the approach. The coefficients of the renormalized models exhibit rich structure, including algebraic time dependence and incomplete similarity.

Jacob Price
University of Washington
jrp14@uw.edu

Panos Stinis
Pacific Northwest National Laboratory
panagiotis.stinis@pnnl.gov

MS148

Uncertainty in Electrostatics and Solvation Calculations

Modeling the electrostatic potential and solvation free energies in systems comprised of biomolecules is an essential step for understanding molecule interactions and designing medicines. Because of limits to computational power, it is challenging to engage such modeling using an explicit solvent model. Therefore, implicit solvent models and their applications have been the main subject in electrostatics and solvation calculations. In implicit solvent electrostatics and energy calculations, atomic radii and charges are two major parameters. The optimization problem for charges and radii is underdetermined, leading to uncertainty in the values of these parameters and the results of solvation energy calculations using them. This study presents a new method for quantifying this uncertainty in implicit solvation calculations of small molecules using surrogate models based on generalized polynomial chaos expansions. The surrogate models for different atom types may be constructed using least-squares fitting because of the low-dimensional spaces. Meanwhile, the construction of surrogate models for the charge parameter space requires compressed sensing combined with an iterative rotation method to enhance problem sparsity. We have tested this

method in the statistical assessment of modeling of proteins and ligands challenge community. The method also provides a framework for efficiently quantifying uncertainty in a diverse range of force field parameterization problems.

Peiyuan Gao, Xiu Yang, Huan Lei, Nathan Baker
Pacific Northwest National Laboratory
peiyuan.gao@pnnl.gov, xiu.yang@pnnl.gov, huan.lei@pnnl.gov, nathan.baker@pnnl.gov

MS148

Computation of Electrostatic Binding Energy of Solvated Protein Complexes using the TABI Poisson-Boltzmann Solver

The Poisson-Boltzmann (PB) equation is a popular framework for computing electrostatics of solvated biomolecules. Our recently developed treecode-accelerated boundary integral (TABI) solver enables accurate and efficient PB computations on the triangulated molecular surface, yielding the electrostatic solvation energy of the system, ΔG_{solv}. The present work extends TABI to compute the electrostatic binding energy, $\Delta\Delta G_{\text{bind}}$, and we compare two surface triangulation options, MSMS and NanoShaper. Since the binding energy is the difference between the free energy of the complex and the two independent monomers, it is more sensitive to the accuracy of the PB solver and requires higher triangulation density to achieve a given accuracy. To address this issue we obtain significantly improved accuracy at low computational cost by extrapolating binding energy values computed at low density, and we find that NanoShaper is more robust for this purpose. Our results are benchmarked with the well-established high-order Matched Interface and Boundary (MIB) PB solver for a set of 51 biomolecular complexes. The resulting code facilitates biomolecular binding energy computations and it is publicly available.

Robert Krasny
University of Michigan
Department of Mathematics
krasny@umich.edu

Leighton Wilson
University of Michigan
lwwilson@umich.edu

Jingzhen Hu, Jiahui Chen
Department of Mathematics
Southern Methodist University
journeyh@smu.edu, jiahuic@smu.edu

Weihua Geng
Southern Methodist University
wgeng@smu.edu

MS148

A Consistent Meshless Method for Modeling Electrokinetic Flows

We present a consistent meshless, Lagrangian method based on implicit incompressible smoothed particle hydrodynamics (I2SPH) for solving the fully coupled Navier-Stokes, Poisson-Boltzmann, and advection-diffusion equations subject to Dirichlet or Robin boundary conditions. It is applied to model various two and three dimensional electrokinetic flows in simple or complex geometries. The accuracy and convergence of the numerical solutions are examined via comparison with analytical solutions, mesh-based numerical solutions, or empirical models. The new method provides a framework to explore broader applications of meshless methods in microfluidics and complex fluids with charged objects, such as colloids and biomolecules, in arbitrary complex geometries.

Wenxiao Pan
University of Wisconsin Madison
wpan9@wisc.edu

MS148

Inverse Problem for the Poisson-Bolzmann Equation

Dielectric permittivity is one of the defining parameters of the biomolecular electrostatics. In implicit solvent models, this value is particularly critical because distinct values are used for solute and solvent. Here we report an inverse problem of the Poisson-Boltzmann equation and related numerical procedure for determination of dielectric permittivity. Our method allows one to calculate a dielectric permittivity for implicit solvent models such that the computed electrostatic potential or solvation energy will be consistent with explicit solvent models.

Yongcheng Zhou
Department of Mathematics
Colorado State University
yzhou@math.colostate.edu

MS149

On Optimal Interpolation with Monogenic Functions

A system of basis functions is called optimal with respect to certain nodes if the interpolationg function constructed by the basis function coincides with the best L_2-approximation. The main problem in the interpolation with monogenic functions or polynomials, respectively, is caused by the non-commutativity of the multiplication in Clifford algebras. This leads to the fact that the product of two monogenic functions is not again monogenic and the usual methods for constructing interpolation polynomials fail. We will present a variational method that leads to optimal basis functions and does not need the commutativity of the multiplication. Two examples will be shown. One is based on a system of shifted fundamental solutions of a generalized Cauchy-Riemann operator and the second works on a special basis of monogenic functions. The idea can be extended to the interpolation of solutions to partial differential equations by simple solutions of the same equation or the monogenic functions are used as building blocks for the solutions of more complicated equations.

Klaus Guerlebeck
Bauhaus Universität, Weimar
klaus.guerlebeck@uni-weimar.de

MS149

Overview of Current Results in Numerical Clifford Algebras

We focus on the application of numerical methods in algebra of quaternions. In order to gain insight into the multidimensional case, we first study the simplest case, i.e. the linear equation in quaternions. We have created an algorithm for the solution based on the fixed point formulation. A natural next step is to study solutions of quadratic

quaternionic equations, or more precisely to search for roots of simple quadratic quaternionic polynomials. Based on the theory of companion polynomials, an algorithm was developed to calculate all roots of simple polynomials of degree n. In general, quaternionic coefficients can be located on both sides of the powers. If so, there are even 5 different zero classes, that are classified according to the rank of a certain real 4×4 matrix. All results can be extended to other noncommutative algebras in R^4. For example, we studied the eigenvalue problem for square matrices with coquaternionic entries. Another generalization is to examine algebras in R^n, $n \geq 4$, for example in R^8. In the paper by Lauterbach and Opfer, Advances in Applied Clifford Algebras 24(2014), the authors constructed an exact Jacobi matrix for functions defined in noncommutative algebraic systems without the use of any partial derivative. The goal was simple application of Newton's method in algebras defined in R^n.

Drahoslava Janovska
University of Chemistry and Technology
drahoslava.janovska@vscht.cz

MS149

Generalizations of Mandelbrot and Julia Sets to Higher Dimensions

The question of what happens when we iterate a function has received much attention, yet many basic problems remain open. Such questions are interesting in itself, but also important in the field of numerical mathematics, e.g. the dynamics of Newton's method. The study of iteration of complex functions was initiated by Julia and Fatou and revived by Mandelbrot and his work on fractal aspects of iteration of quadratic functions. The question is whether these theories have higher dimensional analogues. Here we focus on attempts to obtain generalizations of the complex quadratic case and objects such as the Mandelbrot and Julia sets. The natural generalization via quaternions give trivial results, thus attention has focused on other algebraic structures, such as bicomplex numbers, where analogies to the Julia-Fatou theory exist, coquaternions etc. Especially the amateur community is active in seeking very 'exotic' structures in hope of finding interesting 3D or 4D fractal objects, such as the Tetrabrot set and others. Another approach is to directly generalize the dynamics of complex quadratic polynomials to higher dimensions (Mandelbulb and Mandelbox sets). We give an overview of these attempts and what little is known theoretically. Finally, we present the author's approach using limit sets of three-dimensional Kleinian groups and analogies based on Sullivan's dictionary connecting these sets to holomorphic dynamics.

Vaclav Kucera
Charles University Prague, Czech Republic
kucera@karlin.mff.cuni.cz

MS149

The Relation Between Companion Polynomials and Companion Matrices

Given a polynomial

$$p(z) = \sum_{j=0}^{n} a_j z^j, \text{ where } a_j \text{ are quaternions}, a_n = 1, a_0 \neq 0.$$

Are there zeros of p and how can one find them? The two methods proposed by Serôdio, Pereira, Vitória, Computer. Math. Appl. 42(2001) and by Janovská, Opfer, SIAM J. Numer. Anal. 48(2010) produce the same zeros of p. The first method uses the quaternionic *companion matrix* $\mathbf{C}$ and the second the real *companion polynomial* c of p which has the following consequence. **Theorem:** *The companion polynomial c is the characteristic polynomial of the complex isomorphic matrix $\imath(\mathbf{C})$ derived from the companion matrix $\mathbf{C}$. Or in other words: The roots of the real companion polynomial c are the eigenvalues of the complex matrix $\imath(\mathbf{C})$. The zeros of p are contained in the similarity classes of the roots of c.*

Gerhard Opfer
Universität Hamburg
gerhard.opfer@uni-hamburg.de

MS150

Adventures in Fp16 Arithmetic

The 2008 revision of the IEEE-754 standard defines half precision (fp16) as a storage format. Hardware support for fp16 computation is now available on high-end graphical processing units (GPUs) from AMD and NVIDIA. Recent advances in deep learning exploit fp16 (and even lower precisions) and it is starting to be considered for general purpose scientific computing because of its speed and its low storage and energy requirements. However, the set of fp16 numbers is small and its range is narrow, making underflow or overflow likely. We assess the pros and cons of fp16 arithmetic for scientific computation and provide suggestions on how to overcome its limitations.

Pierre Blanchard
University of Manchester
pierre.blanchard00@gmail.com

Theo Mary
Universite de Toulouse, UPS-IRIT
theo.mary@enseeiht.fr

Nicholas J. Higham
School of Mathematics
The University of Manchester
nick.higham@manchester.ac.uk

MS150

Error Bounds for Iterative Refinement in Three Precisions

Motivated by the emergence of multiprecision capabilities in hardware, we propose a general algorithm for solving an $n \times n$ nonsingular linear system $Ax = b$ based on iterative refinement with three precisions. The working precision is combined with possibly different precisions for solving for the correction term and for computing the residuals. We derive sufficient conditions for convergence and bounds for the attainable forward error and normwise and componentwise backward errors. Our results generalize and unify many existing rounding error analyses. Our results suggest that on architectures for which half precision is efficiently implemented it will be possible to solve certain linear systems $Ax = b$ up to twice as fast and to greater accuracy

Erin C. Carson
New York University

erin.carson@nyu.edu

MS150

Investigating Half Precision Arithmetic to Accelerate Dense Linear System Solvers

The in-hardware acceleration of half precision arithmetic (FP16) in recent GPUs has reinvigorated a great interest in the mixed-precision iterative refinement technique. The technique is based on the use of low precision arithmetic to accelerate the general HPC problem of solving Ax = b, where A is a large dense matrix, and the solution is needed in FP64 accuracy. We present algorithms and their high-performance implementations that enable mixed-precision iterative refinement to use FP16 arithmetic to significantly accelerate FP64- precision Ax = b solvers. We quantify in practice the performance and limitations of the approach. The main hardware target is the Volta V100 GPU, specifically to demonstrate for the first time how to use the V100 Tensor Cores (TC) that provide an additional FP16-TC performance boost amounting to an unprecedented performance of 112 FP16-TC TeraFlops/s (Tflop/s). We show that even a highly optimized FP64-precision solver, running at 6 Tflop/s, can be accelerated up to 4X.

Azzam Haidar
Department of Electrical Engineering and Computer Science
University of Tennessee, Knoxville
haidar@icl.utk.edu

Stanimire Tomov, Panruo Wu
University of Tennessee, Knoxville
tomov@icl.utk.edu, pwu11@icl.utk.edu

Jack J. Dongarra
University of Tennessee, Oak Ridge National Laboratory, USA
dongarra@icl.utk.edu

MS150

IEEE Half precision arithmetic to the rescue for challenging embedded applications on GPUs, FPGAs and ASICs

Algorithms today require a significant amount of computation complexity along with high demand for data transfers between the host (CPU) and the accelerator (GPU/ASIC/FPGA). For embedded efficiency traditionally the only option is to convert the floating-point algorithm to fixed-point before C/HDL implementation. Half-precision arithmetic (16 bit floating-point) provides best of both worlds in terms of higher dynamic range than traditional fixed-point or integer data types and a smaller number of bits compared to single (32)/double(64). This topic discusses numerical algorithms and challenges in building math and trigonometric operators for half-precision types with lower units in the last place (ULP) error and higher simulation and code generation efficiency. This topic also compares design trade-offs of using half-precision to single/double for real-world applications in radar and deep learning applications where floating-point math plays a significant role.

Kiran Kintali
The MathWorks Inc.
Kiran.Kintali@mathworks.com

Srinivas Muddana
MathWorks
srinivas.muddana@mathworks.com

MS151

Seismic Imaging and Multiple Removal via Model Order Reduction

We introduce a novel framework for imaging and removal of multiples from seismic data based on model order reduction. The reduced order model (ROM) is an orthogonal projection of the wave equation propagator (Green's function) on the subspace of discretely sampled time domain wavefield snapshots. The projection can be computed just from the knowledge of the seismic data using the block Cholesky factorization. Once the ROM is found, its use is twofold. First, the projected propagator can be backprojected to obtain an image. ROM computation implicitly orthogonalizes the wavefield snapshots. This highly nonlinear procedure differentiates our approach from the conventional linear migration methods (Kirchhoff, RTM). It allows to resolve the reflectors independently of the knowledge of the kinematics and to untangle the nonlinear interactions between the reflectors. As a consequence, the resulting images are almost completely free from the multiple reflection artifacts. Second, the ROM computed from the original seismic data can be used to generate the Born data set, i.e. the data that the measurements would produce if the propagation of waves in the unknown medium obeyed Born approximation instead of the full wave equation. Obviously, such data only contains primary reflections and the multiples are removed. Consecutively, existing linear imaging and inversion techniques can be applied to Born data to obtain reconstructions in a direct, non-iterative manner.

Alexander V. Mamonov
University of Houston
mamonov@math.uh.edu

Liliana Borcea
University of Michigan
borcea@umich.edu

Vladimir L. Druskin, Mikhail Zaslavsky
Schlumberger-Doll Research
druskin1@slb.com, mzaslavsky@slb.com

MS151

Mathematics of Extended Inversion for Wave Propagation

Seismic full waveform inversion (FWI) was first suggested in the 1980's as a unified and physically consistent approach to interpretation of seismic data. Originally out of reach computationally, it has become in the last ten years an important technique in both industrial and academic geophysics. FWI still faces a major challenge: it is usually posed as a non-convex data-fitting optimization problem that often frustrates efforts to recover from seriously incorrect initial guesses at earth mechanics. In fact, at such poor initial models, small changes in model parameters cannot substantially improve data fit, so local optimization (the only serious algorithmic possibility, due to problem size) fails. As the potential of FWI has become clearer, many researchers have suggested approaches to improved FWI robustness. One of these approaches is the introduction of additional model parameters beyond those provided by basic seismic physics, so that data may be fit throughout the FWI optimization. I will describe one of these *model extensions* explicitly, and explain why it renders the mod-

ified FWI objective is convex over a larger set of models. More precisely, I will show why the original FWI objective is convex only over regions proportional in diameter to a data wavelength, whereas the extended FWI objective is convex over wavelength-independent regions. I will also show computational examples illustrating the enhanced robustness of extended FWI.

William Symes
Rice University
symes@caam.rice.edu

MS151

The Analysis and Application of Optimal Transport Related Misfit Functions in Seismic Imaging

Full Waveform Inversion (FWI) is a PDE constrained optimization in which the variable velocity in a forward wave equation is adjusted such that the solution matches measured data on the surface. L^2 norm is the conventional objective function measuring the difference between simulated and measured data, but it often results in the minimization trapped in local minima. One way to mitigate this is by selecting another misfit function with better convexity, and we proposed using the quadratic Wasserstein distance (W_2) from optimal transport theory. The optimal map defining the quadratic Wasserstein distance can be computed by quicksort (trace-by-trace comparison) or solving a Monge-Ampère equation (global comparison). Theorems pointing to the advantages of using optimal transport over L^2 norm will be discussed, and some large-scale computational examples will be presented.

Yunan Yang
Department of Mathematics
The University of Texas at Austin
yunanyang@math.utexas.edu

Bjorn Engquist
Department of Mathematics and ICES, UT Austin
engquist@ices.utexas.edu

MS151

On Elastic Seismic Inversion: Uniqueness and Conditional Lipschitz Stability

Seismic inversion is to determine properties of the Earths subsurface from seismic waves generated by sources like vibroseis. It can be mathematically formulated as inverse boundary value problems for partial differential equations. That is to determine the coefficients of partial different equations from boundary measurements. In this talk, we focus on time harmonic elastic wave equations, and consider the inverse problem of determining the Lam parameters and the density from the data modeled as local Neumann-to-Dirichlet map. We prove uniqueness and Lipschitz stability of this inverse problem when the Lam parameters and the density are assumed to be piecewise constant on a given domain partition. The uniqueness and stability results suggest a multilevel scheme of numerical inversion, which is guaranteed to converge. Numerical results will be shown.

Jian Zhai
Computational and Applied Mathematics
Rice University
jz59@rice.edu

MS152

Randomization and Sketching

Abstract not available at time of publication.

Alex Gittens
Rensselaer Polytechnic Institute
Computer Science
gittea@rpi.edu

MS152

A Probabilistic Bound for Monte Carlo Computation of Active Subspaces

We analyze a dimension reduction approach for the identification of response surfaces. Given a function f that depends on m parameters, one wants to identify a low-dimensional "active subspace" along which f is most sensitive to change, and then approximate f by a response surface over this active subspace. More specifically, let $X \in \mathbb{R}^m$ be random vectors corresponding to a probability density $\rho(x)$, and let E be the expected value of the "squared" gradient of $f(X)$. An "active subspace" is an eigenspace associated with the strongly dominant eigenvalues E. To reduce the cost, we compute the eigenspace instead from a Monte Carlo approximation S. We present bounds on the number of Monte Carlo samples so that, with high probability, the angle between the eigenspaces of E and S is less than a user-specified tolerance. Our probabilistic approach resembles the low-rank approximation of kernel matrices from random features, but with more stringent accuracy measures. Our bounds represent a substantial improvement over existing work: They are non-asymptotic; fully explicit; allow tuning of the success probability; and do not depend on the number m of parameters, but only on the numerical rank (intrinsic dimension) of E. They also suggest that Monte Carlo sampling can be efficient in the presence of many parameters, as long as the underlying function f is sufficiently smooth.

Ilse Ipsen
North Carolina State University
Department of Mathematics
ipsen@ncsu.edu

Ralph Smith
North Carolina State University
rsmith@ncsu.edu

John Holodnak
MIT Lincoln laboratory
john.holodnak@ll.mit.edu

MS152

New Directions in Randomized Numerical Linear Algebra via the Bootstrap

Randomized Numerical Linear Algebra (RandNLA) is an interdisciplinary research area that exploits randomization as a computational resource to develop improved algorithms for large-scale linear algebra problems. While the motivating applications for RandNLA are in large-scale machine learning and data analysis, most work in RandNLA so far has come from the perspectives of theoretical computer science and numerical linear algebra. This has begun to change, and many of the most exciting current

developments in RandNLA have to do with focusing on statistical and optimization considerations. Here, we describe recent results that use the statistical bootstrap method to yield improved RandNLA algorithms: first, a bootstrap method for error estimation in randomized matrix multiplication; and second, an error estimation for randomized least-squares algorithms via the bootstrap.

Michael Mahoney
UC Berkeley
mmahoney@stat.berkeley.edu

Miles Lopes
UC Davis
melopes@ucdavis.edu

MS152

Sketchy Decisions: Convex Low-rank Matrix Optimization with Optimal Storage

Convex matrix optimization problems with low-rank solutions play a fundamental role in signal processing, statistics, and related disciplines. These problems are difficult to solve because of the cost of maintaining the matrix decision variable, even though the low-rank solution has few degrees of freedom. This talk presents an algorithm that provably solves these problems using optimal storage. The algorithm produces high-quality solutions to large problem instances that, previously, were intractable. Joint work with Volkan Cevher, Roarke Horstmeyer, Quoc Tran-Dinh, Madeleine Udell, and Alp Yurtsever.

Joel A. Tropp
Caltech
jtropp@cms.caltech.edu

MS153

A Lower Bound on the Positive Semidefinite Rank of Convex Bodies

The positive semidefinite rank of a convex body C is the size of its smallest positive semidefinite formulation. We show that the positive semidefinite rank of any convex body C is at least $\sqrt{\log d}$ where d is the smallest degree of a polynomial that vanishes on the boundary of the polar of C. This improves on the existing bound which relies on results from quantifier elimination. The proof relies on the Bézout bound applied to the Karush-Kuhn-Tucker conditions of optimality. We discuss the connection with the algebraic degree of semidefinite programming and show that the bound is tight (up to constant factor) for random spectrahedra of suitable dimension.

Hamza Fawzi
University of Cambridge
h.fawzi@damtp.cam.ac.uk

Mohab Safey El Din
UPMC, Univ Paris 6
Mohab.Safey@lip6.fr

MS153

New Level Set Method for Convex Optimization

First order methods have emerged as an effective solution strategy for tackling large-scale convex optimization problems. The success of these methods has been greatest for such problems with simple feasible sets. We propose a novel level set method that extends the applicability of these methods to convex optimization problems with potentially complicated constraint sets.

Negar Soheili
Carnegie Mellon University
nazad@uic.edu

MS153

On Semidefinite Programming Under Perturbations with Unknown Boundaries

This paper shows that solving a family of semidefinite programming problems under affine perturbations can be converted to solving a system of quasilinear partial differential equations utilizing the Davidenko differential equations within the maximal perturbation set. We develop a second-order sweeping Euler scheme to approximate the boundary of the maximal set of perturbations and solve the SDPs within this set. We prove local and global error bounds for this second-order sweeping Euler scheme and demonstrate numerical results on several examples.

Tingting Tang
University of Notre Dame
ttang@nd.edu

Jonathan Hauenstein
University of Notre Dame
Dept. of App. Comp. Math. & Stats.
hauenstein@nd.edu

MS153

Sieve-SDP: A Simple Algorithm to Preprocess Semidefinite Programs

We introduce Sieve-SDP, a simple algorithm to preprocess semidefinite programs (SDPs). Sieve-SDP belongs to the class of facial reduction algorithms. It inspects the constraints of the problem, deletes redundant rows and columns, and reduces the size of the variable matrix. It often detects infeasibility. It does not rely on any optimization solver: the only subroutine it needs is Cholesky factorization, hence it can be implemented in a few lines of code in machine precision. We present extensive computational results on several problem collections from the literature. We also highlight an issue arising in SDPs with positive duality gap: on such problems SDP solvers may compute a "fake" solution with an arbitrarily small constraint violation, and arbitrarily small duality gap.

Yuzixuan Zhu
UNC Chapel Hill
zyzx@live.unc.edu

Gabor Pataki
University of North Carolina, at Chapel Hill
gabor@unc.edu

Quoc Tran-Dinh
Department of Statistics and Operations Research
UNC-Chapel Hill, USA
quoctd@email.unc.edu

MS154

libEnsemble: A Library for Managing Ensembles

of Calculations

We present libEnsemble, an open-source library for managing ensembles of calculations. libEnsemble can monitor intermediate output from calculations, preempt future calculations, and stop running calculations. Example applications of libEnsemble include coordinating concurrent evaluations of computationally expensive numerical simulations in order to find multiple local optima. We study the computational efficiency of libEnsemble and provide a collection of Python use cases that highlight features of the library.

Jeffrey Larson, Stefan Wild
Argonne National Laboratory
jmlarson@anl.gov, wild@mcs.anl.gov

MS154

A PETSc Framework for PDE Constrained Optimization

Optimization in the field of time dependent Partial Differential Equations (PDEs) is computationally very expensive, since it requires several simulations up until the objective function is minimized (maximized). It is therefore essential to be able to perform the simulation of the underlying PDE in the most efficient fashion. A framework for solving optimization problems at scale has been developed in PETSc over the years and it is now possible to address a wide range of problems. We aim to illustrate how to access these tools on two-dimensional linear and nonlinear PDEs solving complete or incomplete inverse problems, as well as optimization problems. Additionally we shall outline computational bottlenecks as well as efficiency considerations.

Oana Marin, Emil Constatinescu, Barry Smith
Argonne National Laboratory
oanam@anl.gov, emconsta@mcs.anl.gov, bsmith@anl.gov

MS154

Sensitivity Analysis in Computationally Expensive Simulation Optimization

Many science applications involve the numerical simulation of physical phenomena. These simulations contain parameters that must be optimized in order to, e.g., calibrate the simulation model based on observation data or to tune the parameters such that a design objective function is optimized. Simulations are computationally expensive, thus limiting the total number of solution vectors that can be tried. Analytic descriptions of the objective function or the derivatives are generally not available. Often, the influence of many parameters on the optimization objective is not well understood. The larger the number of optimization parameters the more simulation model runs have to be performed in the optimization. For these reasons, scientists focus their calibration and tuning efforts only on a small subset of well-understood parameters which may lead to suboptimal results. In this talk, we investigate how sensitivity analysis methods can be integrated in black box optimization algorithms.

Juliane Mueller
Lawrence Berkeley National Laboratory
julianemueller@lbl.gov

MS154

Bayesian Inference for Model Error Quantification and Propagation with UQTk

The UQ Toolkit (UQTk, sandia.gov/uqtoolkit) is a collection of libraries, scripts and command-line tools for uncertainty quantification (UQ) in computational models. It offers a wide range of intrusive and non-intrusive methods for forward uncertainty propagation, as well as Bayesian methods for inverse UQ. In this talk, we will highlight the inverse modeling components of UQTk. In particular, the core Markov chain Monte Carlo capabilities, together with a higher-level model calibration library, will be detailed. The software enables Bayesian inference of computational model parameters, while allowing for flexible user-defined components such as likelihoods, priors and forward models. An important feature of the software is the capability to perform Bayesian inference with model structural error estimation. The core libraries are implemented in C++, and a Python interface is available for easy prototyping and incorporation in UQ workflows. We will demonstrate the embedded model error methodology, enhanced with surrogate modeling and uncertainty propagation with polynomial chaos, as well as its software implementation on a few DOE SciDAC relevant applications.

Khachik Sargsyan, Xun Huan
Sandia National Laboratories
ksargsy@sandia.gov, xhuan@sandia.gov

Habib N. Najm
Sandia National Laboratories
Livermore, CA, USA
hnnajm@sandia.gov

Cosmin Safta, Kenny Chowdhary
Sandia National Laboratories
csafta@sandia.gov, kchowdh@sandia.gov

Bert J. Debusschere
Chemistry, Combustion and Materials Center
Sandia National Laboratories, Livermore CA
bjdebus@sandia.gov

MS155

Systemic Risk in a Mean-field Model of Interbank Lending with Self-exciting Shocks

In this talk we consider a mean-field model of interacting discussions for the monetary reserves in which the reserves are subjected to a self-and cross-exciting shock modelled by a Hawkes process. The self- and cross-excitement is motivated by the financial acceleration and are sales observed in the market. We derive a mean-field limit for the empirical measure of the monetary reserves using a weak convergence analysis via the limiting martingale problem and an explicit measure-valued process associated with the behavior of a large interbanking system. The convergence analysis is based on a previous result stating that the intensity of a Hawkes process in the limit of a fully connected network of excitations tends to behave as that of a non homogeneous Poisson process. We show that the underlying limit process for the monetary reserves of the nodes has purely diffusive dynamics and the effect of the Hawkes process is reflected in a time-dependent drift coefficient. Then we define several risk indicators and use the weak convergence analysis to derive the law of large numbers approximations to explicitly show the effects of the Hawkes process on the risk in a large interbank network. Finally we will compare the LLN approximations with the actual values simulated through a Monte-Carlo method. We con-

clude that self-exciting shocks increase the systemic risk in the network and their presence in interbank networks should not be ignored.

Anastasia Borovykh, Andrea Pascucci
Universita di Bologna
anasta- sia.borovykh2@unibo.it, andrea.pascucci@unibo.it

Stefano La Rove
NIER Ingegneria
Bologna, Italy
s.larovere@niering.it

MS155

On Mean Field Models with Several Populations

Abstract not available at time of publication.

Mathieu Lauriere
Princeton University
lauriere@princeton.edu

MS155

Optimal Debt-maturity Management

Abstract We solve the problem of a government that wants to smooth financial expenses by choosing over a continuum of bonds of different maturity. The planner takes into account that adjusting debt too fast can affect prices. At the same time, it wants to insure against several sources of risk: (a) income risk, (b) interest rate (price) risk, (c) liquidity risk (prices can become more sensitive to issuance's), and (d) the risks in the cost of default. We characterize this infinite dimensional control problem to aid the design of the debt-maturity profile in response to these forms of risk.

Juan Passadore
Einaudi Institute for Economics and Finance
juan.passadore@eief.it

Saki Bigio
UCLA
sbigio@econ.ucla.ed

Galo Nuño
Banco de Espa{ñ}a
galo.nuno@bde.es

MS156

Analysis of Sparse Approximations in Bayesian Filtering

Bayesian filtering algorithms for systems with nonlinear dynamics and high-dimensional states include ensemble Kalman filters (EnKF), variational approaches, and particle filters. With constraints on computational resources, it is common to deploy these algorithms with structured approximations such as localization and sparse covariance estimation in EnKFs. However, these techniques generally require expensive parameter tuning to optimize algorithms for accurate state estimation. In this presentation, we will explore the bias and variance trade offs resulting from these types of approximations by analyzing the resulting marginal and conditional independence assumptions on the filtering distribution. These errors will be studied and compared in the context of model problems for numerical weather prediction including stochastic turbulence models and chaotic dynamical systems.

Ricardo Baptista
MIT
rsb@mit.edu

Youssef M. Marzouk
Massachusetts Institute of Technology
ymarz@mit.edu

MS156

Improving Particle Filter Performance with a Generalized Random Field Model of Observation Errors

Particle filters are a class of sequential Monte Carlo methods for Bayesian estimation. They suffer from a curse of dimensionality where the number of 'particles' (i.e. Monte Carlo samples, or ensemble members) required for robust uncertainty quantification can be impractical for high-dimensional systems, especially those encountered in discretizations of spatially-extended problems. We describe a method for keeping the required ensemble size manageable in spatially-extended problems by focusing on the large spatial scales, and thereby keeping the 'effective dimension' small. The method uses a generalized random field model of observation errors, and is equivalent to assuming that the smoothed observation errors are spatially uncorrelated. This introduces a bias in the Bayesian posterior distribution, but the bias has a known, controllable character and exists only at small scales. The method effectively applies standard particle methods to an altered Bayesian estimation problem, so classical guarantees of convergence for particle filters still apply, and the convergence rate is significantly faster than for the unaltered, intractable original Bayesian problem. The method only affects the way that importance-sample weights are calculated, so the particles themselves (the ensemble members) are all still simulations of the un-altered model dynamics. We demonstrate the method in the simple setting of a one-dimensional stochastic PDE.

Ian Grooms
Department of Applied Mathematics
University of Colorado, Boulder
ian.grooms@colorado.edu

Gregor Robinson
Univ. of Colorado, Boulder
gregor.robinson@colorado.edu

William Kleiber
University of Colorado at Boulder
Department of Applied Mathematics
william.kleiber@colorado.edu

MS156

Multilevel Monte Carlo for Bayesian Inference

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Kody Law
Oak Ridge National Laboratory
kodylaw@gmail.com

MS156

Using Splitting Techniques to Calculate the Prob-

ability of Intense Tropical Cyclone Formation

A central goal of tropical cyclone (TC) research is to identify tight bounds on the maximum intensity a TC can achieve based on the storms background weather and climate conditions. However, current approaches such as Emanuels (1986) Maximum Potential Intensity theory lead to upper bounds that are too high to be useful, while neglecting important inhibitors of storm intensity such as wind shear. To provide a tighter bound on TC intensity, we use a high-resolution probabilistic weather model to approximate the tail distribution of intense storm behavior from fixed initial conditions. Since a direct sampling approach would be computationally infeasible, we instead use the Weighted Ensemble algorithm from the rare event sampling literature. Weighted Ensemble allows us to generate storms that are much more intense than those from direct sampling, at the same computational cost. We discuss asymptotic convergence of the Weighted Ensemble algorithm, relate Weighted Ensemble to other splitting techniques for rare event sampling, and explain the use of surrogate models to provide approximate confidence intervals and tune parameters. In the future, our approach can be used to study physical limitations on other extreme weather and climate events such as floods, droughts, and heatwaves.

Robert Weber
University of Chicago
rwebber@galton.uchicago.edu

MS157

Weno Simulations of 3D Supersonic Astrophysical Jets

We will survey our WENO simulations of 3D supersonic astrophysical jets, emphasizing the effects of radiative cooling and shock waves, for both proto-stellar jets and for the more massive and powerful jets from AGNs (active galactic nuclei). Physical processes like radiative emission from shocks for proto-stellar jets and star formation by AGN jets will be emphasized. We will compare telescopic images with the WENO simulations for the XZ Tauri, SVS 13, and HH 30 proto-stellar jets (Mach numbers 25-60) and for the Centaurus-A AGN jet (Mach number 3400).

Carl L. Gardner
Arizona State University
School of Mathematical and Statistical Sciences
carl.gardner@asu.edu

MS157

Positivity-Preserving 3D Weno Simulations of Star Formation by Astrophysical Jets

We describe the positivity-preserving version of the WENO-LF method, and parallelization of the 3D gas dynamics code, as applied to star formation by the active-galactic-nucleus astrophysical jet in Centaurus A. Without the incorporation of the positivity-preserving flux limiter, the simulations broke down as soon as the jet bow shock impacted the surrounding dense molecular clouds where star formation takes place. Parallelization is extremely important since the 3D simulations required 100,000 CPU hours (11.4 CPU years). Using 1200 cores though, we were able to get the results within a few days.

Jeremiah Jones
ASU
jrjones8@gmail.com

MS157

Implicit Positivity-preserving High-order Discontinuous Galerkin Methods for Solving Conservation Laws

In this talk we will introduce our recent progress on designing implicit positivity-preserving discontinuous Galerkin methods for solving conservation laws. We consider the Euler backward and the Crank-Nicholson time descritizations. For linear scalar equations, we derive CFL conditions for both methods to be positivity-preserving. For nonlinear equations and systems, numerical examples will be provided to illustrate the applicability of the proposed methods. This work is joint with Prof. Chi-Wang Shu.

Tong Qin
Ohio State University
qin.428@osu.edu

Chi-Wang Shu
Brown University
Div of Applied Mathematics
shu@dam.brown.edu

MS157

Bound Preserving Discontinuous Galerkin Methods for Relativistic Hydrodynamics

In this talk, we demonstrate a discontinuous Galerkin (DG) method to solve the ideal special relativistic hydrodynamics (RHD) and design a bound preserving (BP) limiter for this scheme by extending the idea in (X. Zhang and C.-W. Shu, Journal of Computational Physics, 229 (2010), 8918-8934). For RHD, the density and pressure are positive and the velocity is bounded by the speed of light. One difficulty in numerically solving the RHD in its conservative form is that the failure of preserving these physical bounds will result in ill-posedness of the problem and blowup of the code, especially in extreme relativistic cases. The standard way in dealing with this difficulty is to add extra numerical dissipation, while in doing so there is no guarantee in maintaining the high order of accuracy. Our bound-preserving limiter has the following features. It can theoretically guarantee to preserve the physical bounds for the numerical solution and maintain its designed high order accuracy. The limiter is local to the cell and hence is very easy to implement. Moreover, it renders L^1-stability to the numerical scheme. Numerical experiments are performed to demonstrate the good performance of this bound-preserving DG scheme. Even though we only discuss the bound-preserving limiter for DG schemes, it can be applied to high order finite volume schemes, such as weighted essentially-oscillatory (WENO) finite volume schemes as well.

Tong Qin
Ohio State University
qin.428@osu.edu

Chi-Wang Shu
Brown University
Div of Applied Mathematics
shu@dam.brown.edu

Yang Yang
Michigan Technological University

yyang7@mtu.edu

MS158

Approximate Inference for Bayesian Model Inversion

We present two methods for Bayesian model inversion via approximate inference, with application to systems governed by PDEs with spatially heterogeneous model parameters. We propose employing a parameterized Gaussian process (GP) prior for the model parameters with hyperparameters to be estimated from sparse observations of the system's state. In the first method, we employ a Laplace approximation to the posterior around the maximum a posteriori estimate of model parameters, with the hyperparameters of the GP prior estimated via marginal likelihood estimation. In the second method, we employ a variational expectation maximization approach, with variational parameters and prior hyperparameters estimated via stochastic gradient optimization. The proposed methods are applied to identifying heterogeneous model parameters for a flow problem in porous media.

David A. Barajas-Solano
Pacific Northwest National Laboratory
david.barajas-solano@pnnl.gov

MS158

Dimension Reduction-accelerated Parameter Estimation

A grand challenge in uncertainty quantification is the solution of inverse problem governing by partial differential equations (PDEs). The forward problem is usually characterized by a large dimensional parameter field. As a result, direct solving this hundred to thousand-parameter problem is computational infeasible. Instead we rely on the Bayesian solution to seek the most probable combination of the parameters. The Markov chain Monte Carlo (MCMC) method provides a powerful tool to generate the posterior distributions of the parameters as well as the most probable point in the parameter space. In this work, we also utilize the gPC surrogates and combine the state to the art dimensional reduction technique to accelerate the MCMC evaluation. The data driven dimensional reduction based on the conditional random field provides a tractable approach to estimate the spatial dependent coefficient with only a few measurements.

Jing Li
Pacific Northwest National Lab
jing.li@pnnl.gov

Alexander Tartakovsky
Pacific Northwest National Laboratory
alexandre.tartakovsky@pnnl.gov

MS158

Efficient Model Reduction Methods for High-dimensional Bayesian Inversion Problems

We introduce a sliced-inverse-regression-based model reduction method to effectively reduce the dimensions for Bayesian inversion problems with high-dimensional inputs. For high-dimensional Bayesian inversion problems, which normally suffer the "curse of dimensionality", the proposed method provides a practical way of finding the computationally inexpensive low-dimensional representations for the high-dimensional input. The effectiveness of the proposed approach is illustrated with several subsurface modeling case studies.

jiahao Zhang, Guang Lin
Purdue University
jiahzhang2@outlook.com, guanglin@purdue.edu

MS159

Quantum Annealing Algorithms for Solving the Graph Isomorphism Problem

We present and compare, theoretically and experimentally (using the D-Wave machine), various methods to construct efficient quantum annealing algorithms for the Graph Isomorphism Problem—one of a very few problems in NP that is neither known to be solvable in polynomial time nor NP-complete.

Cristian Calude
University of Auckland
c.calude@auckland.ac.nz

MS159

Quantum Annealing Approaches for Building Sparse Surrogate Models in Uncertainty Quantification

In this talk, we will present a novel use of Quantum Annealing on a D-Wave 2X machine to perform sparse basis selection for the construction of surrogate models for uncertainty quantification applications. We will discuss the formulation of the approach and compare its behavior using both the D-Wave 2X quantum annealer and classical solvers. We will further compare the approach to classical compressed sensing methods, which relax the problem to a convex l1 optimization problem.

Bert J. Debusschere, Khachik Sargsyan, Ojas Parekh
Sandia National Laboratories
bjdebus@sandia.gov, ksargsy@sandia.gov, odparek@sandia.gov

MS159

Navigating a Maze using a Quantum Annealer

Quantum annealers exploit quantum effects in an attempt to minimize a classical Hamiltonian function with a higher likelihood of reaching optimality than can be expected from simulated annealing. The key programming challenge is how to express algorithms in terms of the specific Hamiltonian supported by the quantum-annealing hardware. In this talk, we present an algorithm for finding the shortest path through a maze not via a traditional backtracking mechanism but rather by expressing the shortest path as the globally optimal value of a 2-local Ising-model Hamiltonian function.

Scott Pakin
Los Alamos National Laboratory
pakin@lanl.gov

MS159

Quantum Annealing for Flight Gate Assignment

We report on our efforts to solve a real world problem from airport planning with a D-Wave quantum annealer. The problem is related to the quadratic assignment problem

which is known to be a hard combinatorial optimization problem. As problem instances, we use real data from a mid-size German airport. We present a detailed analysis of the problem and compare quantum annealing solutions to classical approaches. To increase the success probability, we investigate some of the recently introduced features to control the annealing process.

Tobias Stollenwerk
Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR)
tobias.stollenwerk@dlr.de

MS160

Stochastic Modeling of Infectious Diseases

In an infectious disease outbreak, individuals who transmit the disease to a large number of susceptible individuals are know as superspreaders. To investigate the role superspreaders play in an outbreak, we construct both deterministic and stochastic models with two classes of individuals, superspreaders and nonsuperspreaders. We analyze these models and then run numerical simulations for the cases of Middle East respiratory syndrome (MERS) and Ebola. From the analysis and simulations, we gain insight into superspreaders role in the outbreak timeline and severity of the outbreak.

Christina Edholm
University of Tennessee
cedholm@utk.edu

Blessing Emerenini
Department of Mathematics and Statistics
University of Guelph
syno28@yahoo.com

Anarina Murillo
AMLSS-Mathematical, Computation & Modeling Sciences Center
Arizona State University
anarina.murillo@asu.edu

Omar Saucedo
University of Florida
Department of Mathematics
osaucedo1987@ufl.edu

Nika Shakiba
University of Toronto
nikashakiba@gmail.com

Xueying Wang
Washington State University
xueying@math.wsu.edu

Linda J. Allen
Dept. of Mathematics and Statistics
Texas Tech University
linda.j.allen@ttu.edu

Angela Peace
Arizona State University
angela.peace@asu.edu

MS160

Mathematical Models of Autoregulation in the Renal and Cerebral Circulations

Autoregulation contributes to regulation of blood flow during fluctuations in blood pressure through internal adaptive mechanisms independent of central neural control. It is a major factor in the renal and cerebral circulations, both of which must maintain their localized behavior in the presence of global activity. Autoregulatory failure has been linked in recent decades to a large increase in diseases such as hypertension and diabetes and its full mechanism is not well understood. In an attempt to understand this process, we investigate two models for investigating autoregulatory dynamics. We first present a model of renal autoregulation that coupled a system of ordinary differential equations describing nonlinear changes in afferent arteriole vascular smooth muscle tone according to the myogenic and tubuloglomerular feedback responses, to a partial differential equation describing chloride ion transport in the loop of Henle. In the second study, we developed a patient-specific model of differential-algebraic equations describing blood flow in both the cerebral and systemic circulations parameterized by clinical data and used to simulate dynamic changes in cerebrovascular resistance, a marker of autoregulatory behavior.

Laura Ellwein Fix
Virginia Commonwealth University
lellwein@vcu.edu

Julia Arciero
Indiana University-Purdue University Indianapolis
jarciero@iupui.edu

Ashlee N. Ford Versypt
Oklahoma State University
ashleefv@okstate.edu

Elizabeth J. Makrides
Brown University
Division of Applied Mathematics
elizabeth_makrides@brown.edu

Anita T. Layton
Duke University
Department of Mathematics
alayton@math.duke.edu

MS160

Intermittent Preventive Treatment (IPT): Its Role in Averting Disease-induced Mortality in Children and in Promoting the Spread of Antimalarial Drug Resistance

We develop an age-structured ODE model to investigate the role of Intermittent Preventive Treatment (IPT) in averting malaria-induced mortality in children, and its related cost in promoting the spread of anti-malarial drug resistance. IPT has been shown to reduce malaria transmission and deaths in children and pregnant women. However, it can also promote drug resistance spread. Our mathematical model is used to explore IPT effects on drug resistance and deaths averted in holoendemic malaria regions. The model includes drug-sensitive and drug resistant strains as well as human hosts and mosquitoes. The basic reproduction and invasion reproduction numbers for both strains are derived. Numerical simulations show the individual and combined effects of IPT and treatment of symptomatic infections on the prevalence of both strains and the number of lives saved. Our results suggest that while IPT can

indeed save lives, particularly in high transmission regions, certain combinations of drugs used for IPT and to treat symptomatic infection may result in more deaths when resistant parasite strains are circulating. Moreover, the half-lives of the treatment and IPT drugs used play an important role in the extent to which IPT may influence spread of the resistant strain. A sensitivity analysis indicates the model outcomes are most sensitive to the reduction factor of transmission for the resistant strain, rate of immunity loss, and the natural clearance rate of sensitive infections.

Carrie A. Manore
Los Alamos National Laboratory
cmanore@lanl.gov

Miranda I. Teboh-Ewungkem
Lehigh University
mit703@lehigh.edu

Olivia Prosper
University of Kentucky
olivia.prosper@uky.edu

Angela Peace
Arizona State University
angela.peace@asu.edu

Katharine Gurski
Department of Mathematics
Howard University
kgurski@howard.edu

Zhilan Feng
Department of Mathematics
Purdue University
zfeng@math.purdue.edu

MS160

Numerical Simulations of the Aerodynamics of Spider Ballooning

Spider ballooning is one of the most fascinating mechanisms for dispersal. Through ballooning, spiders can travel as far as 3000 km and as high as 5 km. Despite all that is known about ballooning from a biological prospective, the physical mechanisms related to this unique type of dispersal are still poorly understood. A mathematical model that simulates spider ballooning was created through the means of a fully-coupled fluid-structure interaction problem of a flexible dragline moving through a viscous, incompressible fluid. The immersed boundary method has been used to solve this complex multi-scale problem, and particularly an adaptive and distributed-memory parallel implementation of immersed boundary method. This model was used to study the effect physical parameters, such as mass, length of the dragline, and bending modulus, have on the dynamics of ballooning. The model allowed for detailed simulation of the fluid-structure interactions between the spider-dragline system and the air, and it provided a perfect testing environment for a variety of regimes. All three critical stages for ballooning: take-off, flight, and settling, have been simulated and analyzed. The model also revealed the complex transport dynamics when updrafts and eddies are present in the background flow. In this talk, all results of this study will be presented and discussed.

Iordanka N. Panayotova
Boston College
Institute for Scientific Research
iordanka.panayotova@cnu.edu

Longua Zhao
Case Western Reserve University
longhua.zhao@case.edu

Kimberly Sheldon
University of Tennessee - Knoxville
ksheldon@utk.edu

Lydia Bourouiba
Massachusetts Institute of Technology
lbouro@MIT.EDU

Laura A. Miller
University of North Carolina - Chapel Hill
Department of Mathematics
lam9@email.unc.edu

MS161

Modeling Insights into the Mechanical Coordination in the Collective Locomotion of Heart Progenitor Cells

During embryonic development, cells often migrate in groups. The heart progenitors of the ascidian Ciona provide one of the simplest examples of collective migration whereby just two cells migrate with defined leader-trailer polarity. The cells are also capable of migrating individually, albeit by a shorter distance, with imperfect directionality, and with altered morphology. Thus, maintaining the leader-trailer polarity is important for directed migration to the destination. To understand the mechanics of this collective migration phenomenon, we develop a computational model to study the interplay of actomyosin contractility, cell-matrix adhesion, and the resulting leader-trailer polarity maintained for collective migration and combine modeling with imaging of the migrating cells. Two competing hypothesis are tested to understand the mechanical coupling and coordination between leader-trailer cells and the cells in the extracellular tissues: (1) cells act as a single unit in which the leader cell generates actin-driven protrusions while actin polymerization is down-regulated in the contractile trailer cell; (2) alternatively, contraction at the rear of the trailer cell leads to higher osmotic pressure pushing on leader cell. We present insights from modeling explorations of the mechanochemical coordination in this model system for collective locomotion.

Calina Copos
New York University
Courant Institute of Mathematical Sciences
copos@cims.nyu.edu

MS161

Relay from Microenvironment to Cancer Metastasis

In this talk, we leverage biophysics-oriented mathematical modeling of collective cell migration with data-driven inference of gene regulatory networks. In one hand, collective cell migration is homogenized from epithelial single cell motility constituted with intracellular contractility of dipole stress and protrusion, re-orientation of cell polarity, cell-ECM interaction by adhesive resistance, and cell-cell interaction by Maxwell viscoelastic transition. On the other hand, in the deconvolution of gene regulatory net-

work, we utilize time course data of gene expression in transcriptional/RNA level and decompose from many-to-many to one-to-many connectivity for subnetwork reconstruction. These reverse-engineered subnetworks are integrated by global optimization while filtrating kinetics and pathways from upstream micro-environmental cues. We introduce cell fate determination and branching morphogenesis in lung development in the connection between collective cell migration and *in situ* gene regulation, and project translational potentials to metastasis of lung cancer.

Pilhwa Lee
University of Michigan, Ann Arbor
pilee@umich.edu

MS161

Dysregulation of Cellular Hierarchies: Carcinogenesis and Tumor Sensitivity to Chemotherapy

Tissue homeostasis is regulated by feedback loops between cells at various differentiation stages. Here we present a mathematical model of tissue regulation and discuss the type of phenotypic mutations that can lead to abnormal cell proliferation through an escape from these regulatory mechanisms. Many tumors however, are thought to retain certain features of normal tissue cell hierarchies, including the presence of remaining regulatory feedback loops, which can play an important role in determining treatment outcomes. In particular, recent findings indicate that chemotherapy of human bladder cancer xenografts can trigger a wound-healing response that mobilizes quiescent tumor stem cells into active proliferation. This process can result in a loss of sensitivity to chemotherapy due to an increase in the number of tumor stem cells, which typically respond less well than more differentiated cells. Using mathematical models, we show that details of the tumor cell hierarchy can be crucial for determining tumor sensitivity to drug therapy, when stem cell enrichment is the basis for the drug resistance.

Ignacio A. Rodriguez-Brenes
University of California Irvine
ignacio.rodriguezbrenes@uci.edu

MS161

The Role of Backward Cell Migration in the Stem Cell Niche in Tumorigenesis

In colon and intestinal crypts, the backward cell migration from border stem cells (BSCs), which are located between CeSCs and transit amplifying cells (TAs), to central stem cells (CeSCs), which are at the very bottom of the crypt, has been observed. In this project, we develop a bi-compartmental stochastic model for the cell dynamics in the stem cell niche to investigate the role of backward stem cell migrations in the probability of two-hit mutant production. The model suggests that the probability of double-hit mutant production rises when the frequency of backward cell migration increases. Moreover, a small non-zero probability of backward cell migration leads to the largest range of optimal values for the rate of symmetric divisions and the percentage of divisions at each stem cell compartment in terms of delaying two-hit mutant production. Furthermore, the probability of two-hit mutant production is more sensitive to the probability of symmetric division than to the frequency of backward cell migrations. The highest probability of two-hit mutant production corresponds to the case when all stem cells divisions are asymmetric.

Leili Shahriyari
Mathematical Biosciences Institute, Ohio State University
leili.shahriyari@gmail.com

Audrey Bollas
Ohio State University
bollas.12@buckeyemail.osu.edu

MS162

Quantized Compressed Sensing with Structured Matrices

I will present how one can use noise-shaping schemes, including Sigma-Delta and distributed noise-shaping, to quantize compressed sensing measurements arising from bounded orthonormal ensembles and partial circulant matrices. I will show that these methods yield a reconstruction error that decays with the number of measurements, when using convex optimization for reconstruction. Specifically, for Sigma-Delta schemes, the error decays polynomially in the number of measurements, and it decays exponentially for distributed noise-shaping schemes based on beta encoding. These results are near optimal and the first of their kind dealing with bounded orthonormal systems. This is joint work with Rayan Saab.

Thang Huynh
University of California, San Diego
Dept. of Mathematics
tlh007@ucsd.edu

MS162

Optimal Sampling Strategies for Compressive Imaging

Compressive imaging combines sparse sampling strategies with compressed sensing techniques to recover images from a reduced number of measurements. Recent works have shown that in certain examples, so-called multilevel Fourier sampling outperforms the commonly used Gaussian random sampling; a highly unexpected and previously unexplained result. The earlier work in this area had given strong numerical evidence and intuition, but lacked a rigorous theoretical explanation. This work quantitatively describes multilevel random sampling in Fourier space, and proves that it outperforms Gaussian random sampling in desirable smoothness classes for imaging. For these cases, we show that one can achieve quasi-best approximations with optimally few numbers of measurements. As a result, we have fully explained (in the one-dimensional case) the striking numerical results in the literature, and have laid the groundwork for the higher-dimensional setting.

Matthew M. King-Roskamp, Benjamin Adcock, Simone Brugiapaglia
Simon Fraser University
mkingros@sfu.ca, ben_adcock@sfu.ca, simone_brugiapaglia@sfu.ca

MS162

Statistical Tests for Total Variation Regularization Parameter Selection

Total Variation (TV) is an effective method of removing noise in digital image processing while preserving edges. The choice of scaling or regularization parameter in the TV

process defines the amount of denoising, with value of zero giving a result equivalent to the input signal. Here we explore three algorithms for specifying this parameter based on the statistics of the signal in the total variation process. The Discrepancy Principle, an empirically Bayesian approach and a method based on a χ^2 test for the regularized residual. These approaches are advantageous for nonlinear or computationally large problems because they automate selection of a regularization parameter, and give statistical justification that takes away guesswork when manually adjusting or iterating it to zero.

Jodi Mead
Boise State University
Department of Mathematics
jmead@boisestate.edu

MS162

Reducing the Effects of Bad Data using Variance Based Joint Sparsity

Much research has recently been devoted to jointly sparse (JS) signal recovery from multiple measurement vectors (MMV) using $\ell_{2,1}$ regularization, which is often more effective than performing separate recoveries using standard sparse recovery techniques. However, JS methods are difficult to parallelize due to their inherent coupling. In a recent paper the *variance* based joint sparsity (VBJS) algorithm was introduced. VBJS is based on the observation that the pixel-wise variance across signals convey information about their shared support, motivating the use of a *weighted* ℓ_1 JS algorithm, where the weights depend on the information learned from calculated variance. Specifically, the ℓ_1 minimization should be more heavily penalized in regions where the corresponding variance is small, since it is likely there is no signal there. This paper expands on the original method, notably by introducing weights that ensure accurate, robust, and cost efficient recovery using both ℓ_1 and ℓ_2 regularization. Moreover, this paper shows that the VBJS method can be applied in situations where some of the measurement vectors may misrepresent the unknown signals or images of interest, which is illustrated in several numerical examples.

Theresa A. Scarnati
Arizona State University
School of Mathematical & Statistical Sciences
tscarnati24@gmail.com

Anne Gelb
Dartmouth College
Department of Mathematics
annegelb@math.dartmouth.edu

MS163

Using Tropical Geometry to Characterize the Algebraic Matroid for Rank-2 Matrix Completion

Tropical geometry offers us a set of tools for illuminating the combinatorics of an algebraic matroid. I will discuss how one might use these tools for problems in rigidity theory and matrix completion. In particular, I will show how to obtain a combinatorial description of the rank-2 completion matroid by using tropical geometry to reduce this to a problem about phylogenetic trees which can then be solved.

Daniel I. Bernstein
North Carolina State University
dibernst@ncsu.edu

MS163

Unassigned Vectors: New Point Reconstruction Methods Driven by Experimental Advances

Patterson's original paper showed that if one takes a Fourier transform of intensity data from an oriented single crystal, it provides the vectors of interatomic separations [T. Weber, A. Simonov. The three-dimensional pair distribution function analysis of disordered single crystals: basic concepts. Zeitschrift fur Kristallographie-Crystalline Materials 227, 238-247 (2012)]. However at that time, the experimental technology was not able to achieve vector PDFs to high resolution. Instead, scalar PDFs developed first and are now routinely measured by averaging over angles which is usually achieved by using samples with many grains or particles having random orientations. Our previous theoretical and computational work has focused on these scalar PDFs where the mathematical formulation reduces to attempting to find the location of a set of points from an unassigned set of interpoint distances; which we call the unassigned distance geometry problem [P.M. Duxbury, L. Granlund, S.R. Gujarathi, P. Juhas, S.J.L. Billinge. The unassigned distance geometry problem. Discrete Applied Mathematics 204, 117-132 (2016).]. Recently the focus of the experimental community has returned to the vector PDF case; raising interesting new mathematical questions. To address these questions, we define the unassigned vectors problem and present our recent theoretical and computational approaches to study it.

Phil Duxbury
Michigan State University
duxbury@pa.msu.edu

Simon Billinge
Columbia University and Brookhaven National Laboratory
sb2896@columbia.edu

MS163

Distance Geometry in 5D for Protein Structure Determination

We will discuss a new model to represent molecular structures using the 5D Conformal Space and a language more powerful than Linear Algebra: Geometric Algebra. The Conformal Model can be seen as an extension of the Projective Model, widely used in Computational Geometry. Geometric Algebra seeks algebraic representations for geometric objects, recognized by the physicists as a tool of great importance. The beauty and power of Geometric Algebra are related to its capacity for unification, simplification and generalization of several mathematical objects that involve geometric concepts. All this will be exemplified with a problem of real importance in Distance Geometry: the determination of 3D structure of protein molecules using distance information between nearby atoms provided by NMR experiments.

Carlile Lavor
State University of Campinas
Department of Applied Mathematics

clavor@ime.unicamp.br

MS163

Barvinok's Naive Algorithm in Distance Geometry

In 1997, A. Barvinok gave a probabilistic algorithm to derive a feasible solution of a quadratically (equation) constrained problem from its semidefinite relaxation. We generalize this algorithm to handle matrix (instead of vector) variables and to two-sided inequalities, and derive a heuristic for the distance geometry problem. We showcase its computational performance on a set of instances related to protein conformation.

Leo Liberti
CNRS LIX Ecole Polytechnique
liberti@lix.polytechnique.fr

Ky Vu
Chinese University of Hong Kong
vukhacky@gmail.com

MS164

Shape Optimization with Multiple Overlapping Meshes

An important step in shape-optimization algorithms constrained by partial differential equations (PDE) is to adapt the geometry during each optimization iteration. Traditional approaches, such as re-meshing or mesh-deformation, often have to trade off robustness and computationally expensive. In this talk, we present a new approach, in which the computational domain is represented by multiple, non-matching meshes. Each mesh may be freely moved, and hence this approach avoids the need of re-meshing or mesh deformations in cases where the geometry changes consists of rigid motions or scaling. To solve the PDE on all meshes, we employ the finite element method for overlapping meshes, which uses Nitsche terms to weakly enforce continuity over each mesh interfaces. The shape-sensitivities are obtained with an optimize then discretize approach, employing the Hadamard formulas and the adjoint method. If general geometry changes are needed, our method can be combined with mesh-deformation or re-meshing techniques. We demonstrate the robustness and efficiency of the method on several numerical examples. The optimization algorithm, and the finite element method for overlapping meshes has been implemented with the open-source software FEniCS.

Jørgen Dokken
Simula Research Laboratory
dokken@simula.no

Simon W. Funke
Center for Biomedical Computing
Simula Research Laboratory
simon@simula.no

August Johannson
Simula Research Laboratory
august@simula.no

MS164

Automatic Decomposition of Piecewise Smooth Problems

We investigate the problem of non-smooth PDE constrained optimization, where all non-differentiablilities are assumed to be given by piecewise smooth functions such as abs(), min() and max(). These kinds of optimization problems arise in many applications and their efficient as well as robust solution requires numerical simulation combined with specific optimization algorithms. We formally define a new concept for solving optimal control problems constrained by non-smooth PDEs where standard optimal control techniques for obtaining first-order optimal points cannot be applied. The key idea of the optimization method under consideration is locating stationary points by appropriate decomposition of the original problem into smooth branch problems. Subsequent successive exploitation of the corresponding dual variables leads to the next branch and thus to successive reduction of the function value. Numerical results illustrate the proposed approach and the applicability of the method is demonstrated by considering several non-smooth PDEs.

Olga Ebel
Paderborn University
ebelo@math.upb.de

Stephan Schmidt
University Würzburg
stephan.schmidt@mathematik.uni-wuerzburg.de

Andrea Walther
Universität Paderborn
andrea.walther@uni-paderborn.de

MS164

Algorithmic Differentiation for Domain Specific Languages with Applications

Algorithmic Differentiation (AD) can be used to automate the generation of derivatives in arbitrary software projects. This will generate maintainable derivatives that are always consistent with the output of the software. If a domain specific language (DSL) is used in a software, the state of the art approach is to differentiate the DSL library with the same AD tool as used for the software which calls the library. The drawback of this solution is the reduced performance, since the compiler is no longer able to optimize(e.g. SIMD operations). The approach can also lead to a large overhead from AD, since operations in an DSL are not treated properly. A solution of a linear system is one example, where a specialized handling for AD is much more appropriate than the state of the art treatment. Our new approach, presented in this talk, is the development of a generalized AD tool that can be adjusted to any DSL. The new AD tool is partly generated from a specification of the DSL which, enables the AD tool to directly operate on the types and operators of the DSL. Furthermore, this approach enables the compiler to optimize again (e.g. for SIMD operations), since all calculations are still performed with the original data types. Then, it is also possible to handle DSLs, which could not be differentiated with the current state of the art approach.

Max Sagebaum, Nicolas R. Gauger
TU Kaiserslautern
max.sagebaum@scicomp.uni-kl.de,
nicolas.gauger@scicomp.uni-kl.de

MS164

Femorph: Symbolic Shape Differentiation and Au-

tomatic Code Generation

Computational fluid dynamics is an area where shape optimization problems arise naturally, such as finding airfoil designs of least possible drag. Furthermore, these types of problems offer a dense structure, which can be exploited. Examples here are the use of weak or strong form derivatives or how to deal with mesh sensitivities. As such, the semi-automatic creation of derivative formulations that exploit these structures is discussed. To this end, we exploit the area between algorithmic differentiation (AD), symbolic calculations and automatic code generation. Ideally, this creates an environment, where the shape derivative and adjoint equation is automatically created in human readable form, yet at the same time the corresponding computer program is also created. To achieve this, we consider graph transformations of the UFL domain specific language and the FEniCS framework. The talk concludes with the automatic construction of a shape Newton higher order optimization scheme for optimizing shapes in incompressible Navier-Stokes flows.

Stephan Schmidt
University Würzburg
stephan.schmidt@mathematik.uni-wuerzburg.de

MS165

Multiscale Adaptive Approximations to Functions Near Low-dimensional Sets

High-dimensional data arise in many fields of contemporary science and introduce new challenges in statistical learning due to the well-known curse of dimensionality. Fortunately, many real-world data sets in image analysis and signal processing exhibit a low-dimensional structure. I will present the regression problem of approximating functions on high-dimensional data that concentrated on a low-dimensional manifold. We will build multiscale approximations to the function and prove performance guarantees depending on the intrinsic dimension of the manifold. Moreover, our estimator is adaptive to the regularity of the function even when this varies at different scales or locations.

Wenjing Liao
Georgia Institute of Technology
wliao60@gatech.edu

MS165

Principal Graph and Structure Learning Based on Reversed Graph Embedding

Many scientific datasets are of high dimension, and the analysis usually requires retaining the most important structures of data. Many existing methods work only for data with structures that are mathematically formulated by curves, which is quite restrictive for real applications. To get more general graph structures, we develop a novel principal graph and structure learning framework that captures the local information of the underlying graph structure based on reversed graph embedding. A new learning algorithm is developed that learns a set of principal points and a graph structure from data, simultaneously. Experimental results on various synthetic and real world datasets show that the proposed can uncover the underlying structure correctly.

Li Wang
Department of Mathematics
University of Texas at Arlington
li.wang@uta.edu

MS165

The Separation of Signal Components: Geometric Interpretation and Random Dynamics

The separation of two wave-like components in a single signal record has wide applications in medical data, materials science, geophysics, etc. Traditional research focuses on sparse representation after a linear or nonlinear transformation; with the help of optimization or auto-regression, many methods have been proposed for the separation of signal components. This talk introduces the separation conditions and algorithms it is difficult to obtain sparse representation using existing techniques. We interpret the separation condition in terms of time-frequency geometry and propose a separation algorithm from the point of view of random dynamics.

Jieren Xu
Duke University
jieren.xu@duke.edu

Haizhao Yang
National University of Singapore
matyh@nus.edu.sg

Ingrid Daubechi
Duke University
ingrid@math.duke.edu

MS165

Data Clustering Based on Langevin Annealing with a Self-consistent Potential

We introduce a novel data clustering algorithm based on Langevin dynamics, where the associated potential is determined according to the density distribution of data points. The Langevin equations take a classical Gibbs distribution as the invariant measure, where the peaks of the distribution coincide with minima of the potential surface, and are considered as cluster centers. Clustering is achieved when subsets of the data aggregate as a result of the Langevin dynamics for a moderate period of time in the neighborhood of a particular potential minimum. The algorithms feasibility is first established based on several illustrating examples, followed by a stricter evaluation using a standard benchmark dataset. Clustering performance achieved a maximum Jaccard Score of 90% when evolving the benchmark data at relatively low temperature. Finally, to demonstrate the feasibility of our approach using a real dataset, it was applied to a quantitative imaging radiomics problem. Here, our findings suggest that information encoding pulmonary function may be buried deep within anatomic x-ray CT images.

Kyle Lafata, Zhennan Zhou, Jian-Guo Liu, Fang-fang Yin
Duke University
kyle.lafata@duke.edu, zhennan@bicmr.pku.edu.cn, jliu@phy.duke.edu, fangfang.yin@duke.edu

MS166

A Sampling Theorem for the Deconvolution of Point Sources

In the 70s and 80s geophysicists proposed using l1-norm regularization for deconvolution problem in the context of reflection seismology. Since then such methods have

had a great impact in high-dimensional statistics and in signal-processing applications, but until recently their performance on the original deconvolution problem was not well understood theoretically. In this talk we provide an analysis of optimization-based methods for the deconvolution problem, including results on irregular sampling and sparse corruptions that highlight the modeling flexibility of these techniques.

Brett Bernstein
New York University
brettb@cims.nyu.edu

MS166

Conjugate Phase Retrieval by Real Measurements

Classical phase retrieval on $\mathbb{C}^M$ attempts to recover signals up to a global phase factor. However, since conjugate of complex vectors cannot be distinguished using real measurement, such recovery is not possible if the only admissible measurements are real. In this talk, we propose and study in detail the notion of conjugate phase retrieval and show that it is possible to recover complex vectors by real measurements up to global phase and conjugacy. This is a joint work with Luke Evans.

ChunKit Lai
San Francisco State University
cklai@sfsu.edu

MS166

Near Optimal Performance Guaranteesfor Phase Retrieval of Low-rank Matrices

Phase retrieval reconstructs signals from their magnitude-only measurements. We are interested in a particular scenario where the unknown signal is rearranged as a low-rank matrix. Low-rank phase retrieval can be useful in several applications. For example, it enables blind calibration in optical imaging, synchronization-free system identification, and subspace learning from streaming data. We demonstrate that if the matrices involved in the measurement process follow certain distributions, the regularized anchored regression, which is a convex optimization formulation for low-rank phase retrieval without lifting, combined with a simple spectral initialization provides performance guarantees at near optimal sample rates. Our results can be compared to those for sparse phase retrieval where known initialization schemes have been shown guaranteed at suboptimal sample rates proportional to the square of the number of nonzeros.

Kiryung Lee
University of Illinois at Urbana-Champaign
kiryung@ece.gatech.edu

Sohail Bahmani
Georgia Institute of Technology
sohail.bahmani@ece.gatech.edu

Yonina C. Eldar
Technion and Stanford
yonina@ee.technion.ac.il

Justin Romberg
School of ECE
Georgia Tech
jrom@ece.gatech.edu

MS166

Approximate Noisy Super-resolution via Convex Optimzation

Abstract not available at time of publication.

Gongguo Tang
Colorado School of Mines
gtang@mines.edu

MS167

Simulating Solutions to the Generalized Langevin Equation using LAMMPS

Generalized Langevin dynamics (GLD) arise in the modeling of a number of systems, ranging from structured fluids that exhibit a viscoelastic mechanical response, to biological systems, and other media that exhibit anomalous diffusive phenomena. Molecular dynamics (MD) simulations that include GLD in conjunction with external and/or pairwise forces require the development of numerical integrators that are efficient, stable, and have known convergence properties. In this talk, we discuss the implementation of numerical integrators for the extended variable formulation of the Generalized Langevin equation (GLE) in the LAMMPS MD software package. Capability is demonstrated with respect to accuracy in canonical examples, stability in certain limits, and an exemplary application in which the effect of a harmonic confining potential is mapped onto a memory kernel.

Stephen D. Bond, Andrew D. Baczewski
Sandia National Laboratories
sdbond@sandia.gov, adbacze@sandia.gov

MS167

Homogenization for a Class of Generalized Langevin Equations

In this talk, I will present some results of our recent work on homogenization for a class of generalized Langevin equations (GLEs) with state-dependent coefficients. One of our main results says that in the limit, in which all the characteristic time scales of the system modeled by the GLEs vanish at the same rate, the position variable of the system converges to a homogenized process. The homogenized process is described by a stochastic differential equation containing additional drift terms induced by the noise in the considered limit. This is joint work with Jan Wehr.

Soon Hoe Lim
The University of Arizona
Department of Mathematics
shoelim@math.arizona.edu

MS167

Simulating Equilibrium and Non-equilibrium Variants of the Generalized Langevin Equation: Ergodic Properties and Efficient Numerical Discretization

In this talk I discuss ergodic properties and numerical integration schemes for systems which can be described by a quasi-Markovian generalised Langevin equation. Traditionally, in thermal equilibrium, one assumes (i) the forces in the generalised Langevin equation (GLE) are given as

the gradient of a potential and (ii) a fluctuation-dissipation relation holds between stochastic and dissipative forces; these assumptions ensure that the system samples a prescribed invariant Gibbs-Boltzmann distribution for a specified target temperature. In this talk I will relax these assumptions, incorporating non-stationary noise and temperature parameters and allowing nonconservative force fields, for which the form of the stationary state is typically not known a priori. I will discuss theoretical issues such as the existence of stationary states and ergodic properties of such systems. I will also introduce a class of numerical integrators which allow efficient simulation of such systems. Under certain technical assumptions geometric ergodicity for the respective discrete dynamics is shown and an asymptotic error analysis of the discretisation error in ergodic averages is provided. The analysis is supported by numerical experiments.

Matthias Sachs
Duke University, Mathematics
msachs@math.duke.edu

Benedict Leimkuhler
University of Edinburgh
b.leimkuhler@ed.ac.uk

MS168

Fast Algorithms for the Electrostatic Interaction in Charged Systems with Dielectric Boundaries

We introduced fast algorithms for investigating the electrostatic interaction for charged physical/biological systems in the presence of dielectric boundaries. Specifically, we present efficient, tailored, numerical or semi-analytical methods for solving the 3D Poisson's equation with special interface geometries such as spheres, planes or spheroids. Involved techniques including Boundary element method with extrapolation and singularity subtraction; spherical harmonic expansion; image charge method, etc. We further use these methods to explore the role of dielectric effect in varies problems such as colloidal like-charge attraction, self-assembly, and protein-protein interaction. We will show that the dielectric effect can play an important role in these charged physical/biological systems.

Zecheng Gan
Department of Mathematics, University of Michigan
zecheng@umich.edu

Erik Luijten
Department of Engineering Sciences and Applied Mathematics
Northwestern University
luijten@northwestern.edu

Weihua Geng
Southern Methodist University
wgeng@smu.edu

Robert Krasny
University of Michigan
Department of Mathematics
krasny@umich.edu

MS168

Hierarchical Combinatorial Deep Learning Algorithm and Architecture for Pancreas Segmentation of Medical Computed Tomography Cancer Images

Efficient computational recognition and segmentation of target organ from medical images are foundational in diagnosis and treatment, especially the diagnosis of pancreas cancer. However, the structures of previous networks, such as the richer feature convolutional network (RCF), are too coarse to segment the object (pancreas) accurately, especially the edge. In this paper, we extend the RCF, proposed to the field of edge detection, for the challenging pancreas segmentation, and put forward a novel pancreas segmentation network with multi-layer up-sampling structure. By employing multi-layer up-sampling structure replacing the simple up-sampling operation in all stages, the proposed network fully considers the multi-scale detailed texture information of object (pancreas) to perform per-pixel segmentation. Additionally, using the CT scans, we supply and train our network and get an effective pipeline. Working with our pipeline with multi-layer up-sampling model, we achieve better performance than the richer feature convolutional network (RCF) in the task of single object (pancreas) segmentation. Besides, combining with multi scale input, we achieve the 76.36% DSC (Dice Similarity Coefficient) value in testing data. The result of our experiment shows that our advanced model works better than previous network in our dataset by catching detailed texture information, which has practical meaning in computational automative diagnosis.

Xinqi Gong
Renmin University
xinqigong@ruc.edu.cn

MS168

Finite Element Simulations of the Solvation of Membrane Channel Proteins and the Transport of Solvated Ions in a Channel

A Finite Element solver is developed to study the Laterally Periodic Poisson-Boltzmann model for Membrane Channel Proteins. Studies shows taht all the factors, the membrane thickness, the length of periodic box, membrane dielectric constant, pore region dielectric constant, and ionic concentration, have individually considerable influence on the solvation energy of a channel protein. In addition, the ion's Born energy is incorporated into the PNP model (BPNP), which is shown to be able to successfully simulate the selective permeation of K+ in KcsA channel.

Benzhuo Lu
Institute of Computational Mathematics, China
bzlu@lsec.cc.ac.cn

Nan Ji
Institute of Computational Mathematics
jinan14@lsec.cc.ac.cn

MS168

Accelerating the 3D-RISM Implicit Solvent Model using Treecode and Multigrid Methods

A great advantage of the 3D reference interaction site model (3D-RISM) theory of molecular solvation is its ability to quantitatively model solvent density distributions, forces, and thermodynamics for a wide range of biomolecular systems using explicit solvent models. However, 3D-RISM remains much more computationally expensive than other implicit solvent models, such as generalized-Born or Poisson-Boltzmann. To accelerate 3D-RISM, we have tar-

geted the calculation of the long-range electrostatic interactions and convergence of the density distribution, which is the primary result of the theory. For all long-range electrostatic interactions, including long-range asymptotics and forces, we have implemented a cluster-particle treecode approach, which offers $O(N \log N)$ scaling when dealing with N solute charges. This provides significant improvements over the direct-sum scaling of $O(N^2)$. Convergence of the density distribution currently scales as $O(N \log N)$ due to the modified direct inversion of the iterative subspace (MDIIS) but is still computationally costly on typical grid sizes. By coupling MDIIS with a multigrid approach, we reduce the number of fine grid iterations by 50 to 90%. Together, these methods provide $O(N \log N)$ scaling for 3D-RISM and accelerate solutions by a factor of 10 or more for large proteins.

Tyler Luchko
Dept. of Physics & Astronomy
California State University, Northridge
tluchko@csun.edu

Leighton Wilson
University of Michigan
lwwilson@umich.edu

Robert Krasny
Department of Mathematics
University of Michigan
krasny@umich.edu

Garrett Limon
Dept. of Physics & Astronomy
California State University, Northridge
garrett.limon.719@my.csun.edu

MS169

Quasi-monogenic Functions and their Application in Image Processing

Quasi-monogenic functions are generalized monogenic functions which have the similar properties as monogenic functions. They are constructed in Fourier domain based on the decomposition of the classical Dirac operator D in $\mathbb{R}^n$ as $D = |D|\mathcal{H}$, where $\mathcal{H}$ is the Riesz-Hilbert transform. We construct a quasi-monogenic Riesz-Hilbert transform that is a singular integral operator, i.e., a Fourier multiplier in $L^p, 1 < p < \infty$, and the Fourier transform of it is a homogeneous polynomial of degree zero. Hilbert, Riesz, and Riesz-Hilbert transform have been widely used in image processing for analyzing images. We will demonstrate that the quasi-monogenic Riesz-Hilbert transform is a singular integral operator that fulfills similar properties as the analytic signal, introduced by Gabor, depending on the specific operator. Furthermore, we construct quasi-monogenic frames which unify the construction of monogenic wavelets and monogenic shearlets.

Swanhild Bernstein
Freiberg University of Mining and Technology
Institute of Geomathematics and Geoinformatics
swbernstein@gmail.com

MS169

Clifford Algebras, Möbius Transformations and Simplicial Complexes

We consider a construction of Clifford algebras providing a functor from a category of finite simplicial complexes to a category of differential modules. In this context, Möbius transformations for simplicial complexes can then be defined. The properties we discuss follows directly from the concept of Möbius transformations in high dimensions, together with recent developments of combinatorial Clifford algebras. The contribution of this note is to indicate new perspectives for manipulating functions on simplicial complexes, by taking advantage of the geometrical properties of Möbius transformations. This setting is inspired by classification problems in machine learning and signal processing.

Mijail Guillemard
Technical University Hamburg
mijail.guillemard@tuhh.de

PP1

Automatic Extraction of Cell Nuclei from Pathological Images

Pathological examination has been done manually by visual inspection of hematoxylin and eosin (H&E)-stained images. However, this process is labor intensive, prone to large variations, and lacking reproducibility in the diagnosis of a tumor. We aim to develop an automatic workflow to classify cells found in cancerous tumors portrayed in H&E-stained images. For a given image, we propose a segmentation technique based on a convolutional neural network (CNN). The network is trained to classify each pixel (in the context of a patch centered at that pixel) from an image. In such a network, a mix of convolutional and pooling layers is used to combine and summarize the data obtained from the RGB coordinates, followed by fully-connected layers and a softmax loss function to obtain a pixelwise probability map (indicating how likely a pixel belongs to a nucleus). Finally, active contour based method, together with morphological operations and watershed transform, are applied on the probability map to identify the cell nuclei. The proposed method is helpful to analyze the morphological properties of the tumor cells and predict further progress of the cancer.

Alsadig A. Ali, Brendan Caseria
The University of Texas at Dallas
aaa150830@utdallas.edu, brendan.caseria@utdallas.edu

Yan Cao
The University of Texas at Dallas
Department of Mathematical Sciences
yan.cao@utdallas.edu

Yifei Lou
Department of Mathematical Sciences
University of Texas at Dallas
yifei.lou@utdallas.edu

Guanghua Xiao
University of Texas Southwestern Medical Center
guanghua.xiao@utsouthwester.edun

PP1

Fourier Spectral Exponential Time Differencing Methods for Multidimensional Space-fractional Reaction-diffusion Equations

We propose two numerical methods for solving the space-fractional reaction-diffusion equations, which are based on a Fourier spectral approach in space and exponential time differencing schemes in time. The advantages of the approaches are that they attain spectral convergence, pro-

duce a full diagonal representation of the fractional operator, and the extension to multiple spatial dimensions is the same as the one-dimensional space. That can overcome the constraints associated with many of the numerical schemes for these equations such as the computational efficiency caused by the non-locality of the fractional operator, which results in full, dense matrices. Moreover, The proposed schemes are second-order convergent, unconditionally stable, and highly efficient due to the predictor-corrector feature when comparing them with the existing method . It is observed that the scheme based on using Padé(1,1) approximations to the matrix exponential function introduces oscillations with non-smooth initial data for some time steps due to high-frequency components present in the solution which diminish as the fractional order decreases. However, the scheme based on Padé(0,2) approximations to the matrix exponential function is oscillation-free for any time step. Numerical experiments for well-known models from the literature are performed to show the reliability and the effectiveness of the proposed methods.

Saham S. Alzahrani, A. Q. M. Khaliq
Middle Tennessee State University
ssa3g@mtmail.mtsu.edu, abdul.khaliq@mtsu.edu

PP1

A Manager for Engineering Projects Based on the Moise Model and Building Information Modeling

The Industrial Revolution triggered a number of changes and processes throughout world. This caused a major change in relations and means of production and in the educational system during that time. Since then, there has been a requirement for good quality and low cost to achieve the desired results without wasting any time. Considering the difficulty faced by professionals and students in the field of engineering to manage the various phases of a project, this work presents some features included in a System for Engineering Design Modeling. This system is perfectly suited for use on mobile devices (avoiding the use of paper) and is designed for easy viewing and editing of project information, named SiMoPE. Moreover, strategic planning offers attainable solutions that enable minimizing the effort needed to achieve the desired results in all projects. As a study tool in this work, we consider Building Information Modeling and the Moise+ Model organization

Mariane C. Amaral
FURG
marianecamaral@gmail.com

PP1

Efficient Solvers for Some Conic Variational Problems

"In this research, we studied few numerical methods for solving conic programming problems that involve constraints on Fourier modes. Pair interaction problems can be found in variety of natural phenomena like biological aggregation, colloids, liquid crystals, and self-assembly. Finding the global minimum and stable solution to a dynamical system is more challenging when there are many particles in the system, as the total energy from the interaction of all particles becomes highly non-convex. In our approach instead of minimizing the original non-convex functional, we find minimizers to the lower bound functional of it, which is convex. Now, the so-called relaxed problem can be solved using linear programming techniques. The nature of constraints in our problem allows us to exploit structure in order to find a faster algorithm."

Mahdi Bandegi
NJIT
mb495@njit.edu

David Shirokoff
New Jersey Institute of Technology
david.g.shirokoff@njit.edu

PP1

Modeling of Porous Metal Oxide Layer Growth

Under suitable conditions anodic metal oxidation leads to growth of complex porous structures. M. Habera in his diploma thesis suggests an electrochemical model to describe such an oxidation and proposes a numerical method leading to interesting outputs. However, the process itself is still not well understood. From the mathematical point of view, it can be modelled by a non-linear elliptic (in the stationary case) PDE for a potential, which admits jumps between several parts of the domain (electrolyte - oxide - metal). Moreover, the non-linearities are of exponential and jumping type. For these reasons, existence of a solution even in the stationary case is an interesting problem. To solve it, we introduce certain spaces related to Orlicz spaces and use the framework of maximally monotone graphs.

Michal Bathory
Charles University
bathory@karlin.mff.cuni.cz

Michal Habera
University of Luxembourg
michal.habera@uni.lu

PP1

Algebraic Vision Based Face Reconstruction and Mapping

In this poster lecture we will introduce an algebraic vision approach to identify and map face features. The features are purely based on polynomial singularities and other points of interest in the polynomial approximation of face imagery. Further, those features are generic enough to identify the same locales for a broad variety of different faces. In a final reconstruction step the features are used to deform low-polygonal face meshes to best approximate the real face geometry. A polynomial approch is then employed to texturemap the input imagery of the face onto the loe-polygonal face mesh.

Kai U. Berger
Genius Sports Media
berger.cg@gmail.com

PP1

Choosing the Number of Components for PLSGR Models: Influence of Missing Values

Partial Least Squares Regression (PLSR) is a multivariate model for which two algorithms (SIMPLS or NIPALS) can be used to estimate its parameters. The NIPALS algorithm has the interesting property of being able to cope with incomplete data and this has been extensively studied in the case of principal component analysis for which

the NIPALS algorithm has been originally devised. The NIPALS algorithm was extended (ENIPALS) to deal with univariate generalized linear responses, hence giving birth to Partial Least Squares Generalized Linear Regression (PLSGLR). Nevertheless, the literature gives no clear hints at the amount and patterns of missing values that can be handled by the PLSGLR and to what extent the model parameters estimates are reliable. We study the behavior of the ENIPALS algorithm, when used to fit PLSGLR models, for various proportions and pattern of missing data (at random or completely at random). Comparisons with multiple imputation are done. The ENIPALS algorithm tolerance to incomplete data sets depends on the sample size, the proportion of missing data and the chosen component selection method and a proportion of missing data will be given as an empirical maximum for a reliable components number estimation. The PLSGLR logistic models are often used to find relevant latent variables in binary classification, e.g. in genomics or economics, whereas the PLSGLR Poisson models are used for count modeling, e.g. in biology, ecology or actuarial science.

Frederic Bertrand
Universite de Strasbourg
fbertran@math.unistra.fr

Myriam Maumy-Bertrand
Universite de Strasbourg
IRMA
mmaumy@math.unistra.fr

PP1

A Computational Method for Modeling Anisotropy in the Earthquake Cycle

We have developed a computational method for incorporating and studying the effects of anisotropy when simulating cycles of earthquakes over many thousands of years. The method is developed for a vertical fault embedded in a 2D volume which serves as a frictional interface separating heterogeneous material. Inertial terms are dropped from the elastic anisotropic wave equation to obtain a steady state problem. This resulting equilibrium equation is discretized with summation-by-parts finite difference operators. Boundary conditions are enforced weakly to ensure a provably stable discretization. A nonlinear rate-and-state friction law is enforced at the fault. Time stepping is adaptive to capture highly varying time scales, and as such is able to produce self-consistent initial conditions prior to each earthquake. The accuracy of the method is verified via convergence tests for a manufactured solution. For the case of orthotropic anisotropy the method is consistent with observations of fault perpendicular fast directions. We quantify how anisotropy affects such features as surface velocity, surface displacement, and event duration, relative to an isotropic reference simulation. We find that for a large region of parameter space, anisotropy increases the recurrence interval between earthquakes. We are further developing the method to study the effects of heterogeneous anisotropy in sedimentary basins.

Maricela Best Mckay, Brittany Erickson
Portland State University
maricela@pdx.edu, berickson@pdx.edu

PP1

Extension Problem and Harnack Inequality For Master Equations

We analyze regularity properties for fractional powers of parabolic operators in divergence form in bounded domains. These equations are fundamental in continuous time random walk models and appear as the generalized master equation. Some other applications include the parabolic Signorini problem and the phenomenon of osmosis in heterogeneous media. These nonlocal problems are studied by using a localization procedure in the spirit of the extension problem of Luis Caffarelli and Luis Silvestre. Indeed, we develop a *parabolic* method of semigroups that allows us to prove an extension problem of parabolic type. As a consequence, we obtain parabolic Harnack estimates, both in the interior and up to the boundary. These results are completely novel for generalized master equations. This is joint work with Marta de León-Contreras (Universidad Autónoma de Madrid, Spain) and Pablo Raúl Stinga (Iowa State University).

Animesh Biswas
Iowa State University
animbisw@iastate.edu

Marta De León-Contreras
Universidad Autónoma de Madrid, Spain
marta.leon@uam.es

Pablo Stinga
Iowa State University
stinga@iastate.edu

PP1

Towards Geometric Multigrid on Unstructured Finite Element Meshes using LibMesh and PETSc

We report on progress towards support of geometric multigrid algorithms on general unstructured meshes using the libMesh finite element library together with the PETSc library. We discuss the approach for both Galerkin multigrid and full approximation scheme and, in particular, how libMesh interfaces with PETSc library to facilitate composable linear and nonlinear solvers. We demonstrate mesh-independent convergence for standard Laplace problems in 1D, 2D, using triangle and quadrilateral elements, and in 3D, using hexahedral and tetrahedral elements. We discuss progress towards scaling to large numbers of degrees of freedom and potential for usage in a variety of challenging problems and modern numerical schemes.

Paul Bauman
Mechanical and Aerospace Engineering
University at Buffalo, State University of New York
pbauman@buffalo.edu

Boris Boutkov
SUNY AT BUFFALO
borisbou@buffalo.edu

PP1

Implementation of a Finite Element Solver for Velocity Current MHD Equations

Magnetohydrodynamics (MHD) studies the movement of conducting fluids under the presence of electromagnetic fields. MHD phenomena range from industrial processes like aluminum casting to studies in astrophysics like the collapse and formation of stars. Of particular interest is plasma fusion and the Czochralski crystal growth pro-

cess for silicon. We discuss the numerical approximation of solutions to a velocity-current formulation of the three-dimensional viscous, resistive magnetohydrodynamics (MHD) equations. Unlike other formulations, the velocity-current formulation accounts for non-ideal boundaries and currents external to the domain. The system of integro-differential equations is linearized, discretized and then approximated using the finite element method. A parallel finite element solver is implemented using the open source academic library deal.II. The system matrix is iteratively solved using GMRES. Effective preconditioning strategies are required and a simple, block-diagonal Schur-complement preconditioner is proposed and tested. Results indicate that the preconditioner scales well.

Keith D. Brauss
Francis Marion University
dbrauss@fmarion.edu

Amnon J. Meir
Southern Methodist University
ajmeir@smu.edu

PP1

Gradient-based Pareto Optimal History Matching for Noisy Data of Multiple Types

The advantages of the simultaneous integration of production and time-lapse seismic data for history matching have been demonstrated in multiple studies. Production data provide accurate observations at specific spatial locations (wells), while seismic data enable global, though filtered/noisy, estimates of state variables. In this work we present a fast and efficient computational tool for history matching, in which data misfits of both the production and seismic measurements are minimized using an adjoint-gradient approach. This enables us to obtain a set of optimal solutions embodying the trade-off between the production and seismic data misfits (which are, to some extent, conflicting). We will discuss the existence of the (best) trade-off solution that surpasses other solutions in its ability to forecast future reservoir production. We also demonstrate quantitatively that, in the best trade-off solution, the negative effects of noise in the seismic data are effectively counteracted by information from the production measurements.

Vladislav Bukshtynov
Florida Institute of Technology
Department of Mathematical Sciences
vbukshtynov@fit.edu

Oleg Volkov
Stanford University
ovolkov@stanford.edu

Louis J. Durlofsky
Stanford University
Dept of Energy Resources Engineering
lou@stanford.edu

Khalid Aziz
Stanford University
Department of Energy Resources Engineering
aziz@stanford.edu

PP1

Exploring Homology through the Particle Model

For a given space we can define a set of topological invariants called homology groups. These groups provide information about the holes in the spaces being considered, and as such, can be used to distinguish spaces that we want to think of as different. On the other hand, there is a collection of spaces called Eilenberg-MacLane spaces that can be used as building blocks for other spaces. They are simple in that an Eilenberg-MacLane space has only one nontrivial homotopy group, but they are also often infinite dimensional. Cartan showed that the homology groups of certain Eilenberg-MacLane spaces have a nice addition and multiplication on them. We will be looking at some of these spaces, specifically ones with fundamental group Z/pZ, through the particle model (essentially a configuration space), to visualize the generators and relations of these homology groups.

Rachel Chaiser
University of Puget Sound
rchaiser@pugetsound.edu

PP1

Mathematical Model of Gender Bias and Homophily in Professional Hierarchies

Women have made great strides in business, academia, and government, yet the dearth of women at the highest levels of leadership remains. Sociologists have attributed the leaky progression of women through professional hierarchies to various cultural and psychological factors (such as self-segregation) as well as promotion bias. Here, we present a minimal mathematical model that reveals the relative role that bias and homophily (self-seeking) play in the ascension of women through professional hierarchies. To validate the model, we analyze a database of gender fractionation over time for several dozen professional hierarchies. By quantifying the degree of homophily and bias in each professional hierarchy, we propose specific interventions to achieve gender parity more quickly.

Sara M. Clifton
Northwestern University, USA
smc567@illinois.edu

Kaitlin Hill
University of Minnesota Twin Cities
khill@umn.edu

Avinash Karamchandani
Northwestern University
avinashkaramchandani2012@u.northwestern.edu

Patrick McMahon, Grace Sun, Alan Zhou
University of Illinois at Urbana-Champaign
pfmcmah2@illinois.edu, gsun8@illinois.edu, alanz2@illinois.edu

PP1

Linear Stability and Transient Behaviour of Viscoelastic Fluids in Boundary Layers

The behavior of many real fluids is well described by Navier-Stokes theory that is based on the assumption of

a Newtonian constitutive equation. Specifically, the extra-stress tensor can be expressed as a linear, isotropic function of the velocity gradients. Many common fluids such as water and air can be assumed to be Newtonian. However, rheologically complex fluids such as polymer solutions, soaps, blood, paints, shampoo are not adequately described by a Newtonian constitutive equation. Viscoelastic fluids are examples of non-Newtonian fluids, they exhibit both viscous and elastic properties when undergoing deformation. The aim of my research is to understand the stability behavior of such fluids in boundary layers. First, we consider a Rivlin-Ericksen fluid of second grade in a two-dimensional configuration of a flow over a semi-infinite wedge. A linear stability analysis leads to a modified Orr-Sommerfeld equation that is solved by a Chebyshev collocation method. The numerical experiments conducted show that elasticity in this model has a stabilizing effect. A second analysis demonstrates that, when a three-dimensional configuration is considered, elasticity can induce an instability in the form of stream-wise vortices. Furthermore, results on transient behavior show that elasticity generally increases the energy of the perturbations over short time periods. The stability analysis is extended to more complicated models of viscoelastic fluids.

Martina Cracco, Christopher Davies, Timothy Phillips
Cardiff University
craccom@cardiff.ac.uk, daviesc9@cardiff.ac.uk, phillipstn@cardiff.ac.uk

PP1

Fast Algorithms for Cosmic Microwave Background Radiation Data on Healpix Points

Faintly glowing at the edge of the observable universe, the Cosmic Microwave Background Radiation (CMBR) represents the first light to travel during the early stages of the universe's development. After about 379,000 years, the forming universe cooled enough to allow photons to move freely through space, creating a sphere of relic radiation that gives the strongest evidence for the Big Bang theory to date. Further analysis of the CMBR data can lead to revolutionary developments in understanding the nature of dark matter and dark energy. Since the discovery of the CMBR in 1964, scientists have worked to measure it in full detail, most recently using a Hierarchical Equal Area isoLatitude Pixelization scheme on the sphere. While these HEALPix points allow for a quasiuniform discretization of the sphere, they are not well suited for the fast algorithms necessary for mining the prodigious amounts of CMBR data. Utilizing the Double Fourier Sphere method, we transform the HEALPix grid to a Cartesian grid while preserving crucial symmetry and periodicity. We then use this to develop fast algorithms for analyzing CMBR data collected at the HEALPix points. Results illustrating the effectiveness and advantages of these algorithms over current methods are presented.

Kathryn P. Drake
Boise State University
kathryndrake@u.boisestate.edu

Grady B. Wright
Department of Mathematics
Boise State University, Boise ID
gradywright@boisestate.edu

PP1

A Look into the Dimensionality of Recurrent Neural Networks

Neural response trajectories, formed by the activity of many neurons simultaneously recorded in the brain, are revealing aspects of neural organization and computation beyond those that can be seen through observations of single neurons [Elsayed2017]. Theoretical studies of neural network models are furthering our understanding of how neural circuits might work [Barral2016], but fundamental questions remain about their basic behavior. This work takes a geometric perspective, seeking to better understand network trajectories through their dimensionality. We make the counter-intuitive observation that high-dimensional recurrent neural networks favor low-dimensional responses, both in the case of random connections and in the case when the network is trained to perform a classification task.

Matthew Farrell
Department of Mathematics
Cornell University
themattatk@gmail.com

PP1

Optimization Modeling in Matlab

The new problem-based workflow for optimization problems has made it much easier to model and solve linear and mixed-integer linear problems in MATLAB. Optimization variables are identified and defined as the first step. Next, objectives and constraints are defined via expressions of the optimization variables. The optimization solver is then selected automatically based on the type of constraints and objective. Large and complex optimization models can be expressed compactly using MATLAB arrays to index optimization variables and expressions. We will review design considerations, including extensions of familiar MATLAB objects in our implementation, and demonstrate with examples.

Mary Fenelon, Paul Kerr-Delworth, Aurèle Turnes
MathWorks
mary.fenelon@mathworks.com,
paul.kerr-delworth@mathworks.com,
aurele.turnes@mathworks.com

Steve Grikschat
Mathworks
steve.grikschat@mathworks.com

Adam Hug
Adam.Hug@mathworks.com
mathworks

PP1

An OSC Discretization of the Pressure Poisson Refomulation of the Navier-Stokes Equations

We present a numerical method for the pressure Poisson reformulation of the Navier-Stokes equations in two space variables. The reformulation decomposes the Navier-Stokes equations into two parts: Burgers' Equation (with homogeneous Dirichlet boundary conditions) and Poisson's equation (with non-homogeneous Neumann boundary conditions). Burgers' equation can then be solved by discretizing by alternating direction implicit (ADI) extrapolated Crank-Nicolson in time and orthogonal spline collocation (OSC) in space, giving the numerical solution for the velocity. At each time step, Poisson's must be solved

in order to update the pressure. A matrix decomposition algorithm (MDA) is used to solve for the OSC to Poisson's equation. Separately, we have obtained analytical results demonstrating optimal order accuracy in the H^1 norm for the ADI extrapolated Crank-Nicolson solution to Burgers' Equation and the OSC solution to Poisson's satisfying the prescribed boundary conditions using splines of $r \geq 3$. Thus, we expect optimal order accuracy for the overall scheme. Numerical experiments confirm this expectation. Moreover, the combination of ADI and MDA yields a numerical scheme which is both efficient and relatively straightforward to implement.

Nick Fisher, Bernard Bialecki
Colorado School of Mines
nfisher@mines.edu, bbialeck@mines.edu

PP1

Multigrid Method as Convolutional Neural Network

We propose a method to represent a multigrid algorithm as a convolutional neural network. Training our network to approximate the inverse corresponds to optimizing parameters in the restriction and prolongation. The significance of optimizing the parameters via a neural network is that prior knowledge is not required for construction and there is the potential for greater accuracy given comparable efficiency to traditional multigrid methods. Our approach seeks to utilize the sparsity pattern of the network, along with the action of the operator, to represent the inverse. Unlike a conventional deep network, our network has an aggressive reduction to small coarse layers that require fewer parameters and less expense for the network to learn the inverse. The coarsening and prolongation steps are done with convolutional layers and specific padding criteria. We are looking in the context of discretized PDEs and comparing to known multigrid techniques.

Sarah K. Gage, Jed Brown
University of Colorado Boulder
sarah.gage@colorado.edu, jed.brown@colorado.edu

PP1

To B(oussinesq), or Not to B(oussinesq)

In this project we consider a model for geothermal flows, such as those present in natural geyser sites. We work with a Darcy scale model and a coupled energy equation. The question of interest is the use of Boussinesq approximation for the buoyancy terms, and the incorporation of phase transitions in a coupled numerical scheme.

Diana Gonzalez
Oregon State University
gonzadia@oregonstate.edu

PP1

Application of El$_1$-Minimization Methods in Low-rank Approximation of a Tensor

The canonical decomposition of a tensor has a wide range of applications in sciences such as machine learning, signal processing, etc. The main goal of the poster is to present an algorithm to approximate a given tensor by a sum of rank-1 tensors. The related optimization problem can be split into smooth and non-smooth parts. We suggest a practical algorithm for computing the optimal solution via proximal operator tools. The analysis for the convergence of our algorithm will be presented afterwards.

Ramin Goudarzi Karim
Department of Mathematics
University of Alabama at Birmingham
ramin@uab.edu

PP1

Droplet Spreading, Chemically Treated Surfaces and Mathematics

Whether its the raindrops on your car's windshield, or the water running off a plant leaf, we frequently encounter the rich physics behind droplet motion and yet remain unaware of its impact on the modern world. For many decades this class of phenomena has fascinated academics from all areas of science and engineering, furthermore, this interest has brought the development of new technologies such as inkjet printers, and the design of self cleaning surfaces. From a mathematical point of view this area leads to some interesting and yet complex equations, where solutions rely on powerful computers with long simulation times. In many configurations where large amounts of simulations are required we cannot afford these high computing costs, therefore emphasis must also be placed on powerful mathematical methods, such as matched asymptotic analysis, to develop simpler models that retain key physical mechanisms. Using these methods we can determine solutions to the complicated equations at much faster rates, with an example simulation being 250,000 times faster than a supercomputer simulation. This simpler model can potentially assist in the design of surface features for experimental study, help us further understand the key physics behind droplet motion, and advance the development of new technologies.

Danny Groves
Cardiff University
grovesd2@cardiff.ac.uk

Nikos Savva
School of Mathematics, Cardiff University
savvan@cardiff.ac.uk

Usama Kadri
Cardiff University
kadriu@cardiff.ac.uk

PP1

Ecotoxicological Dynamics Subject to Stoichiometric Constraints

The development of ecotoxicological models over the last couple decades have significantly contributed to interpreting how contaminants impact organisms and cycle through food webs. However, there is increasing evidence that organisms experience interactive effects of contaminant stressors and food conditions, such as resource stoichiometry and nutrient availability. Stoichiometric Ecotoxicology modeling efforts shed light on nutrient and chemical contaminant cycling and ultimately can help improve toxicological risk assessment protocols. We are formulating a series of empirically testable and robust models of algae-Daphnia population dynamics subject to concurrent nutritional and contaminant stressors. In parallel to developing the models we are conducting laboratory experiments manipulating the nutritional content of algae fed to Daphnia exposed to Cadmium, Arsenic, and Copper. Here, we

present modeling and empirical results and discuss the synthesis of the two approaches.

Md Nazmul Hassan
Texas Tech University
md.nazmul.hassan@ttu.edu

PP1

Numerical and Bayesian Inference Solutions to the Hodgkin-Huxley ODE Model of Neuronal Action Potential

The most biophysically accurate models, in terms of a mathematical description of ion gates and membrane potentials, are widely accepted to be those derived from the original Hodgkin and Huxley ODE system created in 1952. The coupled, non-linear, system of equations has an incredible ability to simulate the spiking characteristics of neurons, but lacks computational efficiency and scalability. This consequence is partially derived from the characteristics of the equations themselves, because the stiffness of the system increases as neurons and simulation times expand. In an attempt to best solve these equations for voltage and rate constants, several numerical methods, including forward Euler, backward Euler, MATLABs ODE45, Adams-Bashforth-Moulton predictor-corrector, fourth order Runge-Kutta have been utilized in previous work. This project implements all of these methods in MATLAB and also explores spectral deferred correction method to advance the existing techniques. In addition to these forward methods, recent research has used Approximate Bayesian Computational Inference techniques on experimental data to solve for the unknown parameters. The goal of this poster is to explore existing techniques for the approximation of parameters and numerical solutions for computational efficiency and accuracy in both single HH neural models and those in a network.

Kyle Henke
University of New Mexico SIAM Student Chapter
khenke3@unm.edu

PP1

Frame Codes for Cosmic Communication

In this presentation, we introduce two-dimensional frame codes in the space $Mat_{m\times s}(F_q)$ endowed with the frame metric of order $p \times r(1 \leq p \leq m, 1 \leq r \leq s)$ and present their properties. The theory of frame codes will be useful in bursty channels cosmic environment such as deep state communication, satellite communication, aircrafts and spacecrafts, etc.

Shantanu Jain
Hindustan Institute of Technology and Science
Chennai
shantanujain@gmx.com

PP1

Why There May be More Slow-fast Systems than you Thought

Geometric singular perturbation theory (GSPT) provides a well established framework for the study of slow-fast dynamical systems. For the most part, this framework has been applied only for systems in which the slow-fast structure derives from a separation of slow/fast variables. Not all slow-fast systems have such a structure, however, and applications of GSPT to slow-fast systems without a slow/fast variable splitting are rare in the literature. We show how the traditional theory can be generalised so that it may be applicable to a larger class of problems, and illustrate the method by applying it to prove results about a slow-fast limit cycles and so-called "canard explosions" which cannot be studied classically.

Samuel Jelbart
Sydney University
sjel7292@unisydney.edu.au

PP1

Offline-Enhanced Reduced Basis Method Through Adaptive Construction of the Surrogate Training Set

The Reduced Basis Method (RBM) is a popular certified model reduction approach for solving parametrized partial differential equations. However, a large number of parameter inputs diminish the attractiveness of RBM algorithms since this proportionally increases the cost of the offline phase. In this work we propose novel strategies for offline RBM algorithms that mitigate the computational difficulty of maximizing error estimates over a training set. The main idea is to identify a subset of the training set, a Surrogate Training Set (STS), on which to perform greedy algorithms. The STSs we construct are much smaller in size than the full training set, yet our examples suggest that they are accurate enough to induce the solution manifold of interest at the current offline RBM iteration. We propose two algorithms to construct the STS: Our first algorithm, the Successive Maximization Method (SMM) method, is inspired by inverse transform sampling for non-standard univariate probability distributions. The second constructs an STS by identifying pivots in the Cholesky Decomposition of an approximate error correlation matrix. We demonstrate the algorithm through numerical experiments, showing that it is capable of accelerating offline RBM procedures without degrading accuracy, assuming that the solution manifold has rapidly decaying Kolmogorov width.

Jiahua Jiang
University of Massachusetts, Dartmouth
jjiang@umassd.edu

Yanlai Chen
Department of Mathematics
University of Massachusetts Dartmouth
yanlai.chen@umassd.edu

Akil Narayan
University of Utah
akil@sci.utah.edu

PP1

Convex Bilinear Inversion from Entrywise Product of Signals with Known Signs

We consider the bilinear inverse problem of recovering two vectors, $\mathbf{x}$ and $\mathbf{w}$, in R^L from their entrywise product. For the case where the vectors have known signs and belong to known subspaces, we introduce the convex program BranchHull which is posed in the natural parameter space and does not require an approximate solution or initialization in order to be stated or solved. Under the structural assumptions that $\mathbf{x}$ and $\mathbf{w}$ are members of known K and N dimensional random subspaces, we present a recovery guarantee which shows BranchHull is robust to small dense

noise with high probability when $L = \Omega(K + N)$. We also consider an L1 version of the BranchHull program for the case where the vectors are sparse w.r.t. to the known subspaces. BranchHull is motivated by the sweep distortion removal task in dielectric imaging, where one of the signals is a nonnegative reflectivity, and the other signal lives in a known wavelet subspace. Another application is removing shadow from an image, where the image of interest is nonnegative, and the shadow signal lives in an incomplete DCT subspace.

Babhru Joshi, Paul Hand
Rice University
bj12@rice.edu, hand@rice.edu

Alireza Aghasi
Georgia State University
aaghasi@gsu.edu

Ali Ahmed
Information Technology University
Lahore
ali.ahmed@itu.edu.pk

PP1

Examining Redistricting and Gerrymandering using Mathematical Algorithms

Gerrymandering is a problem that is frequently discussed in the media and the court system. This gives rise to the question of how can one best detect gerrymandering and how might one prevent it in the future. In this poster presentation, we present several different mathematical algorithms for drawing congressional district lines and measure the extent of gerrymandering with each new map using recently proposed mathematical techniques.

Nicholas J. Joyner, Michele Joyner
East Tennessee State University
joynern@etsu.edu, joynerm@etsu.edu

PP1

A Nonlinear Non-monotonic Effective Diffusion Coefficient for a Neural Mixed-mode Oscillator

The mitral cells of the mammalian olfactory bulb feature mixed-mode oscillations (MMOs) with both the large amplitude spikes typical of neurons and small amplitude, subthreshold oscillations (STOs). They receive noisy input from sensory neurons, which can strongly perturb the patterns of spikes and STOs displayed by each mitral cell and greatly affect the cells' spike-driven interactions. As a result, the commonly used weak-coupling theory for coherent dynamics in coupled oscillator systems breaks down even for small levels of noise. We find, however, that we can define and measure an effective diffusion coefficient for the phase of each cell's oscillation. We demonstrate that applying this quantity, which is strongly nonlinear and non-monotonic in the input noise strength, greatly extends the applicability of the weak-coupling theory. To elucidate the origin of the effective diffusion coefficient and its features, we investigate the extreme sensitivity of the spike times to noisy inputs. We find that the sequences of the interspike intervals (ISIs) are strongly correlated over a long time scale. Comparing the ISIs from the full MMO model and a reduced version, we identify one slow variable as key to the correlations, giving a Markovian description for the stochastic dynamics. Through this picture, we reveal how subtle features of the slow variable's dynamics have robust and substantial effects on the effective diffusion.

Avinash J. Karamchandani
Department of Engineering Sciences and Applied Mathematics
Northwestern University
avijka@u.northwestern.edu

Hermann Riecke
Applied Mathematics
Northwestern University
h-riecke@northwestern.edu

PP1

Multiresolution Analysis of S&P500 Time Series

Time series analysis is an essential research area for those who are dealing with scientific and engineering problems. The main objective, in general, is to understand the underlying characteristics of selected time series by using the time as well as the frequency domain analysis. Then one can make a prediction for desired system to forecast ahead from the past observations. Time series modeling, frequency domain and some other descriptive statistical data analyses are the primary subjects of this study: indeed, choosing an appropriate model is at the core of any analysis to make a satisfactory prediction. In this study Fourier and wavelet transform methods are used to analyze the complex structure of a financial time series, particularly, S&P500 daily closing prices and return values. Multiresolution analysis is naturally handled by the help of wavelet transforms in order to pinpoint special characteristics of S&P500 data, like periodicity as well as seasonality. Besides, further case study discussions include the modeling of S&P500 process by invoking linear and nonlinear methods with wavelets to address how multiresolution approach improves fitting and forecasting results.

Deniz K. Kilic
Middle East Technical University
Institue of Applied Mathematics / Financial Mathematics(Phd)
deniz.kenan.kilic@gmail.com

PP1

Interaction of Water Waves with a Submerged Inclined Elastic Plate in Deep Water

The interaction of linear water waves with an inclined elastic plate as a breakwater is analyzed when it is clamped at the upper end and moored at the lower end. The assumption of Euler-Bernoulli beam model for the plate allows obtaining the normal derivative of the potential function across the plate boundary. On the other hand, using Greens integral theorem, another expression is evaluated for the same. The comparison between these two forms provides a hypersingular integral equation of the first kind in the potential difference along the plate, which is solved by the expansion-collocation method. The solution of the hypersingular integral equation is used to find the reflection and the transmission coefficients and the hydrodynamic force components. The results are presented for different inclination angle, different submergence depth of the plate, variable length and different flexural rigidity of the plate.

Souvik Kundu
Indian Institute of Technology Kharagpur
kundusouvik@iitkgp.ac.in

Rupanwita Gayen
Indian Institute of Technology Kharagpur,
Kharagpur-721302
West Bengal, India
rupanwita.gayen@gmail.com

Ranadev Datta
Indian Institute of Technology Kharagpur
ranadev@naval.iitkgp.ernet.in

PP1

Numerical Approximations of the Non-Newtonian Fluid Flows Cross a Square Cylinder using Adaptively Weighted Least-squares Finite Element Methods

The work concerns least-squares finite element methods for the non-Newtonian fluid flow problems cross a square cylinder. The LS method uses the L^2-norm of the residuals of the continuity equation multiplied by appropriately adjusted weights. We employ an adaptive weight iteration approach based on a residual type a posteriori error estimator for the LS functional. Numerical results indicate that we can apply the LS method to flow problems and discuss the physical parameter effects.

Hsueh-Chen Lee
General Education Center
Wenzao Ursuline University of Languages, Taiwan
87013@mail.wzu.edu.tw

PP1

Bifurcations and Dynamics in a Growth-first Discrete-time Host-parasitoid Model

We investigate the dynamics of a specific discrete-time host-parasitoid model originally proposed by May et. al. (1981). While the model includes standard functional forms for parasitism and density dependent growth in the host species, the timing of these events in the life cycle leads to unexpected dynamics for certain parameter values. We discuss and analyze the bifurcations in the model, including an unexpected cyclic fold bifurcation resulting in bistability.

Kelsey Marcinko, Mark Kot
University of Washington
kmar517@uw.edu, mark_kot@comcast.net

PP1

Determination of Optimal Closures for Hydrodynamic Models

This investigation is motivated by the question about performance limitations characterizing certain common closure models for nonlinear models of fluid flow. The need for closures arises when for computational reasons first-principles models, such as the Navier-Stokes equations, are replaced with their simplified (filtered) versions such as the Large-Eddy Simulation (LES). In the present investigation we focus on a simple model problem based on the 1D Kuramoto-Sivashinsky equation with a Smagorinsky-type eddy-viscosity closure model. The eddy viscosity is assumed to be a function of the state (flow) variable whose optimal functional form is determined in a very general (continuous) setting using a suitable adjoint-based variational data-assimilation approach. In the presentation we will review details of the formulation of the computational approach and will discuss some computational results.

Pritpal Matharu
McMaster University
mathap1@mcmaster.ca

Bartosz Protas
Dept of Mathematics and Statistics
McMaster University
bprotas@mcmaster.ca

PP1

Robustifying Partial Least Square Generalized Linear Regression

The NIPALS algorithm is commonly used to fit the Partial Least Squares Regression (PLSR) model and has the key property of being able to cope with collinear explanatory variables. It was extended (ENIPALS) to deal with univariate generalized linear responses, hence giving birth to Partial Least Squares Generalized Linear Regression (PLSGLR). The ENIPALS algorithm can still naturally cope with collinear explanatory variables, yet it is sensitive to outliers or influential observations that often contaminate real datasets. We propose various robust extensions of the ENIPALS: using Mallows or Huber type robust estimators or conditionally unbiased bounded influence robust fit. The PLSGLR logistic models are often used to find relevant latent variables in binary classification, e.g. in genomics or economics, whereas the PLSGLR Poisson models are used for count modeling, e.g. in biology, ecology or actuarial science. We will provide example of fit improvements on several datasets and especially in MS/MS proteomics where it is well known the use of regularized robust methods can greatly improve the inference of the abundances of proteins for the peptide intensities.

Myriam Maumy-Bertrand
Universite de Strasbourg
IRMA
mmaumy@math.unistra.fr

Frederic Bertrand
Universite de Strasbourg
fbertran@math.unistra.fr

PP1

Efficient Estimation of Uncertainties in Coastal Flooding Forecasts

We present a methodology for fast variance estimation in spatio-temporal problems in coastal applications, where computing model ensembles may be too costly in time to render effective results. The methodology is applied here to the approach of tsunami waves due to submarine mass failure near coastlines, where variance estimation may be used to inform risk analysis for coastal engineering design. We use a linearized perturbation model for the shallow water equations to simulate tsunamis, where a fully nonlinear solution has been given as the mean result. We use the linearized model to produce Green's function calculations for generating waves with perturbed initial conditions, with resulting data recorded for a grid of points of interest along the coast. The Green's function approach allows very efficient calculations of ensemble members and variances, which are then interpolated to the entire domain using Gauss-Markov kriging. The methodology is applicable to other similar dynamic problems. This project was developed during a year long fellowship program called the

NSF Research Traineeship, which builds interdisciplinary teams to solve problems in marine science.

Will D. Mayfield, Harrison Ko, Michael Dumelle
Oregon State University
mayfielw@math.oregonstate.edu, koh@oregonstate.edu, dumellem@oregonstate.edu

PP1

Accurate Surface Normals From Photographs using Computational Imaging

Reflectance Transformation Imaging was developed in 2001 by Malzbender at HP Labs. The technique aims to model the reflectance of an object under varying light conditions using a simple bi-quadratic polynomial. The process involves capturing images of a static scene from a stationary camera whilst moving a light source around in an equidistant (hemispherical) sequence. The method is inexpensive as it only requires a camera and a light source, and can obtain surface normal measurements more accurate than laser scanning for low relief variances in a surface. The technique is popular with cultural heritage imagers, who often are interested in qualitative analysis rather than quantitative. For this reason the technique has remained largely unchanged with end users since its conception. Methods to improve the accuracy of the surface normals obtained from the technique have been investigated. Chiefly, the mathematics make a false assumption that the light rays from the illumination source (a handheld torch or LED in a dome rig) are parallel across the image plane. This incorrect assumption makes the computation time much faster, but can result in surface normals being severely distorted around the image periphery (particularly for larger scenes as compared to close ups of ancient coinage). A method to correct these distortions has been developed, and the results show a marked improvement in surface normal data after correcting for the fact that the light rays are not parallel.

Matthew Mcguigan
University of Exeter
mm757@exeter.ac.uk

Jacqueline Christmas
Supervisor
j.t.christmas@exeter.ac.uk

PP1

The Underlying Structure of Particulate Matter Concentrations

Functional data analysis continues to greatly attract attention because technological advances in many fields, such as the environmental sciences, have permitted measurements to be made from continuous processes at finer discretizations. Particulate matter continues to be among the most harmful air pollutants, and the relatively high frequency of daily particulate matter sampling enables us to treat the data as functional data. We discuss the separation of the phase and amplitude variation in particulate matter and explore its underlying structure using functional data analysis methodologies. The results improve the understanding of the spatial-temporal behavior of particulate matter.

Eduardo Montoya
California State University, Bakersfield
emontoya2@csub.edu

PP1

Controllability of Functional Classes in the Genetic Regulatory Network of *E. Coli*

While the traditional methods in control theory are computationally expensive for large systems, more recent work that takes a graph theoretical approach to control has been able to make such computations possible. These methods are breifly described through the lens of a paper published by researchers at Northeastern University and Massachusetts Institute of Technology (Liu, Slotine and Barabasi, Nature 2011). This is followed by an exploration into the controllability of the genetic regulatory network of the bacterium, *E. coli* using a data set containing 3277 genes and 8740 interactions. The genetic regulatory network of *E. coli* has been previously shown to be not easily controllable. Therefore, the possibility that organisms do not need highly controllable genetic regulatory networks is entertained. This is done by focusing on the target controllability of specific classes of genes. It is seen that the target controllability of some of these classes can be understood in terms of the biological functionality of the class.

Ananthan Nambiar
Reed College
annambiar@reed.edu

PP1

A Smoothed Newton Method for Support Vector Machines with ℓ^1 Penalty

A method for the solution of large-scale soft-margin Support Vector Machine (SVM) with an ℓ^1 penalty is presented. This method is inspired by the method of Osborne, Presnell and Turlach (2000) for the Lasso. The unpenalized objective function for the soft-margin SVM is piecewise linear. In order to develop a Newton type method for this problem, we use a smoothing procedure with a smoothing parameter that is systematically modified to enable rapid convergence to the solution of the original unsmoothed problem. This method can be easily parallelized. Numerical results showing the competitiveness of our method will be presented.

Suely P. Oliveira, Jeffrey Hajewski
University of Iowa
Department of Computer Science
oliveira@cs.uiowa.edu, jeffrey-hajewski@uiowa.edu

David Stewart
University of Iowa
Department of Mathematics
david-e-stewart@uiowa.edu

PP1

Optimal Control Analysis for Constant Flux Microfiltration

Microfiltration is a filtration method that clears the pollutants and microorganisms efficiently from the liquid. It is used in urban water treatment, dairy industry and pharmaceutical industry. Flat-sheet membrane and hollow-fiber membrane micro filters are commonly used in water treatment. Hollow -fiber is more advantageous than flat-sheet membrane filter because of longer operation time, slower fouling rate, and higher volumetric capabilities. These

filtrations are generally carried out in constant pressure and constant flux mode. Even if constant flux mode is more widely used in industrial settings, majority of the researches are based on constant pressure mode. The common problem for all filtration process is accumulation of pollutants on the filter surface. In order to regenerate the filter the flow is reversed periodically which is called backwashing operation. Dr. Cogan and Jian Li created a model for constant pressure flat-sheet membrane filter and used optimal control analysis for optimal timing and duration of backwashing cycles. In this project our scientific goal is that first test the model and do the optimal control analysis for constant flux flat-sheet filter then regenerate a model and dynamical system for constant flux hollow-fiber membrane filter.

Deniz Ozturk
Florida State university
dozturk@math.fsu.edu

PP1

An Asymptotic-Preserving Spectral Method Based on the Radon Transform for the PN Approximation of Radiative Transfer

The equation of radiative transfer is an integro-differential equation in a five-dimensional phase space for the specific intensity of a radiation field. The equation models the transport of the radiation field, the energy loss due to absorption, the energy gain due to emission, and the redistribution of energy due to scattering. In the PN approximation, the specific intensity is replaced by a truncated spherical harmonics expansion, which results in replacing the five-dimensional integro-differential equation by a three-dimensional system of coupled partial differential equations. The resulting system of PDEs is hyperbolic, although the system becomes a parabolic heat equation in the vanishing mean-free path limit (i.e., the scattering dominated regime). A desirable feature of numerical methods for the PN system is that they remain stable and accurate if we fix the mesh parameters and take the vanishing mean-free path limit—in the literature this has been dubbed the "asymptotic-preserving" property. In this work, we develop a Chebyshev pseudo-spectral method for solving the PN system. The time-stepping is done using an L-stable scheme that guarantees that the overall numerical method is asymptotic-preserving. In the multi-dimensional implementation of the method, we make use of the Radon transform to reduce the computational complexity of the matrix inversion. Several numerical tests are presented in order to demonstrate the feasibility of the resulting method.

Lindsey M. Peterson, James A. Rossmanith
Iowa State University
Department of Mathematics
lindseyp@iastate.edu, rossmani@iastate.edu

PP1

A Numerical Method for the Quantum Liouville-BGK Equation

This poster will introduce a numerical scheme for solving the quantum Liouville-BGK equation, where the equilibrium in the relaxation term is obtained by minimizing a free energy functional under local constraints . The equation forms a system of coupled nonlinear PDEs and models the dynamics of a many-particle system. The numerical difficulties lie in the nonlinear coupling between the PDEs, and are addressed by using a splitting scheme in which the nonlinearity becomes a perfectly linear term. The specifics of the splitting scheme will be presented, along with the associated convergence analysis and supporting numerical results.

Sophia Potoczak
Colorado State University
sophia.potoczak@gmail.com

PP1

Predicting Statistical Response in Uncertainty Quantification through Reduced-order Models

The capability of using imperfect statistical and stochastic reduced-order models to capture crucial statistics in turbulent flow and passive tracers is investigated. Much simpler and more tractable block-diagonal models are proposed to approximate the complex and high-dimensional turbulent flow equations. The imperfect model prediction skill is improved through a judicious calibration of the model errors using leading order statistics. A systematic framework of correcting model errors with empirical information theory is introduced, and optimal model parameters under this unbiased information measure can be achieved in a training phase before the prediction. It is demonstrated that crucial principal statistical quantities in the most important large scales can be captured efficiently with accuracy using the reduced-order model in various dynamical regimes of the flow field with distinct statistical structures.

Di Qi
New York University
qidi@cims.nyu.edu]

Andrew Majda
Courant Institute NYU
jonjon@cims.nyu.edu

PP1

Data Fusion Reconstruction of Spatially Embedded Complex Networks

Inferring networks from data (e.g., estimation of brain connectivity via fMRI "[E. Bullmore and O. Sporns, "Complex brain networks: graph theoretical analysis of structural and functional systems," Nature Revi. Neurosci. 10, 186–198 (2009).]') is important in many practical applications, especially when direct invasive measurements are infeasible. Given time series data collected on the nodes of a spatial network, the problem is to infer the underlying interaction structure of the network "[J. Sun, D. Taylor, and E. M. Bollt, SIAM Journal on Applied Dynamical Systems 14(1), 73–106 (2015).]'.A main challenge is that the amount of data in practice is typically small comparing to the size of the network, rendering reliable inference a difficult and sometimes impossible task. Recognizing that many real world networks are spatially embedded "[M. Barthelemy, "Spatial networks,"]', this project utilizes such information to develop a kernel-based spatial network inference framework that significantly improves inference outcome. Our new approach enables efficient and accurate reconstruction of large spatial networks from limited data even when the exact spatial distribution of the embedded edges are not known. The results have potential impacts on biological and engineering applications where big data is being continuously collected.

Fernando J. Quevedo

Department of Mathematics
Clarkson University
QuevedFJ@Clarkson.edu

PP1

Advanced Mathematical Approaches for Modeling Animal Movement through Landscapes

An important component of population ecology is understanding the impact on animal movement. Modeling animal movement helps us understand how this impact manifests itself in animal behavior and habitat selection as well as human impact on wildlife. Correlated movement and heterogeneous landscapes add complexity to these models and are often neglected. How do landscape features condition population movement and habitat choice? I answer this question by showing that motility does play a significant role in population dynamics. The ecological telegrapher's equation (ETE) incorporates both variable landscape and correlated movement. The solution to the ETE predicts the PDF of future locations. I use this PDF in a maximum likelihood process to parameterize the ETE with simulated data. In this work, I develop code to generate test data by simulating trajectories with a correlated random walk on a simulated terrain. I determine the accuracy of the MLE procedure by parameterizing the ETE with the simulated data and comparing with the assigned values in the simulated landscape. Applying the same MLE procedure to actual telemetry data from mule deer in Southern Utah will yield the impact of different landscape types on mule deer.

Molly Robinson, Ian McGahan, Thomas Edwards, James Powell
Utah State University
mollyrob15@gmail.com, ian.mcgahan@aggiemail.usu.edu, t.edwards@usu.edu, jim.powell@usu.edu

PP1

New Approach to Tensor Completion

We propose a new method for solving tensor completion. We are applying low rank tensor decomposition using sparse optimization. The tensor optimization model is the alternating least squares method, and an l1-minimization on the diagonal entries of the tensor. We demonstrate the performance of our algorithm through several images and videos.

Fatoumata Sanogo
UNIVERSITY OF ALABAMA AT BIRMINGHAM
sanogof1@uab.edu

Carmeliza Navasca
Department of Mathematics
University of Alabama at Birmingham
cnavasca@gmail.com

PP1

Regularization of a Nonlinear Transport Model of Methane Gas with Space-dependent Flux Function, and Numerical Approximation

Methane is a greenhouse gas, and extraction of methane from subsea sediment has been of interest for energy sources. Under low temperature and high pressure, methane and water form methane hydrate, an ice-like substance present in subsea sediments. We study a transport model of methane gas with space-dependent flux functional. The first challenge is that the model has a multivalued graph, and we used a change of variable to rewrite the model. Another challenge is that the obtained flux function is not smooth and depends on two variables. We use regularization to obtain a smooth concave flux function and discuss the seemingly unphysical, and at first glance, unexpected blow-up behavior of this problem. We also discuss the convergence of the numerical solution to this problem using the Godunovs scheme with local phase behavior solver.

Choah Shin
Oregon State University
Department of Mathematics
shinc@oregonstate.edu

Malgorzata Peszynska
Department of Mathematics
Oregon State University
mpesz@science.oregonstate.edu

PP1

Critical Slowing Down Indicators in a Mutualistic Network

Critical slowing down (CSD) is known to generically precede tipping points related to certain bifurcations. However, the evidence of CSD depends nontrivially on the exact system under study. In particular, high-dimensionality and heterogeneous coupling among dimensions demand more principled understanding. In this work we examine the relationships between the structural features of certain mutualistic ecological networks and the covariances between species abundances as the ecosystem approaches a tipping point.

Jordan Snyder
University of California, Davis
jasnyder@math.ucdavis.edu

PP1

Fast Algebraic Multigrid Preconditioners for Radiative Transport and Fully Kinetic Plasma

A new algebraic multigrid (AMG) algorithm has been developed recently based on an approximate ideal restriction (AIR), which has demonstrated potential as a fast, parallel solver for scalar hyperbolic PDEs. Here, we use AIR as an integral part in developing preconditioners for high-dimensional, hyperbolic systems of PDEs. First, we look at coupling AIR with the diffusion synthetic acceleration (DSA) approach to solving the radiative transport equation. Because AMG scales well in parallel, AIR promises better parallel scaling than a traditional transport sweep associated with the DSA algorithm. This is especially promising in the context of curvilinear meshes, which often yield non-triangular matrices that are difficult for traditional sweeping algorithms. Then, we explore the potential of developing a DSA-like algorithm for implicit discretizations of the full Vlasov-Maxwell description of plasma, based on AIRs capability to solve the Vlasov equation and standard AMG to resolve the Maxwell equations. Due to the high dimensionality of the Vlasov-Maxwell system and a lack of fast linear solvers for implicit discretizations of Vlasov, implicit time stepping for kinetic plasma discretizations is largely unexplored. AIR provides such a solver, opening new doors for implicit discretizations of Vlasov-Maxwell and other hyperbolic PDEs, with tractable

computational cost.

Ben Southworth
Department of Applied Mathematics
University of Colorado, Boulder
ben.southworth@colorado.edu

Tom Manteuffel
University of Colorado, Boulder
tmanteuf@colorado.edu

PP1

An Equation-free Multi-scale Time Integration Approach to Fusion Plasma Simulation

Physical processes relevant to magnetically confined fusion plasmas occur over a large range of time and spatial scales. This presents a challenge for the numerical simulation of long-time scale, macroscopic processes since resolution requirements are generally restricted by the physics occurring on the shortest and fastest scales. Here we present a multi-scale time integration method based on equation-free modeling [1]. In this approach, a 4D gyrokinetic neoclassical simulation is taken as an example system. The 4D particle distribution function (2 configuration space variables and 2 velocity variables) is evolved over short time intervals by performing fully resolved simulations with the gyrokinetic, particle-in-cell code XGCa [2]. The distribution function is then restricted to a set of low-order, 2D fluid moments, which are extrapolated over a large time step. Finally, the fluid moments are transformed back to a 4D distribution function using the particle distribution function information in the previous cycle, using a weighted orthogonal polynomial expansion in the two velocity space variables, to continue the simulation at the next large time step. We demonstrate the accuracy of this method by comparing to fully-resolved long time simulations in XGCa for a test problem modeling ion heat transport and report on the computational savings achieved. [1] I. G. Kevrekidis et. al., Comm. Math. Sci., 1(4), 715-762. [2] R. Hager and C. S. Chang, Phys. Plasmas 23 (2016) 042503.

Benjamin Sturdevant
Princeton Plasma Physics Laboratory
bsturdev@pppl.gov

Scott Parker
University of Colorado at Boulder
sparker@colorado.edu

Robert Hager
Princeton Plasma Physics Laboratory
rhager@pppl.gov

Julien Dominski
PPPL
jdominsk@pppl.gov

Choong-Seock Chang, Seung-Hoe Ku
Princeton Plasma Physics Laboratory
cschang@pppl.gov, sku@pppl.gov

PP1

A Backward Stable Quadratic Eigenvalue Solver

The eigensolver `quadeig` for the complete solution of the quadratic eigenvalue problem $Q(\lambda)x = 0$ with $Q(\lambda) = \lambda^2 M + \lambda D + K$ is backward stable when Q is not too heavily damped, i.e., $\|D\|_2^2 \leq \|M\|_2|K\|_2$. For heavily damped quadratics, we show that a special linearization combined with a scaling strategy and appropriate recovery of the eigenvectors leads to computed eigenpairs with small backward errors. Here perturbations are measured relative to each coefficient matrix.

Francoise Tisseur
The University of Manchester
School of Mathematics
francoise.tisseur@manchester.ac.uk

PP1

Flexible Preconditioned Iterative Method for Least Squares Problems

Iterative methods are often imperative for solving large least squares problems, such as LSQR and LSMR based on the Golub-Kahan bidiagonalization process. Choosing a good right preconditioner can speedup the convergence of these methods. In this poster, we propose a flexible preconditionend iterative method for least squares problems. Instead of selecting a fixed preconditioner, we introduce an inner-iteration in the Golub-Kahan process that results in different preconditioners for each iteration, which are called flexible preconditioners. We analyze the flexible preconditioned LSQR and LSMR, and numerically demonstrate the superiority of this new idea.

Mei Yang
University of Texas at Arlington
mei.yang@mavs.uta.edu

Ren-Cang Li
University of Texas - Arlington
rcli@uta.edu

PP1

Consistent Bayesian Inversion with Stochastic Maps

Consistent Bayesian inversion is a recently developed method for constructing a posterior distribution on model input parameters whose push-forward distribution matches a known or specified distribution on model outputs. This method estimates the posterior by combining a prior distribution with the ratio of the observed data distribution and the push-forward of the prior distribution. In other words, the solution to an inverse problem formulated by this approach immediately follows from the solution of a forward uncertainty quantification problem. Prior exploration of this method has been restricted to applications where the parameter-to-outputs map is deterministic. We develop and analyze a framework for applying this method to stochastic maps. Numerical results are reported and the implications discussed.

Tian Yu Yen, Troy Butler
University of Colorado Denver
tian.yen@ucdenver.edu, troy.butler@ucdenver.edu

PP1

An Asymptotically Compatible Meshfree Quadrature Rule for Non-local Problems with Applications to Peridynamics

We present a meshfree quadrature rule for compactly supported non-local integro-differential equations (IDEs) with

radial kernels. We apply this rule to develop a mesh-free discretization of a peridynamic solid mechanics model that requires no background mesh. Existing discretizations of peridynamic models have been shown to exhibit a lack of asymptotic compatibility to the corresponding linearly elastic local solution. By posing the quadrature rule as an equality constrained least squares problem, we obtain asymptotically compatible convergence by introducing polynomial reproduction constraints. Our approach naturally handles traction-free conditions, surface effects, and damage modeling for both static and dynamic problems. We demonstrate high-order convergence to the local theory by comparing to manufactured solutions and to cases with crack singularities for which an analytic solution is available. Finally, we verify the applicability of the approach to realistic problems by reproducing high-velocity impact results from the Kalthoff-Winkler experiments.

Huaiqian You
Lehigh University
huy316@lehigh.edu

Nathaniel Trask
Sandia National Lab
natrask@sandia.gov

Yue Yu
Department of Mathematics, Lehigh University
yuy214@lehigh.edu

Michael L. Parks
Sandia National Laboratories
mlparks@sandia.gov

PP1

A Wavelets Fast Algorithm to Compute Ruin Probability and Gerber-Shiu Functions

Gerber-Shiu functions and its particular case ruin probability are computationally difficult to calculate because they involve infinitely many convolutions and the probability density functions could have jumps. Current computational methods suffer from slow convergence and undershoots. We have found a wavelets computation algorithm that can compute them to a very accurate scale in a fast speed even for the case where the probability density functions have jumps. Convergence proof and error estimates are also obtained.

Siu P. Yung
Math Dept, University of Hong Kong.
spyung@hku.hk

PP1

Dynamic Pricing in Insurance

We develop a pricing policy that enables an insurance company to find the optimal price and maximize the expected profit. The insurance company sells a single product and adopts prices to learn its customers' responses. The pricing policy is determined by the selling price and other model parameters. The parameters of the underlying model are initially unknown to the insurance company, so each price decision involves a trade-off between learning and earning. Maximum quasi-likelihood estimation (MQLE) is used to estimate the unknown parameters in the model. We build an algorithm that guarantees that MQLE parameter estimates eventually exist and converge to the correct values, which implies that the sequence of chosen prices also converge to the optimal price. The performance of the pricing policy is measured in terms of the *regret*: the expected revenue loss caused by not using the optimal price. The upper bounds on the regret can be achieved by our pricing algorithm. The advantages of this new pricing policy are clear. Firstly, it formulates a learning-and-earning problem, where price is used as a learning tool to explore the demand and claims response to different prices. Secondly, only very limited assumptions are made on the model. Finally, although similar results exist in other domains, this is among the first to consider dynamic pricing problems with model uncertainty in the field of insurance.

Yuqing Zhang, Neil Walton, Kees van Schaik
School of Mathematics
The University of Manchester
yuqing.zhang@manchester.ac.uk,
neil.walton@manchester.ac.uk,
kees.vanschaik@manchester.ac.uk

PP1

Uniqueness of Transformations with Prescribed Jacobian Determinant and Curl-vector

Numerical examples demonstrated that a prescribed positive Jacobian determinant alone can not uniquely determine a diffeomorphism. It is conjectured that the uniqueness of a transformation can be assured by its Jacobian determinant and the curl-vector. In this work, we study the uniqueness problem analytically and propose an approach to the proof of the uniqueness of a transformation with prescribed Jacobian determinant and curl-vector.

Zicong Zhou
University of Texas at Arlington
Department of Mathematics
zicong.zhou@mavs.uta.edu

PP1

CG Methods for General-form Regularization with an Application to Low-field MRI

Inexpensive MRI scanners based on permanent magnets are a promising diagnostic tool for developing countries. A disadvantage is the poor signal-to-noise ratio. An ill-posed system of linear equations has to be solved to obtain an image. Regularization is applied to make this system robust to noise. We consider two well-known regularization techniques: total variation and compressed sensing using a wavelet basis. Both require an ℓ_1 penalty term. The resulting minimization problem can be solved using iterative reweighted least squares. For both types of regularization, a regularized least-squares problem has to be solved in each iteration. As the iteration number grows, the regularization matrix becomes increasingly ill-conditioned due to the reweighting step. In this work, we study the performance of different versions of the conjugate gradient method. In particular, we test the standard approach CGLS and we formulate and evaluate an alternative version of CG that handles the regularization operation in a more stable and efficient way. We simulate the signal generation in a low-field MRI scanner and test the different CG algorithms on this data. The results show that the new approach outperforms the standard CGLS algorithm in terms of number of iterations and robustness. Additionally, in the compressed sensing case, the iterations are carried out faster. These observations lead us to believe that the new approach is a

promising alternative to CGLS.

Merel L. de Leeuw den Bouter
Delft Institute of Applied Mathematics
Delft University of Technology
m.l.deleeuwdenbouter-1@tudelft.nl

Martin B. van Gijzen
Delft Inst. of Appl. Mathematics
Delft University of Technology
m.b.vangijzen@tudelft.nl

Rob Remis
Circuits and Systems Group
Delft University of Technology
r.f.remis@tudelft.nl

PP2

AWM Workshop: A Numerical Study of Steklov Eigenvalue Problem

In this research, we focus on the development of numerical approaches to the forward solver and the shape optimization solver for Steklov eigenvalue problems in two dimensions. This problem has a wide range of applications in engineering and applied mathematics. We proposed numerical approaches via spectral methods or finite element methods. To apply spectral methods, we reformulate the Steklov eigenvalue problem in the complex domain via conformal mappings. For shape optimization problem, we use the gradient ascent approach to find the optimal domain which maximizes k- th Steklov eigenvalue with a given k.

Weaam Alhejaili
Claremont Graduate University
weaam.alhejaili@cgu.edu

Chiu-Yen Kao
Claremont McKenna College
ckao@cmc.edu

PP2

AWM Workshop: Fast Classication of Big Data: Proximal Methods for Sparse Discriminant Analysis

Linear discriminant analysis (LDA) fails when interpreting data where the number of features is larger than the number of observations. To address this issue, Clemmensen et al. (2011) developed a sparse version called sparse discriminant analysis (SDA) which allows feature selection and classification to be performed simultaneously. We propose three techniques to improve the efficiency of SDA. We then demonstrate their effectiveness for classifying times series data and simulated data.

Summer Atkins
University of Florida
srnatkins@ufl.edu

Brendan P. Ames
University of Alabama
Department of Mathematics
bpames@ua.edu

Gudmundur Einarsson, Line Clemmensen
Technical University of Denmark
Department of Applied Mathematics and Computer Science
guei@dtu.dk, clemmensen.line@gmail.com

PP2

AWM Workshop: Automatic Extraction of a Stroke-based Font Representation

Designing fonts and typefaces is a difficult process for both beginner and expert typographers. Existing workflows require the designer to create every glyph, while adhering to many loosely defined design suggestions. This process can be simplified by exploiting the similar character glyph structure across fonts. To capture these correlations, we propose learning a stroke-based representation from a collection of existing typefaces. We develop a stroke-based geometric model for glyphs and a fitting procedure to reparametrize arbitrary fonts to our representation.

Elena Balashova
Princeton University
sizikova@cs.princeton.edu

PP2

AWM Workshop: Stability of Spiral Waves in Cardiac Dynamics

Ventricular fibrillation in the heart is often caused by the formation and breakup of spiral waves in cardiac tissue. The alternans instability, an oscillation in the action potential duration, has been clinically linked to spiral wave breakup. We seek to understand how and why alternans develop and if stable alternans patterns exist. To investigate these questions, we analyze spectral properties of the spiral and use numerical time evolution.

Stephanie Dodson
Division of Applied Mathematics
Brown University
Stephanie_Dodson@Brown.edu

Stephanie Dodson
Brown University
Stephanie_Dodson@Brown.edu

PP2

AWM Workshop: Towards More Efficient Multigrid and Multilevel Methods

Preconditioned Krylov subspace (KSP) methods are widely used for solving large and sparse linear systems arising from PDE discretizations. In this work, we present a systematic comparison of some KSP methods, with different classes of preconditioners including incomplete LU factorization (ILUT, ILUTP and multilevel ILU), and algebraic multigrid (including classical AMG and smoothed aggregation). We will also address multilevel ILU preconditioner for predominantly symmetric systems. This study helps establish some practical guidelines for choosing preconditioned KSP methods and to increase the efficiency and robustness of multigrid methods.

Aditi Ghai
Stony Brook University
aditi.ghai@stonybrook.edu

PP2

AWM Workshop: Subset Selection with an Exten-

sion of DEIM

Index selection via the discrete empirical interpolation method (DEIM) can be used to identify representative subsets of data from a larger data matrix. However, the rank of the data matrix limits the number of representatives that can be in the identified subset–an issue, for instance, when the number of classes present in the data is greater than the number of features observed. This work presents a novel extension of DEIM to allow for the selection of additional representatives along with experimental results that support the use of such an extension.

Emily Hendryx
Rice University
emily.hendryx@rice.edu

PP2

AWM Workshop: Robust Residual-based and Residual-free Greedy Algorithms for Reduced Basis Methods

While the offline-enhanced RBM has demonstrated the potential of efficiently solving large scale parametrized problem by identifying a subset of the training set, many opportunities for extending the scope of RBM remain. In this work, the offline stage of RBM is improved by mitigating the computational cost of error estimate over the training set. We present two error estimation mechanisms: the classical one with enhanced implementation and the RB-coefficient-only error indicator. The former method is a more efficient and accurate implementation of the classical approach rendering it capable of approximating the truth solution to machine accuracy (as opposed to its square root) for coercive problems. The latter error indicator is efficiently evaluated solely from the RB coefficients, which is motivated by the need to minimize the Lebesgue constant. We achieved enhancement of the efficiency while guaranteeing the accuracy of the proposed algorithm, both demonstrated through numerical experiments.

Jiahua Jang
University of Massachusetts Dartmouth
jjiang@umassd.edu

PP2

AWM Workshop: Regularization in Tomographic Reconstruction

Tomographic reconstruction is a non-invasive 2D/3D image recovery technique. It is widely used at the Advanced Photon Source at Argonne National Laboratory. One way of solving this problem is via linear least squares optimization formulation assuming the experimental data follows a Gaussian distribution. Due to limited data, the problem is usually ill-conditioned. We study regularization techniques for tomographic reconstruction and provide a performance comparison among different types of regularizers.

Ratna Khatri
George Mason University
Department of Mathematical Sciences
rkhatri3@masonlive.gmu.edu

PP2

AWM Workshop: Anatomical Biomarker for Alzheimer's Disease Progression in the Transentorhinal Cortex

The purpose of this research was to develop a more robust biomarker for early Alzheimer's disease. We manually segmented for the entorhinal cortex from 3T MRIs and reduced longitudinal variability in boundaries using longitudinal diffeomorphometry. Cortical thickness was estimated using a technique called normal geodesic flow. Permutation tests of resulting model showed significant thickness atrophy localized to the transentorhinal cortex. Linear discriminant analysis confirmed sensitivity/specificity were improved using this thickness of the transentorhinal cortex over global entorhinal cortex thickness and hippocampal volume.

Sue Kulason, Daniel Tward, Chelsea Sicat
Johns Hopkins University
skulaso1@jhu.edu, dtward@cis.jhu.edu,
chelsea@cis.jhu.edu

Arnold Bakker, Michela Gallagher, Marilyn Albert
Johns Hopkins School of Medicine
abakker@jhu.edu, michela@jhu.edu, malbert9@jhu.edu

Michael I. Miller
Johns Hopkins University
Center for Imaging Science
mim@cis.jhu.edu

PP2

AWM Workshop: Semiclassical Sine-Gordon Equation, Universality at Gradient Catastrophe

We consider the semi-classical sine-Gordon equation with a class of initial data. In a neighbourhood of a gradient catastrophe point, the solution behave like modulated plane waves in one region and localize like "spikes" in other. The "spike" locations correspond to the poles of the Tritronqueé solution. We give first correction of the solution near the catastrophe, and study the shape of the localized structures. The asymptotic behaviour is nonsensitive to initial data.

Bingying Lu, Peter D. Miller
University of Michigan
bylu@umich.edu, millerpd@umich.edu

PP3

Minisymposterium: Existence of a Weak Solution to an FSI Problem with Signorini Boundary Conditions

Our main problem is to determine the existence of weak solution to blood flow through medium-to-large arteries with the Signorini boundary conditions. We use Signorini boundary conditions for the outlet boundary, a generalization of the free traction conditions. These arise naturally out of the systems energy inequality (Zhou and Saito, 2015). To prove the existence of a weak solution we discretize in time, and break down the problem into fluid and structure sub-problems. The fluid sub-problem uses Robin-type boundary conditions on the structure boundary and Signorini boundary conditions on the outlet boundary. The structure sub-problem is modeled as a linear Koiter shell. We prove the existence of a weak solution by using Lie splitting (Muha and Canic, 2012). Preliminary results will be shown.

Prajakta P. Bedekar

University of Houston
pbedekar@math.uh.edu

Suncica Canic
Department of Mathematics
University of Houston
canic@math.uh.edu

PP3

Minisymposterium: Heart Modeling with the Immersed Boundary Finite Element Method

In this work, we describe the development of a fluid/structure model of cardiac mechanics. This model includes the heart, valves, and great vessels, with geometry derived from cardiac MRI data. The heart, great vessels, and valves are modeled as hyperelastic solids, with viscoelasticity provided by the background fluid. Blood is modeled by the incompressible Navier Stokes equations. A Lagrangian finite element method is used to approximate the displacement of the solid, and a finite difference scheme is employed for the fluid discretization. The immersed boundary methodology couples the fluid and solid through spreading and restriction operators.

Charles Puelz, Margaret Anne Smith, Simone Rossi, Boyce Griffth
Department of Mathematics
University of North Carolina at Chapel Hill
cpuelz@unc.edu, masmath@email.unc.edu, srossi@email.unc.edu, boyceg@email.unc.edu

PP3

Minisymposterium: Fluid-Structure Interaction Between Blood Flow and Coronary Artery Treated with Stents on a Moving Heart

This work is motivated by fluid-structure interaction between a coronary artery treated with a stent, pulsatile blood flow, and heart contractions. The fluid is modeled by the incompressible, viscous Navier-Stokes equations, the vascular walls are modeled as multi-layered composite elastic stuctures, and the presence of a stent is modeled by changing the density and elasticity coefficients of the structure in the inner-most layer, corresponding to the intima, where the stent is located. To include the effects of heart contractions, external force was applied to model the change in artery curvature. The fluid and composite structure are fully coupled via kinematic and dynamic coupling conditions, which describe continuity of velocity and balance of contact forces. The contractions of the heart are modeled by adding a periodic external force to the structure's outer surface. A loosely coupled partitioned scheme combined with an ALE approach is used to solve this nonlinear FSI problem. Four types of commercially available coronary stents are considered, and their performance compared and quantified. Based on the simulations, two out of four stents are considered to be more suitable for coronary angioplasty with stenting in curved, or tortuous arteries. Our results correlate well with clinical results. This is a joint work with Suncica Canic, Martina Bukac and Josip Tambaca.

Yifan Wang
University of Houston
ywang111@uh.edu

Suncica Canic
Department of Mathematics
University of Houston
canic@math.uh.edu

Josip Tambaca
University of Zagreb
tambaca@math.hr

Martina Bukac
University of Notre Dame
mbukac@nd.edu

PP4

Minisymposterium: Performance of Amrex's Multi-grid Poisson Solver in Flash Code

FLASH is a high performance application code developed at University of Chicago and capable of simulating highly complex multi-physics scientific problems. It makes use of Adaptive Mesh Refinement (AMR) to solve problems on multi-resolution meshes. In the next generation of FLASH, we are adopting AMReX to enable octree based block-structured AMR. Fast and accurate solution of Poisson equation is critical in many physical problems of interest to FLASH users such as (1) gravity field solution and (2) incompressible fluid flow. In this work, we interface the multi-grid linear solver from AMReX into FLASH and study its performance using a standard test problem in comparison with the native multi-grid solver of FLASH. The performance characteristics of these solvers are presented in terms of overall solution time as well as scaling on Argonnes Bebop clusters.

Saurabh Chawdhary
Argonne National Laboratory
9700 S Cass Ave, Argonne, IL-60439
sauc@anl.gov

Anshu Dubey
Argonne National Laboratory
adubey@anl.gov

PP4

Minisymposterium: Sundials Suite of Time Integrators and Nonlinear Solvers

SUNDIALS is a suite of robust and scalable solvers for systems of ordinary differential equations, differential-algebraic equations, and nonlinear equations. The suite consists of six packages: CVODE(S), ARKode, IDA(S), and KINSOL. Each package is built on common vector and linear solver APIs allowing for application-specific and user-defined data structures, encapsulated parallelism, and algorithmic flexibility. As part of the DOE's Exascale Computing Program and FASTMath Institute, SUNDIALS is enabling time integrators for exascale architectures. In this poster we present an overview of the SUNDIALS suite, recent enhancements, and current development efforts. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-744910

David J. Gardner, Carol S. Woodward
Lawrence Livermore National Laboratory
gardner48@llnl.gov, woodward6@llnl.gov

Daniel R. Reynolds
Southern Methodist University

Mathematics
reynolds@smu.edu

Alan Hindmarsh
Lawrence Livermore National Laboratory
hindmarsh1@llnl.gov

Slaven Peles
Lawrence Livermore Natinoal Laboratory
peles2@llnl.gov

PP4

Minisymposterium: Strumpack - A Fast Direct Solver and Preconditioner using Hierarchical Matrices and Randomized Sampling

In this poster we present recent results with a sparse direct solver and preconditioner based on approximate LU factorization. The fill in the triangular factors is compressed using hierarchical matrices, a data-sparse format which uses matrix partitioning and low-rank decompositions. Low rank approximations are computed with adaptive randomized projection or sampling. The solver achieves near optimal complexity for a range of PDE problems and is typically used as a preconditioner for linear systems arising from PDE discretizations. The hierarchical matrix kernels can also be applied directly to dense matrices from various applications. We consider both general H matrices as well as the Hierarchically Semi-Separable matrix format. We focus on recent performance and scalability improvements as well as a number of applications.

Pieter Ghysels
Lawrence Berkeley National Laboratory
Computational Research Division
pghysels@lbl.gov

Xiaoye S. Li
Lawrence Berkeley National Laboratory
xsli@lbl.gov

Gustavo Chavez, Yang Liu
Computational Research Division, Lawrence Berkeley National
gichavez@lbl.gov, liuyangzhuan@lbl.gov

Chris Gorman
UC Santa Barbara
gorman@math.ucsb.edu

PP4

Minisymposterium: Solving Nonlinear Problems with Padé Approximants

In this poster, we present a strategy for finding nontrivial solutions (λ, x) for a class of nonlinear eigenvalue problems of the form $F(\lambda)x = 0$. We use rational functions to approximate the nonlinear terms of the problem, together with Padé approximants. This leads to a linearization of the original problem, through a generalized eigenvalue of dimension larger than the original problem. We show the impact of the degree of the Padé approximants in the linearization process and convergence, and alternatives for solving the resulting linearized problem. As study cases, we focus on problems related to the modeling of waveguide-loaded accelerator cavities through a finite element discretization of Maxwell's equation, where some of the matrices involved exhibit low-rank properties and favor the rational approximation strategy.

Osni A. Marques
Lawrence Berkeley National Laboratory
Berkeley, CA
oamarques@lbl.gov

PP4

Minisymposterium: Toward an Extreme-scale Scientific Software Ecosystem with the xSDK

Computational science increasingly demands multiscale and multiphysics formulations, which in turn require many high-quality, robust, portable high-performance math libraries. However, without coordination, independent packages often cannot be easily composed. The Extreme-scale Scientific Software Development Kit (see https://xsdk.info) provides infrastructure for a collection of related and complementary software elements—developed by diverse, independent teams throughout the community—that provide the building blocks, tools, models, processes, and related artifacts for rapid and efficient development of high-quality applications. This poster will describe the development of the xSDK, where math library teams are working toward two strategic objectives: building community and building sustainability. We will discuss xSDK community policies that help to improve code quality and compatibility across independently developed packages, while also determining criteria for member packages' inclusion in the xSDK. We will describe the release process and demonstrate the use of the xSDK in application codes.

Lois Curfman McInnes
Mathematics and Computer Science Division
Argonne National Laboratory
curfman@mcs.anl.gov

Michael Heroux
Sandia National Laboratories
maherou@sandia.gov

Xiaoye S. Li
Lawrence Berkeley National Laboratory
xsli@lbl.gov

Jim Willenbring
Sandia National Laboratories
jmwille@sandia.gov

Carol S. Woodward, Ulrike Yang
Lawrence Livermore National Laboratory
woodward6@llnl.gov, yang11@llnl.gov

PP4

Minisymposterium: Better Scientific Software

Better Scientific Software (BSSw) is an organization dedicated to improving developer productivity and software sustainability for computational science and engineering (CSE). This poster will introduce a new website (https://bssw.io)—a new community-driven resource for scientific software improvement exchange. Were creating a central hub for sharing information on practices, techniques, experiences, and tools to improve software productivity and sustainability for CSE. Site users can find information on scientific software topics and can propose to curate or create new content based on their own experi-

ences. The backend enables collaborative content development using standard GitHub tools and processes. We want and need your contributions to build the BSSw site into a vibrant resource, with content and editorial processes provided by volunteers throughout the international CSE community. Join us!

Lois Curfman McInnes
Mathematics and Computer Science Division
Argonne National Laboratory
curfman@mcs.anl.gov

David E. Bernholdt
Oak Ridge National Laboratory
Computer Science and Mathematics Division
bernholdtde@ornl.gov

Michael Heroux
Sandia National Laboratories
maherou@sandia.gov

PP4

Minisymposterium: A Performance Analysis of Nek5000 for Nuclear Applications

Nek5000 is a state of the art spectral element Computational fluid dynamics code with proven scalability beyond one million MPI ranks. In recent years it has been applied with success to a variety of applications: the present work focuses on nuclear engineering applications. In particular, the ExasSMR project is focused on the exascale application of single and coupled Monte-Carlo and CFD physics. Given the sheer scale of nuclear systems, the main algorithmic driver on the CFD side is weak scaling. Full-core fluid calculations aimed at better predicting the steady-state performance will eventually be conducted with zonal hybrid LES-RANS that provides an additional scaling dimension besides the number of assemblies. LES may be used to simulate a portion of a core, while the remainder will be handled by RANS. The present manuscript focuses on assembly level simulations with Nek5000, to assess performance. We discuss the development of a two benchmark problems in: a subchannel problem (single-rod) to assess inter-node performance and a larger full assembly problem representative of Nuclear applications. We finally discuss profiling and scaling results for both Nekbone, the proxy app of Nek5000, and Nek5000. A discussion on current bottlenecks and potential limitations of the approach follows.

Elia Merzari, Paul F. Fischer, Ron Rahaman, Mi Sun Min
Argonne National Laboratory
emerzari@anl.gov, fischer@mcs.anl.gov, rahaman@mcs.anl.gov, mmin@mcs.anl.gov

PP4

Minisymposterium: Progress on Schwarz-type Coupling of Core and Edge-region Magnetic Fusion Simulations

The edge and core regions of magnetic fusion devices differ drastically on many fronts - geometry and collisionality, to name only two among many. It is thus natural that different numerical methods are optimally suited to the simulation of each region. However, this creates a challenge for the pursuit of whole device modeling (WDM): How can one self-consistently couple two distinct codes to achieve a uniformly accurate description of the entire tokamak? In support of the ECP goal of coupling the codes GENE (core) and XGC (edge) for whole device modeling, we present such a coupling scheme inspired by classical additive Schwarz methods. While traditional Schwarz schemes require iteration to convergence inside a single time step, this is computationally intractable in the context of 5-D gyrokinetic simulations. We give evidence - both analytic and empirical - that if one is interested only in long-time averages (as scientists and engineers typically are in this field) then this expensive iteration can be avoided while retaining the scheme's convergence properties. We present numerical results from tests on both a 1-D model problem and 2-D simulations of the Hasegawa-Wakatani equations. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Lee Ricketson
Lawrence Livermore National Laboratory
lee.ricketson@gmail.com

Jeffrey A. Hittinger
Center for Applied Scientific Computing
Lawrence Livermore National Laboratory
hittinger1@llnl.gov

Ammar Hakim
Princeton Plasma Physics Laboratory
ahakim@pppl.gov

PP4

Minisymposterium: Overview of GPU-related Features in PETSc

In this work we present the latest features of the software library PETSc for using graphics processing units (GPUs) as an alternative computing hardware for the scalable solution of linear, nonlinear, and ODE/DAE systems and the computation of adjoints (sometimes called sensitivities) of ODE systems. In particular, we show how users can run their existing PETSc-based codes without further modification on GPUs by merely providing suitable command line parameters. Furthermore, we identify solver configurations and system sizes where GPUs run either particularly well or particularly poor to guide users in selecting the best machine to run their computations.

Karl Rupp
Freelance Computational Scientist
me@karlrupp.net

Richard T. Mills, Hong Zhang
Argonne National Laboratory
rtmills@anl.gov, hongzhang@anl.gov

Barry F. Smith
Argonne National Lab
MCS Division
bsmith@mcs.anl.gov

PP4

Minisymposterium: Algorithms and Numerics for High-order Accurate Interface Dynamics

A panoply of fluid dynamics problems involve surface, boundary, and interface motion playing a pivotal role in the global dynamics; when modeling these problems computationally, a careful and precise treatment of the boundary and interface motion is often necessary. In this poster we

outline some of the DOE-funded research efforts in developing mathematical frameworks and numerical software for high-order accurate interface dynamics. Algorithmic components include high-order accurate quadrature methods for implicitly defined domains; Voronoi implicit interface methods for tracking the evolution of multi-phase interconnected interfaces; k-d trees optimized for codimension-one point clouds; and high-order accurate closest point calculations on implicitly defined surfaces. We also outline an implicit mesh discontinuous Galerkin framework for precisely computing complex fluid-interface dynamics. Highlighted example applications include multi-scale modeling of foams, high Reynolds number bubble oscillation motion, and in collaboration with manufacturers as part of an HPC4Mfg project using tens of thousands of cores, modeling rotary bell atomization at industrial spray-painting conditions.

Robert Saye
Lawrence Berkeley National Laboratory
rsaye@lbl.gov

PP4

Minisymposterium: Performance Optimization of PETSc on Intel Xeon Phi Processor

PETSc is a widely used software library for the scalable solution of linear, nonlinear, ODE/DAE systems and sensitivity analysis. The Intel Knights Landing (KNL) Xeon Phi processor gains traction in exascale computing and has already been used in U.S. Department of Energys supercomputers. Transitioning PETSc solvers and applications to KNL is often smooth because KNL is binary-compatible with other X86 processors. However, extracting good performance requires significant effort and fine restructuring of the code. We will present our work on optimizing PETSc in order to take advantage of the enhanced vectorization capability and the high-bandwith memory feature offered by KNL. Rather than relying on compiler automatic optimization, we have efficiently vectorized the workhorse of Krylov iterative solvers–the sparse matrix-vector multiplication– for some existing matrix types and a newly implemented matrix type that is more SIMD-friendly. We will investigate and compare their performance on real PDE problems on a supercomputer. In addition, we will show how users can benefit from the new KNL-related features in PETSc.

Hong Zhang, Richard T. Mills
Argonne National Laboratory
hongzhang@anl.gov, rtmills@anl.gov

Karl Rupp
Freelance Computational Scientist
me@karlrupp.net

Barry F. Smith
Argonne National Lab
MCS Division
bsmith@mcs.anl.gov

PP5

Minisymposterium: Parallel Aggregation Strategies for Multigrid Preconditioners

Multigrid algorithms have been developed over the last 40 years and have been successful at accelerating the solution of large systems of linear equations. While their parallelization across many compute nodes using mpi is well established more work needs to be done to obtain performant on node parallelization of these preconditioner on modern architectures using manycore processors and/or GPU accelerators. We present algorithms for the aggregation phase occurring in the multigrid setup. An initial set of independent root nodes is obtained leveraging distance 2 graph coloring algorithms. Subsequent aggregate expansion and secondary aggregate creation strategies are also detailed. Performance of these algorithms on many-core and GPU architectures demonstrated on example using Trilinos' MueLu multigrid framework.

Luc Berger-Vergiat
Sandia National Labs
lberge@sandia.gov

Ray S. Tuminaro
Sandia National Laboratories
Computational Mathematics and Algorithms
rstumin@sandia.gov

Mehmet Deveci
Sandia National Laboratories
mndevec@sandia.gov

PP5

Minisymposterium: Thread Parallel Message Packing for Sparse Matrix MPI Communication

An implementation of thread parallel message packing for sparse matrix MPI communication in Trilinos Tpetra package is presented. Thread parallel message packing is achieved using Kokkos parallel data structures and algorithms. The use of Kokkos allows the implementation to run with any of the threading models supported by Kokkos, including OpenMP and Cuda. The adoption of thread parallel message packing led to 1.51x and 2.46x speed ups in finite element assembly times for an 8M element conduction problem using 16 nodes on Intel Haswell and Intel KNL architectures, respectively.

Tim Fuller
Sandia National Labs
tjfulle@sandia.gov

Mark Hoemmen
Sandia National Laboratories
mhoemme@sandia.gov

PP5

Minisymposterium: A Maxwell Solver for Next-generation Platforms

The advent of the next generation of high performance computing platforms will have a significant impact on the layout of large-scale simulations. New programming paradigms are necessary to fully exploit future compute node architectures. We present a method for the efficient solution of Maxwell's equations by a tailored algebraic multigrid method. The solver, implemented in the Trilinos package MueLu, is based on a mimetic gauge reformulation and leverages on-node parallelism through the Kokkos programming framework. By numerical experiments on several present day supercomputer installations, we compare the solver's performance to Trilinos' legacy multigrid package ML as well as a recently proposed augmentation based solver.

Christian Glusa

Brown University
caglusa@sandia.gov

PP5

Minisymposterium: Towards Solution Methods for A Hypersonic Application

While multigrid methods have been successfully applied to subsonic and transsonic flow problems, multigrid methods for hypersonic flow problems are still an open area of research. In this poster, we discuss ongoing efforts to apply linear multigrid methods to hypersonic flow regimes. We provide some background on the motivating problems, algorithmic solution approaches that are currently being considered, details on using Kokkos in compute intensive kernels, and finally numerical examples from Sandia's simulation code SPARC.

Jonathan J. Hu
Sandia National Laboratories
Livermore, CA 94551
jhu@sandia.gov

Ray S. Tuminaro
Sandia National Laboratories
Computational Mathematics and Algorithms
rstumin@sandia.gov

Paul Lin, Chris Siefert
Sandia National Laboratories
ptlin@sandia.gov, csiefer@sandia.gov

PP5

Minisymposterium: A Parallel Addition Kernel for Unsorted Sparse Matrices

We present a parallel sparse matrix addition function for the Tpetra linear algebra package in Trilinos. The function operates on compressed-row storage (CRS) matrices and allows column indices to be in any order. This is useful because the global indices of distributed Tpetra matrices may be mapped to local indices arbitrarily. The function is implemented as a set of Kokkos kernels and can be run in parallel using OpenMP or CUDA. On the Intel KNL architecture in a sample 8000-element FEM problem, the new function gives an 8.3x speedup over its predecessor in serial, and a 37.1x speedup with 64 OpenMP threads. We demonstrate performance results from a Sandia multiphysics simulation, where preconditioning is critically dependent on scalable sparse matrix addition.

Brian Kelley, Chris Siefert
Sandia National Laboratories
bmkelle@sandia.gov, csiefer@sandia.gov

Jonathan J. Hu
Sandia National Laboratories
Livermore, CA 94551
jhu@sandia.gov

PP5

Parallel Distance 2 Graph Coloring for Algebraic Multigrid Preconditioners

Algebraic multigrid (AMG) methods are used extensively as preconditioners and solvers for problems in thermal fluids and electromagnetics. AMG operates by creating a sequence of increasingly coarse matrices in order to accelerate the solution of a fine resolution linear system. The coarsening phase in the Trilinos multigrid library (MueLu) uses a graph that encodes the structure of the matrix to construct node aggregates, each of which contains a root node and its neighbors. A distance-2 graph coloring can be used to generate these aggregates by selecting the nodes sharing the same color as the root nodes. This allows the aggregates to be formed in parallel as the distance-2 coloring guarantees that no aggregates can overlap. We present a new thread-parallel distance-2 coloring heuristic and show how it is used in the coarsening operation within MueLu.

William C. McLendon, Mehmet Deveci
Sandia National Laboratories
wcmclen@sandia.gov, mndevec@sandia.gov

PP5

Minisymposterium: Parallel Bounding Volume Hierarchy Implementation using MPI+KOKKOS

Trees on a set of geometric objects are an important tool used in many scientific applications. For example, many complex applications require interaction of different scientific libraries operating on their own mesh and data. Such situations require fast algorithms to transfer the data between meshes which is typically done through construction of a geometry-based tree and subsequent searches. In this poster, we present a novel implementation of the distributed bounding volume hierarchy (BVH) construction and search algorithms (k-nearest neighbors and radius) using MPI for inter-node and Kokkos for intra-node shared parallelism. We demonstrate its performance on both CPU and GPU, and compare our results with well known Boost rtree and nanoflann libraries.

Andrey Prokopenko
Oak Ridge National Laboratory
prokopenkoav@ornl.gov

PP5

Minisymposterium: Sparse Matrix-matrix Multiplication and Related Kernels on Knights Landing

Sparse matrix-matrix multiplication is a critical kernel in the setup phase of algebraic multigrid, used as part of a Galerkin product in the formation of coarse levels. This is often implemented as a kernel in a library (e.g. MKL or ViennaCL) which multiply two matrices. For algebraic multigrid, we need additional operations which are not represented by these kernels. First, we need a matrix-matrix Jacobi operation (e.g. $(I - \omega D^{1^-} A)B$). Second, we need a matrix-matrix multiply that allows you to multiply by a matrix and its halo at once (used in the MPI parallel context). Both of these kernels can be implemented using other pieces (e.g. matrix-matrix addition), but we show it is more efficient to implement these as "fused' kernels. We present results from the algebraic multigrid setup phase for Trilinos/MueLu.

Christopher Siefert
Sandia National Laboratories
csiefer@sandia.gov

PP6

On Error Estimation of a Nonlinear Least Squares Type Bilevel Optimal Control Problem

Optimal control tasks arise in a variety of applications from, e.g., mechanical or electrical engineering, where one

wants to minimize a certain cost functional with respect to some input function and the resulting state trajectory. Usually, the systems describing the dynamical behavior of these applications are governed by differential equations. Furthermore, in certain applications, e.g., humanoid locomotion, the cost functional descriptions may depend on parameters. The goal is to find a 'good' set of parameters such that the trajectory generated by the corresponding optimal control problem is close to some reference trajectory. This is a nonlinear least squares problem and introduces an upper level of optimization. It can be solved numerically using Gau-Newton type methods. However, one needs to recompute the solution of the inner optimal control problem at every step. Thus, one can save computational effort if one has control over the error in the inner solution. In this poster we will revisit results on error estimation for Gauß-Newton methods. Then, we will apply these result to the structure of our problem and derive an error estimator for the inner problem.

Daniel S. Bankmann
Technische Universität Berlin
bankmann@math.tu-berlin.de

PP6

A Generic Interface for the Computation of Free Boundary Problems

Free boundary problems appear in many areas from materials science to mathematical biology. They are notoriously difficult to compute and require a certain level of expertise which the practitioner may not always posses. Our software, a DUNE module, allows the user to enter and solve a wide range of free boundary problems by entering geometric evolution equations coupled to balance laws. The software symbolically manipulates these equations into a form which can then be solved using the well known phase-field method. The focus of the software is to provide the user with a adequately generic interface for computation without assuming they have any knowledge of the underlying phase-field methodology which is used to solve the resulting system.

Matthew Collins
University Of Warwick
m.t.collins@warwick.ac.uk

Andreas Dedner, Bjorn Stinner
University of Warwick
a.s.dedner@warwick.ac.uk, bjorn.stinner@warwick.ac.uk

PP6

Numerical and Bayesian Inference Solutions to the Hodgkin-Huxley ODE Model of Neuronal Action Potential

The most biophysically accurate models, in terms of a mathematical description of ion gates and membrane potentials, are widely accepted to be those derived from the original Hodgkin and Huxley ODE system created in 1952. The coupled, non-linear, system of differential equations has an incredible ability to simulate the spiking characteristics of neurons, but lacks computational efficiency and scalability. This consequence is partially derived from the characteristics of the equations themselves, because the stiffness of the system increases as neurons and simulation times expand. In an attempt to best solve these equations for voltage and rate constants, several numerical methods, including forward Euler, backward Euler, MATLABs ODE45, Adams-Bashforth-Moulton predictor-corrector, fourth order Runge-Kutta have been utilized in previous work. This project implements all of these methods in MATLAB and also explores spectral deferred correction method to advance the existing techniques. In addition to these forward methods, recent research has used Approximate Bayesian Computational Inference techniques on experimental data to solve for the unknown parameters. The goal of this poster is to explore existing techniques for the approximation of parameters and numerical solutions for computational efficiency and accuracy in both single HH neural models and those in a network.

Kyle Henke
University of New Mexico SIAM Student Chapter
khenke3@unm.edu

PP6

Integrating Vehicle Routing and Scheduling to Optimize Foster Care Visitations

We have partnered with a county in New York State that oversees approximately 100 foster care cases, each requiring the transportation of one or more children to weekly/bi-weekly meetings with one or more biological parents and case workers with an assigned meeting time between these parties. The current driver and case worker assignment system is executed manually by workers in a cumbersome manner. We model this problem using concepts from combinatorial optimization such as the traveling salesman and Dial-A-Ride problems with the goal of maximizing the throughput of cases seen per week. Our goal is to create a decision-support tool to recommend weekly driver/case worker assignments to facilitate the scheduling process of the county, increasing the efficiency and quality of this system.

Caroline Johnston, Shima Azizi, Katherine Dunphy, Renata A. Konrad, Andrew C. Trapp
Worcester Polytechnic Institute
cmjohnston@wpi.edu, sazizi@wpi.edu, akddunphy@wpi.edu, rkonrad@wpi.edu, atrapp@wpiedu

PP6

Duality Principles and a Posteriori Error Estimation for DPG Methods with a View Towards Viscoelastic Fluids

A novel duality theory for finite element methods with trial and test spaces of unequal dimension is used to derive the newly discovered DPG* methods. Motivation for this new theory is taken from a challenging problem in viscoelastic fluid flow modeling and, in particular, goal-oriented adaptive mesh refinement for the drag coefficient therein. A posteriori error estimation, for both DPG and DPG* methods, is essential in understanding such an adjoint-based, goal-oriented strategy and two novel theoretical results on the subject will be displayed.

Brendan Keith
The University of Texas at Austin
The Institute for Computational Engineering and Sciences
brendan@ices.utexas.edu

Leszek Demkowicz
Institute for Computational Engineering and Sciences (ICES)
The University of Texas

leszek@ices.utexas.edu

PP6

Determination of Optimal Closures for Hydrodynamic Models

This investigation is motivated by the question about performance limitations characterizing certain common closure models for nonlinear models of fluid flow. The need for closures arises when for computational reasons first-principles models, such as the Navier-Stokes equations, are replaced with their simplified (filtered) versions such as the Large-Eddy Simulation (LES). In the present investigation we focus on a simple model problem based on the 1D Kuramoto-Sivashinsky equation with a Smagorinsky-type eddy-viscosity closure model. The eddy viscosity is assumed to be a function of the state (flow) variable whose optimal functional form is determined in a very general (continuous) setting using a suitable adjoint-based variational data-assimilation approach. In the presentation we will review details of the formulation of the computational approach and will discuss some computational results.

Pritpal Matharu
McMaster University
mathap1@mcmaster.ca

Bartosz Protas
Dept of Mathematics and Statistics
McMaster University
bprotas@mcmaster.ca

PP6

Chaotic Advection in Active Nematics

The recent surge of research into active materials is an exciting development in soft matter physics. Unlike traditionally studied fluids, active fluids are not in equilibrium. Instead, they continuously consume energy to generate internal mo- tion, which can subsequently produce large-scale flows and rich emergent dynamical structures. These moving defects can wind around one another to generate chaotic mixing. We report here on experimental and theoretical work on a biologically in- spired active nematic liquid crystal. Densely packed microtubules slide antiparallel to each other at a controlled rate due to kinesin molecular motors. The resulting chaotic advection is studied experimentally using the tools of particle tracking, particle image velocimetry, and fluorescence imaging of labeled tracers. Experimental data are analyzed and interpreted in the context of topological dynamics, thereby bridging the fields of chaotic advection and active fluids. We focus on the topo- logical entropy, measured from the braiding of tracer trajectories, and on the local Lyapunov exponent, measured from the divergence of neighboring tracers.

Eric Roberts, Amanda Tan, Linda Hirst, Suzanne Sindi
University of California, Merced
eroberts5@ucmerced.edu, atan25@ucmerced.edu,
lhirst@ucmerced.edu, ssindi@ucmerced.edu

Kevin A. Mitchell
University of California, Merced
Physics
kmitchell@ucmerced.edu

PP6

High-order Perturbation of Surfaces Algorithms for the Simulation of Localized Surface Plasmon Resonances

High-Order Spectral (HOS) methods deliver highly accurate simulations with a relatively small number of degree of freedom. In layered media applications, HOP approaches based on High-Order Perturbation of Surface (HOPS) algorithms have proven to be a compelling choice, and we display how two of these-the Methods of Field Expansions and Transformed Field Expansions-extend to simulations of nanorods. With numerical experiments, including a convergence study and simulations of nanorods, we show the remarkable efficiency, fidelity and high-order accuracy of our algorithms.

Xin Tong, David P. Nicholls
University of Illinois at Chicago
xtong20@uic.edu, davidn@uic.edu

PP6

Influence of Pore Scale Methods on Numerically Upscaled Simulations

Modeling pore scale processes is important for understanding the large scale flow and transport models in the subsurface. These models have become ubiquitous in applications to the geosciences, from fundamental geologic processes to energy resource storage and production. Pore scale changes (e.g. due to phase transitions) impact the critical macro scale variables, permeability and porosity. To incorporate pore scale simulation results in solving core or reservoir scale problems, we utilize numerical homogenization to upscale. In this work, we examine how different numerical methods used at pore scale impact the upscaled results.

Joe Umhoefer
Oregon State University
umhoefej@oregonstate.edu

Malgorzata Peszynska
Department of Mathematics
Oregon State University
mpesz@science.oregonstate.edu

Timothy Costa
Numerical Solutions, Inc.
timothy.costa@numericalsolutions.org

PP7

Permutation-Invariant Consensus Over Crowdsourced Labels

This research project introduces a novel crowdsourcing consensus model and inference algorithm – which we call PICA (Permutation-Invariant Crowdsourcing Aggregation) – that is designed to recover the ground-truth labels of a dataset while being invariant to the class permutations enacted by the different annotators. This is particularly useful for settings in which annotators may have systematic confusions about the meanings of different classes, as well as clustering problems (e.g., dense pixel-wise image segmentation) in which the names/numbers assigned to each cluster have no inherent meaning. The PICA model is constructed by endowing each annotator with a doubly-stochastic matrix (DSM), which models the probabilities that an annotator will perceive one class and transcribe it into another. We conduct simulations and experiments to show the advantage of PICA compared to Majority Vote for three different clustering/labeling tasks. We also explore

the conditions under which PICA provides better inference accuracy compared to a simpler but related model based on right-stochastic matrices. Finally, we show that PICA can be used to crowdsource responses for dense image segmentation tasks, and provide a proof-of-concept that aggregating responses in this way could improve the accuracy of this labor-intensive task. Faculty Advisors: Paffenroth, Randy, rcpaffenroth@wpi.edu; Whitehill, Jacob, jrwhitehill@wpi.edu, Worcester Polytechnic Institute

Michael Giancola
Worcester Polytechnic Institute, USA
mjgiancola@wpi.edu

PP7

Understanding Deep Neural Networks

Deep learning has achieved great success in may machine learning tasks. This talk will focus on the speaker's work on understanding the deep neural networks. The talk will separate to two parts. The first part will about understanding deep generative models from sparse coding's view. We develop a "deep" regularization term via sparse coding. The second part will about differential equation's view on deep neural networks. In this section we will understand the neural network as a numerical scheme approximation to the dynamic system and to understand the neural net, we will think beyond finite layer neural nets. Based on this perspective, we introduce a new type of neural net structure by applying the linear multi-step scheme. In particular, on both CIFAR and ImageNet, LM-ResNet/LM-ResNeXt can significantly compress ($> 50\%$) the original networks while maintaining a similar performance. Faculty Advisor: dongbin@math.pku.edu.cn

Yiping Lu
Peking University
luyiping9712@pku.edu.cn

Zhong Aoxiao
MGH/BWH Center for Clinical Data Science, USA
zhongaoxiao@gmail.com

PP8

Minisymposterium: You Get the Pointer, but Only on My Terms: Control Local Data Access for Better use of Modern Computer Hardware and Programming Models

Many applications have large collections of data, distributed over parallel hardware. Software developers want easy access to "local" data – e.g., local to my MPI process, thread, or GPU. However, WHAT data are local, and WHEN and WHERE the data are up to date, may depend on hardware, programming model, and numerical algorithms. Typical software patterns for answering these questions tangle programmers in a spaghetti state machine. We propose a syntax, "withLocalAccess," that makes it clear WHEN and WHERE programmers access WHAT data. We demonstrate a C++ prototype.

Mark Hoemmen
Sandia National Laboratories
mhoemme@sandia.gov

PP8

Minisymposterium: Speeding up Small Matrix-matrix Multiplication: Just-in-Time Compilation in Intel(R) Math Kernel Library

Small, dense matrix-matrix multiplication often forms a building block for modern scientific applications such as those arising from machine learning, finite element methods, and applied mathematics. Due to the combinatorial explosion of all possible sizes, leading dimensions, transpositions, and scaling values involved in matrix multiplication, it is not feasible for a library to contain specific pre-compiled codepaths for every combination of parameters. However, by utilizing just-in-time compilation to build the particular kernels at run-time, a library can provide computational kernels tuned for the matrix multiplications needed by the application. By storing the generated kernels in a hash table, the cost of the run-time generation can be amortized across many utilizations of the kernels, leading to significant performance improvements in various high-performance computing applications. We describe how the Intel(R) Math Kernel Library can use just-in-time compilation to generate fine-tuned matrix multiplication kernels and consider the performance speedup achieved on modern architectures.

Sarah Knepper, Louise Huot, Kazushige Goto, Arthur Mitrano, Shane Story
Intel Corporation
sarah.knepper@intel.com, louise.huot@intel.com, kazushige.goto@intel.com,
arthur.araujo.mitrano@intel.com, shane.story@intel.com

PP8

Minisymposterium: SLATE: Next Generation ScaLAPACK

The objective of the Software for Linear Algebra Targeting Exascale (SLATE) project is to provide fundamental dense linear algebra capabilities to the US Department of Energy and to the high-performance computing (HPC) community at large. The ultimate objective of SLATE is to replace the venerable Scalable Linear Algebra PACKage (ScaLAPACK) library, which has become the industry standard for dense linear algebra operations in distributed memory environments. However, after two decades of operation, ScaLAPACK is past the end of its lifecycle and overdue for a replacement, as it can hardly be retrofitted to support hardware accelerators, which are an integral part of today's HPC hardware infrastructure. Primarily, SLATE aims to extract the full performance potential and maximum scalability from modern, many-node HPC machines with large numbers of cores and multiple hardware accelerators per node. This is to be accomplished in a portable manner by relying on standards like MPI and OpenMP.

Jakub Kurzak
University of Tennessee, Knoxville
kurzak@icl.utk.edu

Mark Gates
Computer Science Department
University of Tennessee
mgates3@icl.utk.edu

Piotr Luszczek
University of Tennessee
luszczek@icl.utk.edu

Jack J. Dongarra
University of Tennessee, Oak Ridge National Laboratory, USA

dongarra@icl.utk.edu

PP8

Minisymposterium: Truncated SVD Approximation Via Kronecker Summations

In this poster we describe an approach to approximate the truncated singular value decomposition (TSVD) of a large matrix by first decomposing the matrix into a sum of Kronecker products. Our approach can be used to more efficiently approximate a large number of singular values and vectors than other well known schemes, such as iterative algorithms based on the Golub-Kahan bidiagonalization or randomized matrix algorithms. We provide theoretical results and numerical experiments to demonstrate accuracy of our approximation, and show how the approximation can be used to solve large scale ill-posed inverse problems, either as an approximate filtering method, or as a preconditioner to accelerate iterative algorithms.

Chang Meng, Clarissa Garvey, James Nagy
Emory University
chang.meng@emory.edu, ccgarve@emory.edu, jnagy@emory.edu

PP8

Minisymposterium: IR Tools Matlab Package for Large-scale Inverse Problems

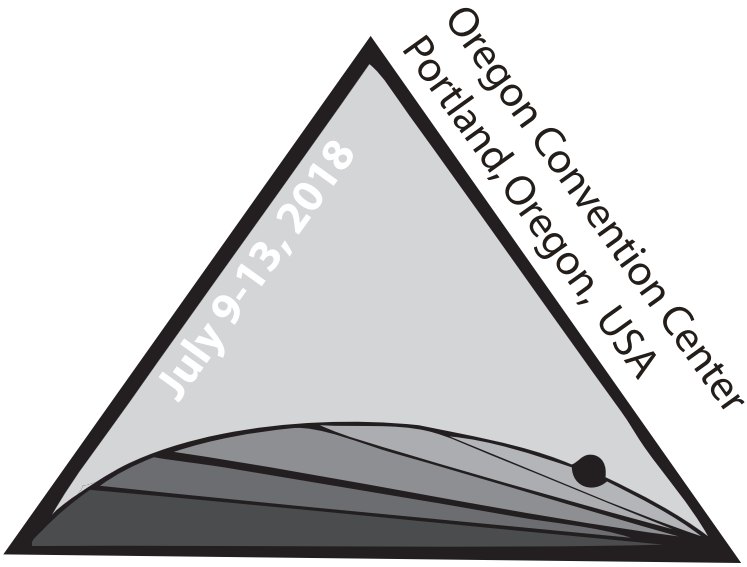
In this poster we describe and demonstrate capabilities of a new MATLAB software package that consists of state-of-the-art iterative methods to solve large scale discretizations of inverse problems. The package allows users to easily experiment with different iterative methods and regularization strategies with very little programming effort. The package includes several test problems and examples to illustrate how the iterative methods can be used on a variety of large-scale inverse problems.

James G. Nagy
Emory University
Department of Math and Computer Science
nagy@mathcs.emory.edu

Silvia Gazzola
University of Bath
s.gazzola@bath.ac.uk

Per Christian Hansen
Technical University of Denmark
DTU Compute
pcha@dtu.dk

MS18 Abstracts



SIAM Conference on

Mathematical Aspects of Materials Science

SP1

The AWM-SIAM Sonia Kovalevsky Lecture: Learning and Efficiency of Outcomes in Games

Selfish behavior can often lead to suboptimal outcome for all participants, a phenomenon illustrated by many classical examples in game theory. Over the last two decades our community developed good understanding on how to quantify the impact of strategic user behavior on the overall performance in many games by analyzing Nash equilibria of these games (including traffic routing as well as online auctions). Learning outcomes emerged in recent years as an attractive alternative to Nash equilibrium, modeling players who havent reached a stable equilibrium, but rather use algorithmic learning. We propose that learning is a good model of behavior in games where the systems has high economic value overall, but where stakes of individual items are low, which makes exploring and learning a good behavior. Such games include both Internet packet routing as well as online auctions. In this talk we consider a few closely related questions: What are broad classes of learning behaviors that guarantee high social welfare in games, are these results robust to situations when the game or the population of players is dynamically changing, and does data from such games suggest that learning is indeed a good behavioral model of the participants.

Eva Tardos
Cornell University
Department of Computer Science
eva@cs.cornell.edu

SP2

The John Von Neumann Lecture: Untangling Random Polygons and Other Things

Suppose we are given a random polygon $\mathcal{P}_0$ with vertices $(x_1, y_1), \ldots, (x_n, y_n)$ that have centroid (0,0). If we connect the midpoints of its edges, then we obtain a new polygon. Assume that the x-values and y-values are scaled after each update so that we always have $\|x\|_2 = 1$ and $\|y\|_2 = 1$. This update process can obviously be repeated to produce a sequence of polygons $\{\mathcal{P}_k\}$. No matter how "criss-crossy' the initial polygon $\mathcal{P}_0$, the $\mathcal{P}_k$ eventually "untangle' and their vertices head towards an ellipse with a 45-degree tilt. Why? It turns out that the sequence of x and y vectors that are produced by this iteration are the result of a power method process that involves a shifted version of the n-by-n downshift matrix S_n. That fact plus a slick SVD analysis of a certain 2-by-2 matrix explains everything. In this talk I will step through the matrix computations that explain the untangling. I will also discuss how I came across this problem and why it is a great metaphor of matrix-based computational science.

Charles F. Van Loan
Cornell University
Department of Computer Science
cv@cs.cornell.edu

SP3

Julian Cole Lectureship: Modeling of Complex Fluids: Wormlike Micellar Solutions, Polymers and Mucins

Complex and viscoelastic fluid properties arise due to immersed mesoscale structures. These structures may be small particles, long chain molecules, or transiently connected networks. This talk will cover elements of macroscale, and of stochastic mesoscale, modeling and simulation of transiently networked fluids; fluids typified by wormlike micellar solutions, polymers and mucins.

Pamela Cook
University of Delaware
cook@udel.edu

SP4

W.T. and Idalia Reid Prize Lecture: Modeling, Simulation, and Control of Differential-Algebraic Port-Hamiltonian Systems

Complex multi-physics, multi-scale systems are at the heart of almost all modern technology developments. A highly relevant example is the real time control of modern energy systems that have to integrate different energy sources (fossil and renewables) and large networks of producers and comsumers. To obtain a systematic approach for modeling, simulation, optimization and control of such complex systems, the concept of port-Hamiltonian systems is ideal. The structure is close to the underlying physics, the interconnection, Galerkin discretization and model reduction preserves the structure and there are nice algebraic properties of the equations and geometric properties of the resulting flow. When such systems contain constraints (such as e.g. Kirchhoff's laws in networks) then the resulting model is best described by (partial) differential-algebraic systems of port-Hamiltonian structure. The analysis, numerical solution, and control of this class of systems will be discussed, new mathematical and computational challenges will be described and the success of the approach will be demonstrated for the synchronization of power networks.

Volker Mehrmann
Technische Universität Berlin
mehrmann@math.tu-berlin.de

SP5

I.E. Block Community Lecture: How Paradoxes Shape Mathematics and Give Us Self-Verifying Computer Programs

A paradox is a seeming contradiction. The liar's paradox is one of the best known: "This statement is a false." If the statement is true, then it is false; if it is false, then it is true. Paradoxes can be so amusing that we might think that paradoxes are nothing more than a game. However, paradoxes triggered a crisis in math a century ago when a paradox similar to the barber paradox was found: a barber named Bertie shaves exactly those who do not shave themselves. Does Bertie shave himself? If he does, then he doesn't; if he doesn't, then he does. Other clever paradoxes show us the disturbing limits of computation and mathematics. These results are mathematical bombshells. Today, we design computer programs that check that other computers programs have no bugs. Can computer programs be fed into themselves to check their own correctness? Or does paradox stop us in our tracks? And can we know that beneficial artificial intelligence will not turn evil when it starts to modify its own computer code?

Thomas Hales
University of Pittsburgh

hales@pitt.edu

JP1

The Mathematics of Wrinkles and Folds

The wrinkling and folding of thin elastic sheets is very familiar: our skin wrinkles; a crumpled sheet of paper has folds; and a flat sheet stretched over a round surface must wrinkle or fold. What kind of mathematics is relevant? The stable configurations of a sheet are local minima of a variational problem involving its elastic energy – which consists of a nonconvex *membrane energy* (favoring isometry) plus a small coefficient times *bending energy* (penalizing curvature). The bending term is a *singular perturbation*; its small coefficient is the sheet thickness squared. The patterns and defects seen in thin sheets arise from energy minimization – but not in the same way that minimal surfaces arise from area minimization. Rather, the analysis of wrinkles and folds involves the *asymptotic character* of minimizers as the sheet thickness tends to zero.

Robert V. Kohn
Courant Institute of Mathematical Sciences
New York University
kohn@cims.nyu.edu

MS1

Grain Structure, Grain Boundary Character Distribution and Grain Growth in Thin Metallic Films

The types and connectivity of grain boundaries strongly influence materials properties. In the macroscopic description of grain boundaries, a general grain boundary is characterized by five parameters: three parameters to specify the lattice misorientation between the adjoining crystals meeting at the boundary and two parameters to specify the inclination of the boundary plane normal. Grain boundary character distribution (GBCD) gives the relative area of boundaries with a given misorientation and a given boundary normal. Using electron back scatter diffraction in the scanning electron microscope, GBCDs of many materials with grain sizes in the micrometer range have been measured. More recently precession electron diffraction in the transmission electron microscope has allowed these measurements to be extended to nanocrystalline materials. In this talk, GBCD of three nanocrystalline metallic films, Al, Cu and W, will be compared with microcrystalline counterparts. Grain structure of the films in the as-deposited and annealed states will be presented and related to crystal structure and bonding. Experimental grain size distributions using image based and crystal orientation mapping based methods in Al and Cu will be compared with the distribution obtained in two-dimensional simulations of grain growth with isotropic boundary energy. The role of structure formation processes during film deposition in the observed difference between experiment and simulation will be noted.

Katayun Barmak
Columbia University
katayun.barmak@columbia.edu

MS1

Polycrystalline Materials and Evolution of Grain Boundaries Network

Cellular networks are ubiquitous in nature. Most technologically useful materials arise as polycrystalline microstructures, composed of a myriad of small crystallites or grains, separated by interfaces, or grain boundaries. The energetics and connectivity of the grain boundaries network plays a crucial role in determining the properties of a material across a wide range of scales. During the coarsening, or growth, process, an initially random grain boundary arrangement reaches a steady state that is strongly correlated to the interfacial energy density. In this talk, we will discuss recent progress on mathematical modeling and analysis of the grain boundaries network's evolution in polycrystalline materials.

Yekaterina Epshteyn
Department of mathematics
University of Utah
epshteyn@math.utah.edu

MS1

An Overview of a Integral Formulation for Grain Growth in 2D

We review a novel integral model for numerical simulation of grain growth in 2D. The integral formulation generates an integro-differential dynamical system that must be solved numerically. Several numerical challenges are addressed, such as numerical computation of the unitary interpolation and its derivatives, and their connection with Chebyshev spectral methods. We compare the output generated with vertex based models and curvature method. We will provide details of the framework built for the numerical computation, which is based en GPU computing. This framework will be freely available to the community.

Claudio E. Torres
University of Delaware
ctorres@inf.utfsm.cl

Alejandro H. Sazo
Departamento de Informática
Universidad Técnica Federico Santa María
asazo@alumnos.inf.utfsm.cl

Dmitry Golovaty
The University of Akron
Department of Mathematics
dmitry@uakron.edu

Maria Emelianenko
George Mason University
memelian@gmu.edu

MS1

The Principle of G-Equivariant Universality

The statistical physics that govern either thermodynamic or driven phase-ordering dynamics continue to intrigue, while unifying principle have remained largely elusive. In this regard, we have introduced the *Principle of G-Equivariant Universality* [1], which states that the dynamical symmetry group G of a Coarsening Dynamical System ($\mathcal{CDS}$) covariantly (equivariantly) acts on that $\mathcal{CDS}$'s universal emergent parameters and probability distributions. We will exhibit this principle for a dynamically chiral $\mathcal{CDS}$, wherein Lorentzian-parabolic dynamical symmetries permit us to theoretically predict a universal coarsening law that goes beyond mere scaling [1]. We will also discuss why the *Principle of G-Equivariant Universality* is the natural generalisation of the dynamic scaling hypothesis, anticipat-

ing that it will find resonance and application well beyond the confines of the exhibited coarsening (ageing) system.
Reference: [1] Stephen J. Watson, *Lorentzian symmetry predicts universality beyond power laws*, EPL, 118 (2017) 56001.

Stephen J. Watson
University of Glasgow
Stephen.Watson@glasgow.ac.uk

MS2

The Skyrmion-bubble Transition in a Ferromagnetic Thin Film

Magnetic bubbles and skyrmions observed in ferromagnetic thin films with perpendicular magnetic anisotropy are close relatives as they can share the same topology. However, their characteristic sizes differ and while classical bubbles present a long lifetime at room temperature, much shorter lifetimes were found for nanometer-sized skyrmions in recent experimental and theoretical works. The case of intermediate-size solitons is more favorable, as stable room-temperature topological solitons with sizes of a few hundred to a few tens of nanometers have been reported in multilayers and even in a single ferromagnetic layer. These topological solitons are sometimes called skyrmion bubbles when the demagnetising energy plays a role in their stabilization. In this context, the necessity to clarify whether a fundamental difference exist between skyrmions and bubbles appears. In previous works, the difference between magnetic bubbles with a large number of collinear spins in their center and skyrmions with a compact core has been described. We derive in the present work an analytical topological soliton model in order to build a skyrmion-bubble phase diagram and obtain a better physical insight of the differences between skyrmions and bubbles. This allows us to calculate skyrmions and bubbles equilibrium solutions out of a single model from nanometer to micrometer radii and demonstrate the existence of transitions between them as a function of magnetic field.

Anne Bernand-Mantel
Institut Néel
CNRS, Grenoble
anne.bernand-mantel@neel.cnrs.fr

Lorenzo Camosi, Alexis Wartelle, Nicolas Rougemaille, Michaël Darques, Laurent Ranno
Université Grenoble Alpes, CNRS
Institut Néel
lorenzo.camosi@neel.cnrs.fr, alexi.wartelle@neel.cnrs.fr, nicolas.rougemaille@neel.cnrs.fr, m.darques@outlook.com, laurent.ranno@neel.cnrs.fr

MS2

Dynamical Skyrmions and Emergent Electromagnetism of Moving Monopoles

Topological defects such as domain walls and skyrmions have gained prominence as they owe their stability to their robustness against continuous deformations, similar to knots in a rope. While most considerations refer to static skyrmions, they can also be stabilized dynamically via a purely precessional mechanism. Such objects may serve as tuneable generators of microwave radiation and may even exist in DMI free materials. As a second example of topologically nontrival dynamical object in DMI free materials, we discuss the rapid motion of hedgehogs in nanowires. The creation of such hedgehogs is intimately related to the irreversibility of magnetization reversal in generic nanoparticles. Their rapid motion gives rise to substantial emergent electric field, thus characterizing these hedgehogs as bona-fide monopoles.

Hans-Benjamin Braun
University College Dublin
beni.braun@ucd.ie

MS2

Chiral Domain Walls and Domain Wall Tilt in Ferromagnetic Nanostrips

Recent advances in nanofabrication make it possible to produce multilayer nanostructures composed of ultrathin film materials with thickness down to a few monolayers of atoms and lateral extent of several tens of nanometers. At these scales, ferromagnetic materials begin to exhibit unusual properties, such as perpendicular magnetocrystalline anisotropy and antisymmetric exchange, also referred to as Dzyaloshinskii-Moriya interaction (DMI), due of the increased importance of interfacial effects. The presence of surface DMI has been demonstrated to fundamentally alter the structure of domain walls. Here we use the micromagnetic modeling framework to analyse the existence and structure of chiral domain walls, viewed as minimizers of a suitable micromagnetic energy functional. We explicitly construct the minimizers in the one-dimensional setting, both for the interior and edge walls, for a broad range of parameters. Using varitional methods we analyze the asymptotics of the two-dimensional magnetization patterns in samples of large spatial extent in the presence of weak applied magnetic fields and present an analytical theory of domain wall tilt. We show that under an applied field the domain wall remains straight, but tilts at an angle to the direction of the magnetic field that is proportional to the field strength for moderate fields and sufficiently strong DMI.

Valeriy Slastikov
University of Bristol
Bristol, UK
Valeriy.Slastikov@bristol.ac.uk

Cyrill B. Muratov
New Jersey Institute of Technology
Department of Mathematical Sciences
muratov@njit.edu

Oleg Tretiakov
Tohoku University
Institute for Materials Research
olegt@imr.tohoku.ac.jp

Alexander Kolesnikov
School of Natural Sciences
Far Eastern Federal University
kolesnickov.a@gmail.com

MS2

Ferromagnetic Domain Wall as a Nonreciprocal String

We present a simple model of a domain wall in a thin-film ferromagnet. A domain wall is represented as a nonreciprocal string, on which transverse waves propagate with different speeds in opposite directions. The model has three parameters: mass density, tension, and a gyroscopic constant quantifying the nonreciprocity. We discuss the un-

usual dynamics of a nonreciprocal string in a strip of constant width.

Oleg Tchernyshyov
Department of Physics and Astronomy
Johns Hopkins University
olegt@jhu.edu

Shu Zhang
Department of Physics
Johns Hopkins University
szhang67@jhu.edu

MS3

Post-Bifurcation and Stability of a Finitely Strained Hexagonal Honeycomb Subjected to Equi-Biaxial in-Plane Loading

The buckling and crushing mechanics of cellular honeycomb materials is an important engineering problem. We review the literature on finitely strained honeycombs subjected to in-plane loading and identify two open questions: (i) How does the mechanical response of the honeycomb depend on the applied loading device? and (ii) What can the "Bloch wave representation" contribute to our understanding of the stability of post-bifurcated equilibrium configurations? We model the honeycomb as a two-dimensional infinite perfect periodic medium and use group theory methods to study the honeycomb's behavior under three different far-field loadings. Using an FEM discretization of the honeycomb walls, we find the principal and bifurcated equilibrium paths for each loading case. We evaluate the structure's stability using two criteria: "rank-one convexity" of the homogenized continuum (long wavelength perturbations) and "Bloch wave stability" (bounded perturbations of arbitrary wavelength). We find that the post-bifurcation behavior is extremely sensitive to the applied loading device. We confirm that the "flower mode" is always unstable, as previously reported. However, our Bloch wave stability analysis shows that the flower mode is stable for all sufficiently short wavelength perturbations. This new result provides a realistic explanation for why this mode has been observed in the finite size specimen experiments of Papka & Kyriakides.

Ryan Elliott
University of Minnesota
relliott@umn.edu

Christelle Combescure
University Paris-Est Marne-la-Vallee
christelle.combescure@u-pem.fr

MS3

Bifurcation Analysis of Pdes and Vis with Deflated Continuation

Computing the solutions u of an equation $f(u, \lambda) = 0$ as a parameter $\lambda \in \mathbb{R}$ is varied is a central task in applied mathematics and engineering. In this talk I will present a new algorithm, deflated continuation, for this task. Deflated continuation has two main advantages. First, it is capable of computing disconnected bifurcation diagrams; previous algorithms only aimed to compute that part of the bifurcation diagram continuously connected to the initial data. Second, its implementation is extremely simple: it only requires a minor modification to any existing Newton-based solver. This means it is straightforward to scale to very large discretisations if a good preconditioner is available. Among other problems, we will apply this to a famous singularly perturbed ODE, Carrier's problem. The computations reveal a striking and beautiful bifurcation diagram, with an infinite sequence of alternating pitchfork and fold bifurcations as the singular perturbation parameter tends to zero. The analysis yields a novel and complete taxonomy of the solutions to the problem, and demonstrates that a claim of Bender & Orszag is not stated correctly.

Patrick E. Farrell
Mathematical Institute
University of Oxford
patrick.farrell@maths.ox.ac.uk

MS3

A One-dimensional Model for the Propagation of Bulges in Cylindrical Balloons

During the inflation of an axisymmetric thin elastic tube subject to a constant axial force and to a variable internal pressure, the initiation and propagation of a localized instability is observed. The initial homogeneous cylindrical configuration becomes unstable shortly after attainment of a maximum pressure. A bulge is then formed while the pressure drops. As the volume of the tube is further increased, the bulge propagates while the pressure remains constant. The value of the pressure at this plateau can be calculated in terms of the hyper-elastic constitutive law of the membrane, based on an analogy with Maxwell's construction for the equilibrium of two phases. In this talk, I will push the analogy between propagating bulges and phase transitions further. I will show that the details of the bulge formation and propagation can be captured accurately by a one-dimension model similar to the diffuse interface model developed in the context of liquid-vapor phase transitions. In our model the energy depends not only on the tube radius but also on its gradient along the tube's axis. This model is derived by a formal expansion starting from the non-linear membrane model. I will compare numerical solutions of this model with solutions of the original non-linear membrane model, and show how it can be used to make analytical predictions on the bifurcation loads and on the post-buckling behavior of the tube while accounting for the finite tube length.

Claire Lestringant
Pierre and Marie Curie University
claire.lestringant@gmail.com

Basile Audoly
Moore Distinguished Scholar
baudoly@gmail.com

MS3

The Wrinkle to Crumple Transition in Confined Sheets

Thin sheets are prone to localizing stress in singular vertices and ridges, like those in a crumpled piece of paper. However, a general set of conditions for stress focusing in confined sheets is not yet known. We present a minimal model system exhibiting a wrinkle-to-crumple transition, consisting of an ultrathin polymer film on a water meniscus. When the interface is flat, lateral compression gives rise to smooth sinusoidal wrinkles. By increasing the hydrostatic pressure, the interface becomes curved and the wrinkles break up into segments that focus stress at their tips. We study how the threshold curvature for this transition depends on the properties of the sheet and the liquid.

We propose a general phase diagram that also describes measurements from spherical and hyperbolic geometries [PNAS 109, 9716 (2012) and PNAS 113, 1144 (2016)].

Joey Paulsen
Syracuse University
jdpaulse@syr.edu

Yousra Timounay
Syracuse University
Dept of Physics
ytimouna@syr.edu

MS4

Relaxation of surface energies with density

We study the behavior of surface energies defined over couples (E,u) where E is a set and u is a density on the boundary of E. Such energies have been considered in the context of materials science for modelling surface diffusion in a way that takes into consideration explicitly the effect of the free atoms moving on the surface (adatoms) in a regime where the elastic energy is negligible. We discuss regular critical points, existence and uniqueness of minimizers and we characterize the relaxation of the energy functional in a suitable topology. Finally, we will present approximations with phase field and discrete energy. This is a work in collaboration with Marco Caroccia and Laurent Dietrich.

Riccardo Cristoferi
Carnegie Mellon University
rcristof@andrew.cmu.edu

MS4

Title Not Available At Time Of Publication

Abstract Not Available At Time Of Publication.

Qiang Du
Columbia University
Department of Applied Physics and Applied Mathematics
qd2125@columbia.edu

MS4

Upscaling in Molecular Solvation

We treat the variational Poisson-Boltzmann model of molecular solvation of discrete polar macromolecules in a nonpolar continuous solvent. We show that as the size of the macromolecules tends to zero and their number to infinity, there are different scaling regimes where either the self-energies of optimal molecule clusters or long-range Coulombic interactions dominate, depending on the relative density. Further, the presence of common ions in the solvent leads to a screening effect between different molecule clusters, negating long-range interactions.

Janusz Ginster
Carnegie Mellon University
jginster@andrew.cmu.edu

MS5

Fluctuating Hydrodynamics for Modeling Electrolytes

Fluctuating hydrodynamics augments the Navier-Stokes equations with stochastic fluxes that represent thermal fluctuations in fluids at small scales. In this talk we discuss the generalization of fluctuating hydrodynamics to electrolytes. The overall formulation is based on a Boussinesq approximation and includes detailed species transport and electrochemistry. We consider some of the analytic properties of the resulting system and introduce a numerical algorithm for solving the system. Finally, we present numerical examples that illustrate the behavior of electrolytes.

John B. Bell
CCSE
Lawrence Berkeley Laboratory
jbbell@lbl.gov

MS5

Fluctuating Hydrodynamics of Reactive Liquid Mixtures

We discuss a low Mach number formulation of the equations of isothermal fluctuating hydrodynamics for multispecies reactive mixtures of miscible liquids, as well as associated computational algorithms and applications. We use a general Maxwell-Stefan-based formulation of multispecies diffusion, and include a quasi-incompressible constraint that allows the density to change with composition. For chemical reactions, we show that the traditional diffusion process description of thermal fluctuations via the chemical Langevin equation does not correctly reproduce the large deviation theory of the chemical master equation (CME). However, a description based on Poisson noise, which can be efficiently simulated using tau leaping, is consistent and no harder to simulate than the Langevin description. While the CME is well known for ideal dilute solutions of reactants in a solvent, we discuss how to generalize it to more general non-ideal mixtures. For spatially-extended systems, we combine a fluctuating hydrodynamics description and numerical model for diffusion with a stochastic description of reactions, and discuss some inherent difficulties associated with a purely local description of reactions. We also account for advection and the coupling between velocity and concentration fluctuations, and discuss some difficulties in handling the fact that reactions typically change the local density of the fluid.

Changho Kim, Andy Nonaka
Lawrence Berkeley National Laboratory
changhokim@lbl.gov, ajnonaka@lbl.gov

John B. Bell
CCSE
Lawrence Berkeley Laboratory
jbbell@lbl.gov

Alejandro Garcia
San Jose State University
alejandro.garcia@sjsu.edu

Aleksandar Donev
Courant Institute of Mathematical Sciences
New York University
donev@courant.nyu.edu

MS5

Fluctuating Hydrodynamics for Ionic Liquids

We will present a mean-field fluctuating hydrodynamics (FHD) method for studying the structural and transport properties of ionic liquids in bulk and near electrified surfaces. The free energy of the system consists of (a) a Ginzburg-Landau functional that models the spontaneous

separation of the ionic groups, and (b) the standard mean-field electrostatic interaction between the ions in the liquid. The numerical approach used to solve the resulting FHD-Poisson equations is very efficient and models thermal fluctuations adequately. Such density fluctuations are sufficiently strong to excite the experimentally observed spontaneous formation of liquid nano-domains. Statistical analysis of our simulations provides quantitative information about the properties of ionic liquids, such as the mixing quality, stability, and the size of the nano-domains. Difference between stochastic and deterministic equations will also be discussed.

Nikolaos Voulgarakis, Konstantinos Lazaridis, Logan Wickham
Washington State University
n.voulgarakis@wsu.edu, k.lazaridis@wsu.edu, logan.wickham@wsu.edu

MS6

Transforming Addition Manufacturing Through Exascale Simulation

The Exascale Additive Manufacturing Project (ExaAM) is an integrated collaboration between U.S. DOE laboratories (ORNL, LLNL and LANL). ExaAM is one of the applications selected by ECP for development on exascale computers. Starting from a top-down approach, an integrated computational materials engineering (ICME) approach can be used to accelerate the qualification and adoption of AM parts by enabling up-front assessment of manufacturability and performance. The project includes an integration of all the computational components of the AM process into a coupled exascale modeling environment, where each simulation component itself is an exascale simulation. In order to expose the physics fidelity needed to enable part qualification, the continuum scale build simulation is tightly coupled to mesoscale simulations of microstructure and defect development and evolution from which location-specific properties are determined for performance simulations. The project is driven by a series of demonstration problems that are amenable to experimental observation and validation. Here, we present our coupled exascale simulation environment for additive manufacturing and its initial application to AM builds. Work performed under the auspices of the U.S. DOE by LLNL, LANL and ORNL under contracts DE-AC52-07NA27344, DE-AC52-06NA25396, DE-AC05-00OR22725, and supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. DOE Office of Science and the NNSA.

James F. Belak
Lawrence Livermore National Laboratory
Lawrence Livermore National Laboratory
belak1@llnl.gov

John Turner
Oak Ridge National Laboratory
Computational Engineering and Energy Sciences
turnerja@ornl.gov

Curt Bronkhorst
Los Alamos National Lab
cabronk@lanl.gov

MS6

Application of the Truchas Code to Additive Manufacturing

Originally developed for simulating metal casting, Truchas is a parallel, open-source multiphysics simulation code that is being adapted and applied to the simulation of melt pool dynamics for additive manufacturing (AM) modeling applications, as part of the Exascale Additive Manufacturing (ExaAM) project. A brief overview of the AM relevant physical models and their implementation will be given, along with current representative simulation results. An overview of current efforts to couple Truchas to both mesoscale codes for predicting microstructure and part-scale codes for predicting final product configuration and performance will also be given.

Matthew Bement
Los Alamos National Laboratory
bement@lanl.gov

MS6

Part-Scale Modeling of Selective Laser Melting at LLNL

Selective Laser Melting (SLM) is a manufacturing process which can realize significant benefits over traditional manufacturing processes, including significantly shortened time between design and manufacture of parts, and the ability to create parts with much more geometric complexity than has previously been tenable, or in some cases, even possible. However, the extreme sensitivity of the results to input parameters results in a process that is difficult to predict, and thus control. Indeed, it is not uncommon for the resulting parts to vary significantly from the desired geometry, due to the influence of extreme and inhomogeneous thermal gradients. The SLM process is difficult to model for several reasons, including the complex, dynamic physical phenomena, as well as its severely multiscale character. The current presentation will describe ongoing work within the parallel, implicit finite element code Diablo, toward several goals: (1) addition of new, or improvement of existing, physics, and (2) improvement of the throughput of simulations, while simultaneously keeping degradation of the solution accuracy to a minimum.

Neil Hodge, Rishi Ganeriwala, Robert Ferencz
Lawrence Livermore National Laboratory
hodge3@llnl.gov, ganeriwala1@llnl.gov, ferencz1@llnl.gov

MS6

A Material Point Method for Marangoni Flow

The Material Point Method (MPM) was originally developed by Sulsky, Chen, and Schreyer for computational mechanics simulations of materials with large deformations. In the last 25 years, it has been further developed and applied to problems in various types of solids, porous media, fracture, fluids, and phase change. In the case of low speed incompressible fluids possessing an interface or a free surface, MPM is particularly attractive due to resolution of the interface by the material points and the associated accurate Lagrangian advection schemes. In addition, multiphysics simulations and phase change are facilitated by the ease of material description by the material points. In powder-scale simulations of additive manufacturing the objective is to create high-resolution simulations of the melting and solidification of the metallic powder. The resulting melt pool dynamics and shape ultimately dictate the microstructure of the manufactured part which in turn

describes its properties and performance. The dynamics of the melt pool are primarily driven by Marangoni flow caused by varying surface tension at the free surface due to large temperature gradients and surfactants. As part of our objective to create an efficient and accurate MPM-based solver for this phenomena, we present an MPM scheme to model Marangoni flow and discuss various aspects of modeling surface tension with MPM.

Stuart Slattery
Computer Science and Mathematics Division
Oak Ridge National Laboratory
slatterysr@ornl.gov

MS7

Islands Correlation Induced by Strain-Dependent Surface Energy

Experiments evidence the correlated growth of SiGe quantum dots in some experimental conditions. We investigate this phenomena through the interactions between quantum dots via their elastic fields, that significantly alter their self-organization. Experiments reveal that the spatial distribution of quantum dots tend to be clustering in low-density dots assembly, indicating some attractive phenomena. The dots interactions are subject simultaneously to the direct elastic energy but also to the strain-dependent surface energy. If the former is mostly repulsive, we theoretically show that the latter can lead to a significant attractive effect. Indeed, the decrease in the surface energy close to an existing island reduces the nucleation barrier and thence increases the nucleation probability close to an existing island. We show by Monte-Carlo simulations that this effect describes well the experimental results, evidencing a new mechanism that may rule the quantum dots nucleation.

Jean-Noel Aqua
Institut des NanoSciences de Paris
aqua@insp.jussieu.fr

MS7

Nanoscale Self-Organization Induced by Ion Bombardment of Solid Surfaces

Bombarding a solid surface with a broad ion beam can produce a variety of self-assembled nanoscale patterns. The spontaneous emergence of these patterns is not just fascinating in its own right: in the future ion bombardment may prove to be an important tool in the fabrication of nanostructures. Under certain conditions, ion-induced erosion of a crystalline solid can be thought of as a kind of "negative epitaxy" and there are intriguing parallels with crystal growth. As an introduction to the field, the question of why oblique-incidence ion bombardment often produces periodic height modulations or "ripples" on a solid surface will be addressed. Next, I will discuss a theory we have developed that explains the genesis of the strikingly regular hexagonal arrays of nanodots that can form when a flat surface of a binary compound is subjected to normal-incidence ion bombardment. In experiments of this kind, a layer at the surface of the solid is amorphized by the impinging ions. When the (001) surface of a crystalline binary material with fourfold rotational symmetry is bombarded at normal incidence, on the other hand, we predict that highly ordered square arrays of nanopyramids can form if the crystal structure remains essentially intact. In this case, our nonlinear continuum equations of motion include the effect of the Ehrlich-Schwoebel barrier, which is known to be important in epitaxial growth.

R. Mark Bradley
Colorado State University
mark.bradley@colostate.edu

MS7

Kinetic and Entropy-Based Modeling of Texture in Polycrystalline Materials

Several kinetic and entropy-based mesoscale models of polycrystalline grain growth have been introduced recently, aimed at describing evolution of grain boundary network statistics through the cascade of coarsening-induced topological changes. Resulting Fokker-Planck, integro-differential and Boltzmann-type equations have each been able to reproduce some steady state and dynamical features of the process, but each faced certain challenges. This talk will focus on elucidating connections and differences between these models and exploring their strengths and limitations, with an overarching goal of developing a unified stochastic theory of materials coarsening capable of fully capturing experimental and simulation-based observations.

Maria Emelianenko
George Mason University
memelian@gmu.edu

MS7

A Fokker-Planck Reaction Model for the Epitaxial Growth and Shape Transitions of Quantum Dots

We construct a Fokker-Planck reaction model which is based on a coupled system of Fokker-Planck equations for growth of different types of quantum dots, with reaction terms describing the shape transitions between islands of different types including asymmetric shapes. This mean-field model enables us to consider the kinetics of asymmetric shape transitions and study the evolution of island shape distributions during the coupled growth and transition process. Through numerical simulations over a range of growth parameters, we find multimodal and unimodal evolution modes of the shape distribution of island arrays, which depend on the external deposition flux rate and temperature rather than the shape transition rate. However, the shape transition rate governs the kinetics of shape transitions and determines the fraction of islands that form via asymmetric states, which has implications for the development of asymmetric composition profiles within alloy islands.

Chaozhen Wei
State University of New York at Buffalo
iasczwei@ust.hk

Brian J. Spencer
State University of New York at Buffalo
Department of Mathematics
spencerb@buffalo.edu

MS8

Packing and Assembling Polyhedra: from Ancient Math to Advanced Materials

Abstract Not Available At Time Of Publication.

Daphne Klotsa
University of Michigan

Current affiliation: University of North Carolina
dklotsa@email.unc.edu

MS8

Crystal Growth Revisited

The discovery of quasicrystals in 1982 not only upset the received notion of "crystal," it also revived dormant questions about their form and growth. Not only has the long-banned icosahedron been readmitted to the crystal kingdom, the tiling paradigm for crystal structure is being seriously challenged by alternate models (e.g., soft packings and nested clusters). This talk draws on recent joint work with Jean Taylor, Erin Teich, Pablo Damasceno, and Yoav Kallus on modeling the growth of complex crystals.

Marjorie Senechal
Smith College
senechal@smith.edu

MS8

Modeling Proteins for Rigidity and Flexibility Analysis: Mathematical Challenges

Modeling of molecules as mechanical linkages permits the application of ideas from rigidity theory to flexibility studies for large large bio-molecules. Kinari is an on-going project which uses the body-bar-hinge model for proteins and the periodic bar-and-joint model for crystalline matter to infer, in each case, rigid cluster decompositions and flexibility parameters with provable mathematical properties. I will survey the mathematical results that underlie the KINARI approach, as well as new mathematical challenges that emerged.

Ileana Streinu
Department of Computer Science
Smith College
istreinu@smith.edu

MS8

Local Structure in Hard Polyhedral Glass-formers

Colloidal systems are capable of self-assembling into a wide variety of ordered structures, ranging from the simple to the exceedingly complex. Often, however, no such assembly occurs, and the system instead may be characterized as a glass-former. Here, we computationally investigate assembly failure in a family of monodisperse, one-component systems, composed of particles of related polyhedral shapes with no interactions aside from those of excluded volume. We study the role that particle geometry and consequent local structure play in dynamical arrest in these entropically-mediated systems, and find that assembly failure arises from a structural identity crisis experienced on a local level. Our work demonstrates the power of considering families of related systems when exploring phase behavior, and additionally probes the long-sought nature of the relationship between structure and dynamics in glass-forming systems.

Erin G. Teich
University of Michigan
Applied Physics Program
erteich@umich.edu

Greg Van Anders, Sharon Glotzer
University of Michigan
grva@umich.edu, sglotzerkjc@umich.edu

MS9

Domain Walls with Prescribed Winding Number in a Nonlocal Model Coming from Micromagnetics

We study a nonlocal Allen-Cahn type problem for vector fields of unit length, arising from a model for domain walls (called Néel walls) in ferromagnetism. We show that the nonlocal term gives rise to new features in the energy landscape; in particular, we prove existence of energy minimisers with prescribed winding number that would be prohibited in a local model. We also determine the interaction energy between the domain walls that governs their position. This is a joint work with Roger Moser, University of Bath.

Radu Ignat
Institut de Mathématiques de Toulouse
Université Paul Sabatier
radu.ignat@math.univ-toulouse.fr

MS9

Numerical and Mathematical Aspects of an Integrodifferential Equation

The Weertman equation is a nonlinear integrodifferential equation which models steadily-moving dislocations in materials science. Its solution can be interpreted as the (unique) traveling wave of an "artificial" dynamical system (a nonlocal reaction-diffusion equation). Under reasonable hypotheses, we prove that, for any initial condition, the dynamical system actually converges to the solution of the Weertman equation. This convergence provides a way of approximating numerically the solution of the Weertman equation.

Marc Josien
CERMICS at Ecole des Ponts ParisTech (France)
marc.josien@enpc.fr

Frederic Legoll
Laboratoire Navier (ENPC) and Inria
frederic.legoll@enpc.fr

Claude Le Bris
Ecole des Ponts ParisTech, France
claude.le-bris@enpc.fr

Yves-Patrick Pellegrini
Commissariat a l'Energie Atomique
Departement de Physique Theorique et Appliquee
yves-patrick.pellegrini@cea.fr

MS9

Numerical Approximation of Time Dependent Advection Fractional Diffusion Systems

In this talk we discuss the numerical approximation of time dependent advection-diffusion problem where the diffusion consists of fractional powers of elliptic operators. The numerical methods put forward are based on Dunford-Taylor representations for both the spectral and integral laplacians. Convergence analysis together with the necessary regularity theory are discussed for linearized advections. In the second part of the talk, we illustrate the efficiency of our algorithm in the context of surface quasi-geostrophic (SQG) and electro-convection systems. The

former model large-scale motions in the atmosphere near the pole, while the latter describes the flow dynamics of electrically charged fluids immersed in electrical fields.

Peng Wei
Texas A&M University
weip@math.tamu.edu

MS10

Machine Learning Materials Physics: Algorithms Predict Precipitate Morphology in An Alternative to Phase Field Dynamics

Machine learning has been effective at detecting patterns and predicting the response of systems that behave free of natural laws. Examples include learning crowd dynamics, recommender systems and autonomous mobility. There also have been applications to the search for new materials that bear relations to big data classification problems. However, when it comes to physical systems governed by conservation laws, the role of machine learning has been more limited. Here, we present our recent work in exploring the role of machine learning methods in discovering, or aiding, the search for physics. Specifically, this talk will focus on using machine learning algorithms to represent high-dimensional free energy surfaces with the goal of identifying precipitate morphologies in alloy systems. Traditionally, this problem is approached by combining phase field models, which impose first-order dynamics, with elasticity, to traverse a free energy landscape in search of minima. Equilibrium precipitate morphologies occur at these minima. Here, we exploit the ability of machine learning methods to represent high-dimensional data, combined with surrogate optimization, sensitivity analysis and uncertainty quantification as an alternate approach to finding minimum energy states. This combination of data-driven methods offers an alternative to the imposition of first-order dynamics via phase field methods, and represents one approach to learning materials physics with machine learning.

Krishna Garikipati
Mechanical Engineering
University of Michigan
krishna@umich.edu

Gregory Teichert
University of Michigan
greght@umich.edu

MS10

QoI-Adapted Stochastic Models for Material Systems

Computational burden is a significant challenge in characterizing the statistical performance of materials systems. We address this challenge by allowing the quantities of interest (QoI) to drive the computational and statistical complexities of the problem, rather than the governing equations and their numerous inputs. Further, several such systems exhibit behaviors across several scales that involve distinct load transfer and failure mechanisms. We address this aspect of the problem by enabling sensitivity calculations across scales and across interacting physical processes. This ability proves to be very valuable for design-based optimization of complex multiscale materials systems. Our approaches are based on delineating manifolds that support the QoI. This is done through both probabilistic learning and adapted vector space projection.

Roger Ghanem
University of Southern California
Aerospace and Mechanical Engineering and Civil Engineering
ghanem@usc.edu

Loujaine Mehrez
Department of Aerospace and Mechanical Engineering
University of Southern California
lmehrez@usc.edu

Ziad Ghauch
University of Southern California
Department of Civil Engineering
ghauch@usc.edu

Venkat Aitharaju, William Rodgers
General Motors Research
venkat.aitharaju@gm.com, william.r.rodgers@gm.com

Praveen Pasupuleti, Arnaud Dereims
ESI Group
praveen.pasupuleti@esi-group.com, arnaud.dereims@esi-group.com

MS10

Adaptive Control of Modeling Error in Multiscale Models of Random Heterogeneous Media: Applications to the Design of New MLMC and MFMC Methods

This lecture describes an adaptive modeling paradigm for the analysis of high-fidelity (HF) stochastic, multiscale models of random heterogeneous materials. The methodology is based on the idea of approximating key quantities of interest (QoI) using a sequence of lower-dimensional surrogate models in which homogenized effective properties exist in subdomains of the exact solution that contribute to errors in the QoIs below a preset tolerance. Rigorous two-sided goal-oriented bounds on the error in the surrogate QoI are derived and used as a basis for an adaptive modeling algorithm. Applications to heat conduction in a random two-phase material are described. The estimates of error in QoIs are used to derive efficient Multi-Level and Multi-Fidelity Monte Carlo methods for solving the stochastic system. Estimates of MLMC bias tolerances and computational costs are discussed.

J. T. Oden
ICES - The University of Texas at Austin
oden@ices.utexas.edu

Danial Faghihi
Institute for Computational Engineering and Sciences
University of Texas at Austin
danial@ices.utexas.edu

Barbara Wohlmuth, Laura Scarbosio
Technical University of Munich
barbara.wohlmuth@ma.tum.de, scarabos@ma.tum.de

MS10

Statistical Learning of Reduced Kinetic Monte Carlo Models of Complex Chemistry from Molec-

ular Dynamics

Complex chemical processes, such as the decomposition of energetic materials or the adsorption of water on titania nanoparticles, are typically studied using large-scale molecular dynamics (MD) simulations. These computations may involve thousands of atoms forming hundreds of molecular species and undergoing thousands of reactions, generating a wealth of data. This data has traditionally been used to calculate some aggregate property of the system being studied, and is then discarded. We propose that MD data can actually be reused to study related systems, and demonstrate how to do this using methods from statistical learning. In this talk, we will develop a statistical framework for constructing kinetic Monte Carlo (KMC) models from MD data. We will also discuss a new and efficient data-driven method for reducing our learned KMC models using L1-regularization. We will show that our KMC models can not only extrapolate the behavior of the chemical system by as much as an order of magnitude in time, but can also be used to study the dynamics of entirely different chemical trajectories with a high degree of fidelity. Importantly, our KMC models require only minutes to simulate systems and timescales that typically require weeks using MD.

Qian Yang
Stanford University
qianyang@stanford.edu

Carlos Sing-Long
Pontificia Universidad Catolica de Chile
casinglo@uc.cl

Enze Chen, Muralikrishna Raju, Evan Reed
Stanford University
enze@stanford.edu, mraju@stanford.edu, evanreed@stanford.edu

MS11

Modeling of Sintering from First Principles

A fundamental challenge in heterogeneous catalysis is to understand the mechanism by which catalysts deactivate. Sintering is one such phenomenon that reduces catalytic activity through significant reduction of the active catalytic surface area. We seek a general understanding of the process by which particles sinter, in order to design systems with improved resistance to deactivation. Our work establishes a framework for simulating the evolution of supported nanoparticles using kinetic Monte Carlo (kMC) simulations incorporating atom-by-atom processes. We have developed a model for predicting the energies of metal atoms in a general configurational space, which requires knowledge only of metal atom identity and individual atoms coordination to other metal atoms. This method can be extended to bimetallic systems, which are more complex due to the larger compositional and configurational space of bimetallic alloys, as well as due to physical phenomena (e.g. preferential segregation of components) not present in monometallic systems. Further, we have developed explicit linear relationships between the adsorption energies of metal atoms (adsorption sites) and the adsorption energies of small molecular and atomic adsorbates on those sites. This allows for the optimization of metal atom stability as a powerful activity descriptor, motivating the further refinement of this approach toward models more representative of true catalytic environments.

Frank Abild-Pederesen
SUNCAT Center, School of Engineering and SLAC
Stanford University
abild@slac.stanford.edu

Luke Roling
Iowa State University
roling@iastate.edu

Lin Li
University of Pittsburg
lil121@pitt.edu

Philipp Plessow
Karlsruhe Institute of Technology
plessow@kit.edu

MS11

Special Solutions to a Non-Linear Coarsening Model with Local Interactions

We study a one-dimensional toy model for coarsening processes with local interactions. The system consists of an infinite lattice of discrete particles $x(k) \geq 0$ that exchange mass between nearest neighbors. The time evolution is given by the spatially discrete backward fast diffusion equation $\partial_t x = -\frac{\beta}{|\beta|}\Delta x^\beta$, with $\beta \in (-\infty, 0) \cup (0, 1]$. Particles with mass zero are deleted from the system, which leads to a coarsening of the mass distribution. A typical problem is to establish upper and lower bounds on the rate of coarsening. The scaling of the equation in the case $\beta \neq 1$ suggests that the average mass of the system typically grows like $t^{\frac{1}{1-\beta}}$, while we expect exponential growth in the linear case $\beta = 1$.
We construct bounded initial data that lead to a very organized coarsening pattern with the expected rate of growth. Moreover, we prove that constant initial configurations can be approximated in ℓ^∞ by this kind of data. The main tool is an analysis of the time-reversed evolution. In particular we establish positivity estimates and long-time equilibrium properties for discrete parabolic equations with bounded non-negative initial data.

Constantin Eichenberg
University of Bonn
eichenberg@iam.uni-bonn.de

MS11

Formation and Coarsening of Nanoclusters on Surfaces: Overview and New Developments

Atoms deposited on flat surfaces diffuse and aggregate into ensembles of nanoclusters or islands, where islands above a critical size i are stable on the time scale of deposition [Surf. Sci. Rep. 61 (2006) 1]. Fundamental ensemble-level questions relate not just to the island size distribution, but also to the spatial arrangement of islands. If the surface is tessellated into capture zones (CZ) surrounding each island, then recent interest has focused on the capture zone area distribution [J. Chem. Phys. 145 (2016) 211911]. We discuss these developments. However, we note that actually a more comprehensive description is provided by the joint island size and CZ area distribution. On a longer time scale, island ensembles coarsen to reduce the energy cost of broken bonds at island peripheries. Coarsening can occur via either Ostwald ripening (OR) or Smoluchowski ripening (island diffusion and coalescence) depending on the system. Homoepitaxial systems provide an ideal platform for fundamental 2D studies

of these classic phenomena as islands have a 2D single-layer high form. However, here we describe deviations from classic behavior: OR in anisotropic systems where islands change shape during coarsening [Phys. Rev. B 88 (2013) 155434]; and OR with impurities where mass transport is facilitated by complex formation, and behavior is described by non-linear reaction-diffusion versus just linear diffusion equations [Phys. Rev. B 91 (2015) 045426].

James Evans
Ames LaboratoryUSDOE
Dep of Physics & Astro and Dep of Math, Iowa State Univ
evans@ameslab.gov

Yong Han
IOwa State University
yhan.ameslab@gmail.com

MS11

Diffusion of Two-Dimensional Clusters on Surfaces and Configurational Combinatorics

For diffusion of 2D homoepitaxial clusters of N atoms on metal (100) surfaces mediated by edge atom hopping, macroscale continuum theory suggests that the diffusion coefficient scales like $D_N \sim N^{-\beta}$ with $\beta = 3/2$. However, dynamics of nanoscale clusters can be distinct from macroscale behavior [J. Chem. Phys. 147 (2017) 201101; Phys. Rev. B 96 (2017) 235406]. Through kinetic Monte Carlo simulation of an appropriate stochastic lattice-gas model, we find different and diverse behavior in multiple regimes. For moderate sizes $9 \leq N \leq O(10^2)$, there are two mechanisms for long-range diffusion depending on island size N: slow nucleation-mediated diffusion with small $\beta \leq 1$, and facile diffusion with large $\beta \geq 2$. For larger $N = O(10^2)$ to $N = O(10^3)$, the above distinct branches merge, and subsequent anomalous scaling with $1 \leq \beta \leq 3/2$ reflects the quasi-facetted structure of clusters. There is always a strong enhancement of diffusivity for short time increments corresponding to back correlation in the cluster motion. Further understanding of this enhancement, of anomalous size scaling behavior, and of the merging of various branches, is facilitated by combinatorial analysis of the number of the ground-state and low-lying excited state cluster configurations, and also of kink populations. In this talk, we describe our simulation model, simulation results, and the application of number-theoretic combinatorial analysis.

King (Alex) C. Lai
Department of Physics & Astronomy
Iowa State University
kclai@iastate.edu

James Evans
Ames LaboratoryUSDOE
Dep of Physics & Astro and Dep of Math, Iowa State Univ
evans@ameslab.gov

Da-Jiang Liu
Ames Lab DOE
dajiang@fi.ameslab.gov

MS12

A Variational Model for Mobility from Optimal Transport Theory

We construct a variational framework for grain boundary mobility based on the principle of maximum dissipation, and inspired in part by the calculus of moving surfaces. The formalism is based on a dual dissipation functional on the surface, corresponding to energy loss as a result of surface motion, and we begin with the ansatz that the surface is driven to maximize dissipation. This formalism leads us to construct a linear component of the dissipation energy resulting in a yield criterion and a nonlinear component resulting in a velocity hardening rule. We construct a dual dissipation potential using optimal transport theory that considers full boundary plane and misorientation degrees of freedom, and use it in our variational model to predict the mobility of several types of grain boundaries. Model predictions are compared to mobilities computed from elastically driven boundary motion in molecular statics simulations.

Ian Chesser
Carnegie Mellon University
ichesser@andrew.cmu.edu

Brandon Runnels
University of Colorado, Colorado Springs
brunnels@uccs.edu

Elizabeth Holm
Carnegie Mellon University
eaholm@andrew.cmu.edu

MS12

Modeling Microstructural Evolution using Discrete, Evolving, Random Points

Discrete microstructural evolution simulations (i.e. the Monte Carlo Potts model, probabilistic cellular automata) are computationally efficient and easy to implement; they suffer, however, from various artifacts of the underlying computational lattice. In contrast, the Material Point Monte Carlo (MPMC) method uses a dynamic random lattice where material points are placed and removed randomly each time step. Eliminating the underlying lattice removes the unphysical effects of lattice anisotropy on interfacial and volumetric energies and enables the correct evolution of systems that undergo shape distortion. MPMC simulations retain most of the computational benefits of other discrete methods and provably reproduce the physics of interface motion by surface and bulk driving forces. As a case study, we examine nanotwinned polycrystalline silver films. In this system, microstructural evolution depends on small differences in interfacial and surface energies. In lattice-based methods, the lattice anisotropy overwhelms they physical energetic anisotropy. However, the MPMC is able to capture the experimentally observed dependence of texture development on film thickness.

Elizabeth Holm
Carnegie Mellon University
eaholm@andrew.cmu.edu

Philip Goins
Army Research Laboratory
philipgoins2011@gmail.com

MS12

Analysis of Thresholding Schemes for Mean-

Curvature Flow

The thresholding scheme – introduced by Merriman, Bence and Osher in 1992 – is an efficient time-discretization for multi-phase mean-curvature flow consisting of two simple operations: linear diffusion on the level of the characteristic function of each phase, and pointwise thresholding. The recent fundamental insight of Esedoglu and Otto that this practical scheme solves a minimizing movements principle draws a curious connection to de Giorgis theory of gradient flows in metric spaces. This minimization principle has a natural generalization to arbitrary surface tensions and to higher codimension, and – as opposed to other minimizing movements schemes – may be localized in space. In this talk, I will present convergence results of the scheme for (networks of) hypersurfaces and for codimension two manifolds. While the results for hypersurfaces are conditioned on the convergence of the total time-integrated energies, the result in codimension two is unconditional and based on a energy estimates away from the codimension two mean-curvature flow. This talk encompasses joint work with Felix Otto and Aaron Yip.

Tim Laux
UC Berkeley
tim.laux@berkeley.edu

Felix Otto
Max Planck Institute for Mathematics in the Sciences
Leipzig, Germany
Felix.Otto@mis.mpg.de

Aaron Yip
Purdue University
yipn@purdue.edu

MS12

Random Walk Theory of Microstructure Coarsening

Microstructure coarsening with corresponding topological reconfigurations can be modeled as a stochastic process with jumps, namely, as a continuous time random walk (CTRW) with time-dependent jumps and waiting times, for which a unified generalized master equation framework has recently been developed [*Torrejon, Emelianenko, Generalized master equations of random walks with time-dependent jump sizes, SIAM J. Appl. Math. (2018)*]. We start with a one-dimensional "toy" model of coarsening. We show that for different interfacial energy functions one can accurately match the master equation solution to numerical experiments and capture intrinsic characteristics of the coarsening model including self-similarity of the statistics. We then extend the CTRW theory to two-dimensional case to describe evolution of the misorientation distribution function (MDF). Results of the new model are compared against the literature as well as large-scale numerical experiments.

Diego Torrejon, Maria Emelianenko
George Mason University
diego.torrejon.medina@gmail.com, memelian@gmu.edu

MS13

The Magnetization Ripple: A Nonlocal Stochastic PDE Perspective

The magnetization ripple is a microstructure formed by the magnetization in a thin-film ferromagnet. It is triggered by the random orientation of the grains in the polycrystalline material. In an approximation of the micromagnetic model, this leads to a nonlocal (and strongly anisotropic) elliptic equation in two dimensions with white noise as a right hand side. However, like in singular Stochastic PDE, this right hand side is too rough for the non-linearity in the equation. In order to develop a small-date well-posedness theory, we take inspiration from the recent rough-path approach to singular SPDE. To this aim, we develop a Schauder theory for the non-standard symbol $|k_1|^3 + k_2^2$.

Radu Ignat
Institut de Mathématiques de Toulouse
Université Paul Sabatier
radu.ignat@math.univ-toulouse.fr

Felix Otto
Max Planck Institute for Mathematics in the Sciences
otto@mis.mpg.de

MS13

Hybrid Three-dimensional Solitons

Chiral magnets (ChMs) comprise a distinct class of magnetic crystals with unique properties, which are significantly distinct from those of other magnetically ordered systems such as common ferro- or antiferromagnets. The presence of natural geometrical confinement of the system provides nontrivial mechanisms for the stabilization of particle-like states that are known as magnetic skyrmions. Recently, we reported that this effect is also responsible for the stabity of other particle-like objects chiral bobbers (ChBs). Such hybrid particles have smooth magnetization vector fields and magnetic singularities Bloch points that are located a certain distance from the surface of the crystal. As a result of the nontrivial spin textures and compact sizes of ChBs, they are interesting objects for fundamental research. Because of unusual static and dynamical properties of ChBs, they are of interest for possible practical applications. For instance, the coexistence of two types of movable particle-like objects gives rise to a new concept of data encoding in novel magnetic data storage, where information can be encoded by a sequence of skyrmions and ChBs that are arranged in chains moving along a guiding stripes.

Filipp Rybakov
KTH
Royal Institute of Technology
prybakov@kth.se

Nikolai Kiselev
Peter Grünberg Institut
Forschungszentrum Jülich
n.kiselev@fz-juelich.de

A. B. Borisov, S Blügel
Institute for Advanced Simulation and Peter Grünberg Institu
Forschungszentrum Jülich
bor1947@gmail.com, s.bluegel@fz-juelich.de

MS13

Solitonic Dynamics in the Presence of Chiral Interactions

We shall discuss new phenomena of conservative magnetization dynamics induced by antisymmetric exchange inter-

action. These include solitonic motion and periodic rotation of skyrmionic propellers. The analysis will be based on variational and topological methods and conservation laws for the Landau-Lifshitz equation.

Christof Melcher
RWTH Aachen University
melcher@rwth-aachen.de

Stavros Komineas
University of Crete
komineas@tem.uoc.gr

Zisis Sakellaris
Department of Mathematics I
RWTH Aachen
sakellaris@math1.rwth-aachen.de

MS13

Edge Domain Walls in Ultrathin Ferromagnetic Films

We study existence and properties of one-dimensional edge domain walls in ultrathin ferromagnetic films with either uniaxial in-plane magnetic anisotropy or exchange bias. In these materials, the magnetization vector is constrained to lie entirely in the film plane, with the preferred directions dictated by the magnetocrystalline easy axis. We consider magnetization profiles in the vicinity of a straight film edge. To minimize the micromagnetic energy, these profiles form transition layers in which the magnetization vector rotates away from the direction of the easy axis to align with the film edge. For uniaxial films, we prove existence of edge domain walls as minimizers of the appropriate one-dimensional micromagnetic energy functional and show that they are classical solutions of the associated Euler-Lagrange equation with Dirichlet boundary condition at the edge. For exchange-biased films, we also prove that minimizers are always one-dimensional within a two-dimensional periodic setting and recover explicit one-dimensional wall profiles via Γ-convergence in an appropriate thin film limit.

Cyrill B. Muratov
New Jersey Institute of Technology
Department of Mathematical Sciences
muratov@njit.edu

Valeriy Slastikov
University of Bristol
Bristol, UK
Valeriy.Slastikov@bristol.ac.uk

Ross Lund
NJIT
ross.lund@gmail.com

MS14

Defect-induced Metric Deformations in Columnar Materials

Incorporating topological defects into a crystalline membrane like graphene, results in metric anomalies that can trigger buckling into cone- or saddle-like geometries. Now a recently uncovered mapping between the inter-element spacing in columnar structures and the metric properties of curved surfaces motivates basic questions about the interplay between defects in the 2D cross section of a columnar bundle and its 3D shape. Such questions are critical to a broad class of filamentous materials, from biological assemblies like protein fibers to nano-structured synthetic materials like carbon nanotube bundles. We describe defect-containing columnar materials using two models. First, the linear instability analysis of a continuum elastic columnar domain reveals previously unknown symmetry-breaking equilibrium shapes, which can be understood as the filamentous analogs to the conical and saddles shapes of defective membranes. Second, the energy minimization of discrete filament bundles with negative defects uncovers a surprising texture that best compensates for the incompatibility between longitudinally constant filament spacings and their tilt pattern. These symmetry breaking transitions possess a non-linear dependence on the sign of the topological disclination charge, which is shown to have a purely geometric origin. Overall, we observe a profoundly asymmetric response to positive and negative topologically charged defects that is without parallel to the membrane analog.

Isaac R. Bruss
Harvard University
ibruss@seas.harvard.edu

Gregory M. Grason
Polymer Science and Engineering
University of Massachusetts Amherst
grason@mail.pse.umass.edu

MS14

Controlling Fracture of Thin Brittle Rods Through Twisting and Quenching

Fracture limits the structural stability of macroscopic and microscopic materials, from beams and bones to microtubules and nanotubes. Despite substantial recent progress, fracture control continues to present practical and theoretical challenges. An interesting longstanding problem is due to Feynman who noted that sufficiently long, brittle elastic rods appear to fragment into at least three pieces when placed under large bending stresses. Feynman's observation raises questions as to the existence and feasibility of quench protocols that can robustly induce binary fracture in elongated brittle materials. Here, using a combination of experiments, simulations and analytical scaling arguments, we demonstrate controlled binary fracture of brittle elastic rods for two distinct protocols based on twisting and nonadiabatic quenching. Our experimental data for twist-controlled fracture agree quantitatively with a phase diagram theoretically predicted from dynamical mode analysis. Furthermore, we derive and validate novel asymptotic scaling relations for quenched fracture of elastic rods.

Jorn Dunkel
Mathematics, MIT
dunkel@math.mit.edu

MS14

The Role of Boundary Conditions in the Buckling of Cylindrical Shells

Abstract Not Available At Time Of Publication.

Yury Grabovsky
Temple University

yury@temple.edu

MS14

On a Boundary Value Problem for Conically Deformed Thin Elastic Sheets

We consider a thin elastic sheet in the shape of a disk that is clamped at its boundary such that the displacement and the deformation gradient coincide with a conical deformation with no stretching there. These are the boundary conditions of a so-called "d-cone'. We define the free elastic energy as a variation of the von Kármán energy, that penalizes bending energy in L^p with $p \in (2, \frac{8}{3})$ (instead of, as usual, $p = 2$). We prove ansatz free upper and lower bounds for the elastic energy that scale like $h^{p/(p-1)}$, where h is the thickness of the sheet.

Heiner Olbermann
University of Liepzig
heiner.olbermann@math.uni-leipzig.de

MS15

A Phase-Field Fracture Model Based on Tracking Fractured Planes

We formulate and characterize a variational phase-field model for brittle fracture that accounts for the direction of the crack through gradients of the order parameter field. Joint with Vaibhav Agrawal and Carlos Mora Corral.

Kaushik Dayal
Carnegie Mellon University
Kaushik.Dayal@gmail.com

MS15

The Wrinkling of a Twisted Ribbon

We explore a specific system in the mechanics of thin elastic? sheets in which geometry and loading conspire to generate fine-scale wrinkling. This system – a twisted ribbon held with small tension – was examined experimentally by Chopin and Kudrolli [Phys Rev Lett 111, 174302, 2013]. There is a regime where the ribbon wrinkles near its center. A recent paper by Chopin, Dmery, and Davidovitch models this regime using a von Krmn-like variational framework [J Elasticity 119, 137-189, 2015]. Our contribution is to give upper and lower bounds for the minimum energy as the thickness tends to zero. Since the bounds differ by a thickness-independent prefactor, we have determined how the minimum energy scales with thickness. Along the way we find estimates on Sobolev norms of the minimizers, which provide some information on the character of the wrinkling.

Ethan O'Brien
Courant Institute of Mathematical Sciences
New York University, USA
obrien@cims.nyu.edu

MS15

Solid-State Dewetting - Variational Modeling, Higher Order Schemes and Applications

We analyse the variational structure for a phase-field model for surface diffusion with increased accuracy, develop higher order numerical schemes and use high performance computing to simulate realistic solid-stete dewetting phenomena [1]. [1] M. Naffouti, R. Backofen, M. Salvalaglio, T. Bottein, M. Lodari, A. Voigt, T. David, A. Benkouider, I. Fraj, L. Favre, A. Ronda, I. Berbezier, D. Grosso, M. Abbarchi, M. Bollani: Complex dewetting scenarios of ultrathin silicon films for large-scale nano-architectures. Science Advances 13, (2017), eaao1472

Axel Voigt
TU Dresden
axel.voigt@tu-dresden.de

MS15

Analysis and Stability of a One-Dimensional Landau-de Gennes Model for Bent-Core Liquid Crystals

We consider an energy functional used in the physics literature to model the switching mechanism seen in a columnar phase of bent-core molecule liquid crystals. In this model, it is possible to reorient the spontaneous polarization by applying an electric field. The reorientation can be achieved by either a rotation around the smectic cone or the molecular axis, or more in general by a combination of both. To study the effects on the reorientation mechanism of the various physical parameters, we will discuss a simplified version of the model, and present some remarks about the full version. We also obtain the existence and stability of positive solutions for the simplified Euler-Lagrange equations.

Feras Yousef
The University of Jordan
fyousef@ju.edu.jo

MS16

A Fluctuating Boundary Integral Method for Brownian Suspensions

We present a fluctuating boundary integral method (FBIM) for Brownian Dynamics of suspensions of rigid particles of complex shape immersed in a Stokes fluid. We develop a linear-scaling algorithm to generate, together, both the deterministic (mean) component of the particle linear and angular velocities that arise in response to the applied forces and torques, as well as the stochastic (fluctuating) Brownian displacements that arise in response to the thermal fluctuations in the fluid. Our approach relies on a first-kind boundary integral formulation of a Stochastic Stokes Boundary Value Problem in which a random surface velocity is prescribed on the particle surface. This random surface velocity has zero mean and covariance proportional to the Green's function for the Stokes flow (Stokeslet). FBIM provides the key ingredient for time integration of the overdamped Langevin equations for Brownian suspensions of rigid particles. We demonstrate that FBIM obeys discrete fluctuation-dissipation balance by performing equilibrium BD simulations of suspensions of starfish-shaped bodies using a random finite difference temporal integrator.

Yuanxun Bao
Courant Institute of Mathematical Sciences
New York University
billbao@cims.nyu.edu

Manas N. Rachh
Applied Mathematics Department
Yale University
manas.rachh@yale.edu

Eric Keaveny

Imperial College
e.keaveny@imperial.ac.uk

Leslie Greengard
Simons Foundation and Courant Institute
New York University
greengar@cims.nyu.edu

Aleksandar Donev
Courant Institute of Mathematical Sciences
New York University
donev@courant.nyu.edu

MS16

Large Scale Brownian Dynamics of Confined Suspensions of Rigid Particles

We introduce new numerical methods for simulating the dynamics of passive and active Brownian colloidal suspensions of particles of arbitrary shape sedimented near a bottom wall. The methods also apply for periodic (bulk) suspensions. Our methods scale linearly in the number of particles, and enable previously unprecedented simulations of tens to hundreds of thousands of particles. We demonstrate the accuracy and efficiency of our methods on a suspension of boomerang-shaped colloids. We also model recent experiments on active dynamics of uniform suspensions of spherical microrollers.

Brennan Sprinkle
Northwestern University
brennansprinkle2013@u.northwestern.edu

Florencio Balboa Usabiaga
Courant Institute of Mathematical Sciences
New York University
fbalboa@courant.nyu.edu

Neelesh Patankar
Northwestern University
neeleshpatankar@gmail.com

Aleksandar Donev
Courant Institute of Mathematical Sciences
New York University
donev@courant.nyu.edu

MS16

Long-Range Interaction Mediated Dynamics of a System of Active Janus Particles: An Integral Equation Approach

The collection of active Janus particles has been studied as a paradigm to understand the thermodynamics of a collection of active particles. Yet the effects of non-local hydrodynamic interactions on the system of active Janus particles has not been investigated. In this work we simulate hydrated active Janus particles by using a combination of fast numerical schemes previously developed for studying the interaction of amphiphilic particles (lipids) in the solvents. In this formulation the coarse-grained lipid molecules interact with each other through an action field that describes their hydrophobic tail-tail interactions. For this action potential, we adopt the integral equation method on solving energy minimizer with specific boundary condition on each Janus particle. Both the QBX (quadrature by expansion) and the fast multipole method (FMM) are used to efficiently solve the integral equation. We also examine the numerical accuracy and qualitative observation from large system simulations.

Yuan-Nan Young
New Jersey Institute of Technology
yuannan.young@gmail.com

Szu-pei Fu
Fordham University
sfu17@fordham.edu

Shidong Jiang
Department of Mathematical Sciences
New Jersey Institute of Technology
shidong.jiang@njit.edu

Rolf Ryham
Department of Mathematics
Fordham University
rryham@fordham.edu

Andreas Kloeckner
UIUC
andreask@illinois.edu

MS17

Abstraction, Acceleration, and Analysis: Integrating CALPHAD and Phase-Field Models for AM Superalloys

CALPHAD databases tantalize phase-field modelers working on multicomponent superalloy systems, but integrating the two techniques can be vexatious. This contribution summarizes some warning signs and shortcuts learned from attempts to quantitatively model solid-state transformations in Inconel 625. Results of semi-quantitative simulations of multiphase reversion will be discussed in terms of phase stability and transformation kinetics.

Trevor Keller
National Institute of Standards and Technology
trevor.keller@nist.gov

Greta Lindwall
MSE
KTH
gretal@kth.se

Ursula Kattner
NIST
ursula.kattner@nist.gov

Jonathan Guyer
NIST
Metallurgy Division
jonathan.guyer@nist.gov

MS17

An Implicit Approach to Phase Field Modeling of Solidification for Additively Manufactured Materials

We develop a fully-coupled, fully-implicit approach to phase field modeling of solidification for additively manufactured materials. Predictive simulation of solidification in pure metals and alloys remains a significant challenge in the field of materials science, as micro-structure formation during the solidification of a material plays an im-

portant role in the properties of the solid material. Our approach consists of a finite element spatial discretization of the fully-coupled nonlinear system of partial differential equations at the microscale, which is treated implicitly in time with a preconditioned Jacobian-free Newton-Krylov (JFNK) method. The approach allows timesteps larger than those restricted by the traditional explicit CFL limit on structured and unstructured 2D and 3D meshes, is algorithmically scalable and efficient due to an effective preconditioning strategy. In addition, we discuss development of a computational tool based on this approach in which a subscale simulation can be utilized to directly inform a process simulation code at the continuum scale, or utilized to support an analytical model at the continuum scale. The computational tool leverages MPI and OpenMP, demonstrates parallel scalability and efficiency and is uniquely targeted to emerging exascale architectures.

Chris Newman, Marianne M. Francois
Los Alamos National Laboratory
cnewman@lanl.gov, mmfran@lanl.gov

MS17

Monte Carlo Simulation of Polycrystalline Additive Manufacturing Microstructures

A Potts Monte Carlo-based simulation method has been recently developed for the prediction of metal additive manufacturing polycrystalline microstructures. The method directly simulates the heat source scan path used in experiment and is capable of modeling hundreds of passes and dozens of build layers in a reasonable runtime. Here, recent developments will be discussed including integrating the microstructure model with multiphysics simulation codes, a new approach to simulating large domains with improved computational efficiency, and ongoing work to tie model parameters to physical values. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energys National Nuclear Security Administration under contract DE-NA0003525.

Theron M. Rodgers, John A. Mitchell, Jonathan D. Madison
Sandia National Laboratories
trodger@sandia.gov, jamitch@sandia.gov, jdmadis@sandia.gov

MS17

Intragranular and Intergranular Microstructure Modeling under Additive Conditions Using the Cellular Automaton (ca) Method

The development of microstructure in Additive Manufacturing (AM) solidification is a complex and multiscale process, depending on input parameters, material selection, and the fluid and heat transport within the molten pool. We apply the cellular automata (CA) method to model both the growth of grains based on an interfacial response function, as well as the solute transport and dendritic growth occurring at the scale of individual grains. In particular, we analyze the applicability of 2D and 3D versions of the model to the wide range of thermal conditions expected in various AM processes, as well as the impact of alloy composition and solidification velocity on microstructural transitions. The impact of heterogeneous and homogenous nucleation on the resulting grain size is also discussed. Additionally, we explore the direct coupling of this model to AM fluid and heat transport models to directly simulate microstructure evolution and compare to experimental results for grain size and morphology.

Matthew R. Rolchigo
Iowa State University
rolchigo@iastate.edu

MS18

Formation of Core-Shell Particles by Solid-State Dewetting of a Binary Alloy Thin Film

A multi-physics PDE model of solid-state dewetting of a heteroepitaxial, binary alloy thin film will be presented. The model (built upon a thermodynamically consistent alloy model of Q. Zhang, P.W. Voorhees, and S.H. Davis, J. Mech. Phys. Solids 100, 21-44 (2017)) accounts for the surface and bulk diffusion of the alloy components, the bulk phase separation, and the surface segregation. I obtained a closed-form analytical relation that expresses the thermodynamic surface segregation of one component of a binary alloy. This relation can be seen as the generalization of the classical McLean model to the bulk phase-separating alloy film with the thermodynamically stable surface. The surface composition obtained from this relation is substituted into the coupled evolution PDEs for the bulk composition and surface morphology. Following this, the stability of a planar film surface with respect to small perturbations of the shape and/or composition is analyzed, revealing the dependence of the particles size on major physical parameters. Computations show various scenarios of the particles formation and the redistribution of the alloy components inside the particles and on their surface. The results of the modeling are semi-quantitatively matched to the recent experiments by Rabkin group in Technion, Israel. (Reference: Journal of Applied Physics 123, 034302 (2018), DOI: 10.1063/1.5011676; preprint at http://arxiv.org/abs/1801.00764)

Mikhail Khenner
Western Kentucky University
mikhail.khenner@wku.edu

MS18

Kinetics of Nanoring Formation on Surfaces of Stressed Deposited Thin Films

Recent experimental studies have reported the formation of nanorings from nanocrystals or quantum dots (QDs) on stressed gold and silver thin-film surfaces upon thermal annealing. Here, we report modeling results on the kinetics of nanoring formation in biaxially stressed deposited thin films and a systematic exploration of the resulting nanoring structures upon processing parameter variation. We have developed a model for the thin-film surface morphological evolution, accounting for curvature-driven diffusion on the film surface, stress in the film, and the wetting potential between the film and the substrate. Self-consistent dynamical simulations capture QD formation on the film surface. Moreover, due to the thermal mismatch between the film and substrate materials, thermal annealing induces additional strain in the film, triggering further morphological evolution and the transformation of QDs into nanorings. Our simulation results provide a fundamental kinetic interpretation of the experimental reports in the literature and determine the effects on nanoring formation of all the relevant processing conditions and material parameters. Our dynamical simulations demonstrate that multiple concen-

tric nanorings can form from sufficiently large QDs at sufficiently high annealing temperatures. Finally, we provide a fundamental explanation of nanoring formation on stressed film surfaces based on weakly nonlinear stability analysis.

Dimitrios Maroudas, Lin Du
University of Massachusetts, Amherst
maroudas@ecs.umass.edu, ldu@umass.edu

Mikhail Khenner
Western Kentucky University
mikhail.khenner@wku.edu

MS18

Corner Wetting and Drop Shapes During Vapor-Liquid-Solid Growth of Nanowires

We consider the corner wetting of faceted nanowires in the context of vapor-liquid-solid growth of nanowires. In particular, we numerically determine the equilibrium shape of a liquid drop on top of wires of hexagonal cross section. In general, for a fixed contact angle the drop contact line approaches the corner as a function of increasing drop volume. The behavior of the liquid surface near the corners of the wire is nearly singular, and we determine the scaling behavior for the drop shape in the vicinity of the corner. A key result for nanowire growth is that for a range of contact angles there is no equilibrium drop shape that completely wets the corner because large drops violate the edge spillover condition before the corners are wetted. Finally, we show that even though the drop has near-singular behavior near the corners, the macroscopic drop shape can be determined from the geometry of the wire cross section.

Brian J. Spencer
State University of New York at Buffalo
Department of Mathematics
spencerb@buffalo.edu

MS18

Morphological Evolution and Composition Segregation During the Growth of Core Shell Nanowires

GaAs-AlGaAs core-shell nanowires with heterostructures have attracted much attention because of their significant advantages and great potentials for creating high-performance nanophotonics and nanoelectronics. A two-dimensional model that accounts for capillarity in the faceted surface limit and deposition has been developed for the evolution of the shell morphology and concentration in AlGaAs alloys. The objective is to understand the mechanisms of the formation of the radial heterostructures in the nanowire shell. There are two issues that need to be understood. One is the mechanism responsible for the morphological evolution of the shells. Analysis and simulation results suggest that deposition introduces facets not present on the equilibrium Wulff shapes. Balance between diffusion and deposition yields the small facets with slowly time-varying sizes, which are stripe structures, whereas deposition dominant growth can lead to quantum dots structures observed in experiments. There is no self-limiting facet size in this case. The other issue is the mechanism responsible for the segregation of Al atoms in the shells. It is found that the mobility difference of the atoms on the {112} and {110} facets together determine the non-uniform concentration of the atoms in the shell. In particular, Al-rich stripes are predicted to form along the {112} facets when the difference of the mobilities of Al and Ga atoms is large enough on {112} facets.

Qian Zhang
Northwestern University
qian.zhang_jennifer@northwestern.edu

MS19

Building Polyhedra by Self-Assembly

This talk is a description of various mathematical models that we have used to model self-assembly of polyhedra. These are most directly connected to experiment in the case of self-folding polyhedra designed by David Gracias lab at Johns Hopkins. I will also describe some subtleties in modeling ad simulating conformational diffusion of polyhedral intermediates.

Govind Menon
Brown University
menon@dam.brown.edu

MS19

Self-Folding Origami

Self-folding structures are a new experimental paradigm in the design of three-dimensional structures from a two-dimensional substrate. These structures are characterized by flat panels joined by hinges that are driven to fold by strain-mismatch or external driving forces. Because they start out flat, origami structures exhibit a bifurcation in their configuration space. I will present evidence that the number of bifurcations is exponential in the number of vertices. Though a partial proof will be presented, many questions about the structure of origami configuration spaces remain open. I will also describe the prospects for designing structures that self-fold robustly (without error).

Christian Santangelo
UMass Amherst
csantang@physics.umass.edu

MS19

Origami, Topology, and Transformers

In this talk, I will discuss experiments, theories, and computations on the physics of folded paper. The basic-sciences aspects of this work address the connection between the simple geometry of an origami folding pattern, the resulting topology of configuration space, and the emergent bulk mechanical properties. The applied-sciences aspect reorients and examines how practical devices can be fabricated from these abstract design principles. While we find mechanical analogs of familiar physical phenomena such as lattice defects, vacancies, and phase transitions, we also uncover a number of unexpected behaviors unique to thin folded sheets. Probing these reprogrammable mechanical metamaterials ultimately leads to new insights and a greater appreciation for the art-form itself.

Jesse Silverberg
Harvard University
Jesse.Silverberg@wyss.harvard.edu

MS19

Associative Memory in Mechanical Systems and Origami

Associative memory is the ability of recurrent neural

networks to retrieve one of several stored configurations ('memories') using only partial or corrupted information about the desired memory. We find the conditions under which associative memory is seen in a general family of mechanical networks that include spring networks and folding sheets (origami). We show that the capacity for associative memory requires strong mechanical non-linearities and grows with the range of interactions and the dimensionality of the system. We classify the different kinds of failure modes when memory capacity is exceeded. In addition to laying out design principles for multi-functional mechanical metamaterials, our work identifies limits on the programmability of energy landscapes arising from mechanical interactions.

Menachem Stern
The University of Chicago
James Franck Institute
nachistern@uchicago.edu

Arvind Murugan
University of Chicago
amurugan@uchicago.edu

MS20

The Effect of Forest Dislocations on the Evolution of a Phase-Field Model for Plastic Slip

We consider a phase field model for dislocations introduced by Koslowski, Cuitino, and Ortiz in 2002. The model describes a single slip plane and consists of a Peierls potential penalizing non-integer slip and a long range interaction modeling elasticity. Forest dislocations are introduced as a restriction to the allowable phase field functions: they have to vanish at the union of a number of small disks in the plane. Garroni and Mller proved large scale limits of these models in terms of Gamma-convergence, obtaining a line-tension energy for the dislocations and a bulk term penalizing slip. This bulk term is a capacity stemming from the forest dislocations. In the present work, we show that the contribution of the forest dislocations to the viscous gradient flow evolution is small. In particular it is much slower than the timescale for other effects like elastic attraction/repulsion of dislocations, which, by recent results due to del Mar Gonzales and Monneau/Patrizi and Valdinoci is already slower than the time scale from line tension energy. Overall, this leads to an effective behavior like a gradient flow in a wiggly potential. On the other hand, when adding a driving force in the direction of increasing slip, one needs to spend the energy to overcome the obstacles. The forest dislocations thus act like a dissipation for increasing the amount of slip, but their effect on the propagation is absent when the amount of slip is decreasing.

Patrick Dondl
Albert-Ludwigs-Universität Freiburg
patrick.dondl@mathematik.uni-freiburg.de

MS20

The Dirichlet Problem for a Nonlocal System of Equations

The focus of this talk is the Dirichlet problem associated with a strongly coupled system ofm nonlocal equations. The system of equations comes from a linearization of a model of peridynamics, a nonlocal model of elasticity. The system is a nonlocal analogue of the Navier-Lame system of classical elasticity. The leading operator is an integral operator characterized by a distinctive matrix kernel which is used to couple differences of components of a vector field. In this talk we will present well posedness of the system of equations and demonstrate optimal interior Sobolev regularity of solutions. We apply Hilbert space techniques for well posedness.

James Scott
University of Tennessee, Knoxville
jscott66@vols.utk.edu

MS20

Consistent Boundary Conditions for Nonlocal Models

It is well known that nonlocal models should be complemented with nonlocal boundary conditions that are not in the conventional sense in order for the nonlocal problem to be well-posed. In this talk, we discuss the suitable notion of nonlocal Dirichlet and Neumann boundary conditions such that the nonlocal models are consistent with the classical local models in the zero limit of the nonlocal interaction. In addition, we introduce the heterogeneous localization of nonlocal interactions at the boundary so that the classical local boundary conditions can be attached.

Xiaochuan Tian
University of Texas at Austin
xtian@math.utexas.edu

MS21

DFT is a Coarse-grained Theory

I will explain what I mean by the title, how we know this, and how many aspects of modern DFT can be understood this way. I will also describe our small-data machine-learned attempts to improve DFT. For background, please see publications at http://dft.uci.edu.

Kieron Burke
University of California, Irvine
kieron@uci.edu

MS21

Accurate Thermal Properties Using Machine Learned Interatomic Potentials

I will show our recent results in fitting interatomic potentials to DFT data using the SOAP/GAP framework, that is based on an invariant representation of atomic environments and Gaussian process regression. The talk will focus on finite temperature properties of various elemental materials, including silicon, carbon and iron, and demonstrate exquisite accuracy with respect to the underlying DFT reference.

Gabor Csanyi
University of Cambridge
gc121@cam.ac.uk

MS21

Predictive Models for Organic Materials

The recent progress in machine learning (ML) and statistical inference methods can be viewed as a revolution in artificial intelligence. Most ML methods, such as neural networks and Bayesian optimization, were developed decades

ago but did not find widespread until very recently. Today, these methods are behind many commercial applications such as Internet searches, natural language translation, and image and speech recognition. Very recently, ML techniques have emerged in physics, chemistry, and biology as a powerful computational tool that complements analytical methods. The problems that ML has been successfully applied include searches for molecules with specific properties, discoveries of chemical reaction pathways, modeling of excitation dynamics, analysis of wave functions of complex systems, and identification of phase transitions. However, a systematic understanding of which ML methods are optimal for scientific computation and what their limitations are is yet to be developed. In this talk, I will overview recent developments of our team in the prediction of organic materials properties. I will discuss how the intrinsic hierarchy of physics phenomena allows for splitting the property optimization problem into a set of interconnected subproblems with different descriptors. Finally, I will outline how the developed methods can be integrated into a broader platform for materials discovery.

Semion Saikin
Harvard University
saykin@fas.harvard.edu

MS21

Non-additive, Non-interacting, Non-decomposable Kinetic Energy Functionals: Why They Matter

Approximations of the non-additive non-interacting kinetic energy (NAKE) as an explicit functional of the density are the basis of several electronic structure methods that provide improved computational efficiency over standard Kohn-Sham DFT calculations. However, within most fragment-based formalisms, there is no unique exact NAKE, making it difficult to develop general, robust approximations for it. I will explain how these fragment-based formalisms can be adjusted to guarantee uniqueness of the NAKE. Numerically accurate inversions allow us to investigate the behavior of the *exact* NAKE and assess the performance of approximations. I will show how standard approximate functionals for the NAKE fail to reproduce its correct behavior in various bonding regimes. Finally, I will describe our progress toward new, accurate approximations for the NAKE, and why this matters.

Adam Wasserman
Purdue University
awasser@purdue.edu

MS22

Particle System Models for Two-dimensional Grain Boundary Coarsening

We construct a family of particle systems which model the coarsening of two-dimensional networks whose edges evolve by mean curvature. The limiting kinetic equations of these models, describing distributions of grain areas and topologies, are shown to be well-posed. Evidence for the exponential convergence of the empirical densities of the particle system to solutions of the kinetic equations is provided through several minimal models. The framework for the particle system is general enough to allow for various assumptions suggested in the 1980's and 1990's concerning facet exchange and first order neighbor correlations. Multiple particle system models are compared against a level set method.

Joe Klobusicky
Rensselaer Polytechnic Institute
klobuj@rpi.edu

MS22

Mathematical Modeling of Epitaxially Grown Multilayers of 2D Materials

Vertical stacking of monolayers via van der Waals (vdW) interaction opens promising routes toward engineering physical properties of two-dimensional (2D) materials and designing atomically thin devices. However, due to the lack of mechanistic understanding, challenges remain in the controlled fabrication of these structures via scalable methods such as chemical vapor deposition (CVD) onto substrates. In this paper, we develop a general multiscale model to describe the size evolution of 2D layers and predict the necessary growth conditions for vertical (initial + subsequent layers) versus in-plane lateral (monolayer) growth. An analytic thermodynamic criterion is established for subsequent layer growth that depends on the sizes of both layers, the vdW interaction energies, and the edge energy of 2D layers. We develop a phase field formulation and find that the adatom flux from vapor and temperature-induced variation of the kinetic coefficients are primary criteria affecting the self-assembled growth. The proposed model clearly demonstrates the distinct roles of thermodynamic and kinetic mechanisms governing the final structure. Our model agrees with experimental observations of various monolayer and bilayer transition metal dichalcogenides grown by CVD and provides a predictive framework to guide the fabrication of vertically stacked 2D materials.

John Lowengrub
University of California, Irvine
lowengrb@math.uci.edu

John Lowengrub
Department of Mathematics
University of California at Irvine
lowengrb@math.uci.edu

Zhenlin Guo
University of California - Irvine
zhenling@math.uci.edu

Han Ye, Vivek Shenoy
University of Pennsylvania
yehan@seas.upenn.edu, vshenoy@seas.upenn.edu

MS22

Temporal Oscillations in a Coagulation-fragmentation Model

The long-time behavior of coagulation-fragmentation equations is known to admit runaway growth (gelation) or atomization in different cases depending on the rate kernels. I will describe preliminary work on a model that exhibits stable temporal oscillations as indicated by numerics and a formal bifurcation analysis. This work is in collaboration with B. Niethammer and J. Velazquez.

Robert Pego
Carnegie Mellon University

rpego@cmu.edu

MS23

Homogenized Stray-field of a Crystalline Array of Nanoparticles

We are interested in system of small particles with constant magnetization, where all nanoparticles have some general shape and are arranged into some sort of an array. This kind of systems has been experimentally realized by growing magnetic materials in porous media, or by growing magnetic nanotubes/pillars on a non-magnetic substrate. In this work we present a simplified model for these kinds of systems, where the arrangement is assumed to be periodic and the particles within the periodic cell may have general shapes. For this model we study the homogenized macroscopic behaviour of the energy and the homogenized stray-field operator.

Elsie Araujo
ITESO, Mexico
elsie.araujo@gmail.com

Antonio Capella
Mathematics Institute, UNAM, Mexico
capella@im.unam.mx

Victor Carrera, Armando Encinas
IPICyT, Mexico
victor.carrera@ipicyt.edu.mx, armando.encinas@ipicyt.edu.mx

MS23

Skyrmionic Strings in Chiral Magnets

Skyrmions in nanosamples of chiral magnets in the first approximation can be considered as two-dimensional particle-like states. Detailed description of their properties and morphology requires three-dimensional consideration where skyrmions looks like tubes. In bigger samples such tubes are more like strings and may exhibits sophisticated morphology and behavior. We present the results of a detailed study of such skyrmionic strings and their properties.

Filipp Rybakov
KTH
Royal Institute of Technology
prybakov@kth.se

Nikolai Kiselev
Peter Grünberg Institut
Forschungszentrum Jülich
n.kiselev@fz-juelich.de

MS23

Energy Barriers in Nano-structured Permanent Magnets

Permanent magnets in hybrid and electric cars operate at elevated temperature. Classical micromagnetic simulations take into account temperature only by the temperature-dependent intrinsic materials properties. Thermal fluctuations that may drive the system over a finite energy barrier are neglected. From the energy barrier as function of the applied field the temperature dependent coercive field can be computed. We apply the string method to compute thermal switching taking into account the granular microstructure of the magnets.

Thomas Schrefl
Zentrum für Integrierte Sensorsysteme
Donau-Universität Krems
thomas.schrefl@donau-uni.ac.at

MS23

A Nonlocal Isoperimetric Problem with Dipolar Repulsion

We study a functional in which perimeter and regularized dipolar repulsion compete under a volume constraint. In contrast to previously studied similar problems, the nonlocal term contributes to the perimeter term to leading order for small regularization parameters. Indeed, below a critical value for the dipolar strength, the limiting functional is a renormalized perimeter and for small, positive regularization parameters the minimizers are balls. At critical dipolar strength, we identify the next-order Gamma-limit and discuss the existence and properties of its minimizers.

Cyrill B. Muratov
New Jersey Institute of Technology
Department of Mathematical Sciences
muratov@njit.edu

Thilo Simon
Department of Mathematical Sciences
NJIT
thilo.m.simon@njit.edu

MS24

A Corrected Sadowsky Functional for Inextensible Elastic Ribbons

The classical theory of ribbons, developed by Sadowsky and Wunderlich, has recently received a renewed attention. In this talk we will discuss the rigorous derivation, by means of Γ-convergence, of the limit energy of an inextensible elastic ribbon, as the width goes to zero. The energy deduced in this way generalises and corrects the classical Sadowsky functional.

Maria Giovanna Mora
Università degli Studi di Pavia
Dipartimento di Matematica
mariagiovanna.mora@unipv.it

Lorenzo Freddi
Università di Udine
Italy
lorenzo.freddi@dimi.uniud.it

Peter Hornung
TU Dresden
peter.hornung@tu-dresden.de

Roberto Paroni
Università degli Studi di Sassari
paroni@uniss.it

MS24

The Design and Kinematics of Generalized Miura Origami

Gauss's Theorema Egregium informs us that a sheet can-

not bend in two directions without incurring some stretch. Thus, smooth isometric deformations are restricted to variations in essentially only one direction. Alternatively, by the careful design of crease patterns, origami enables a diverse range of complex shapes not easily achieved by other means. But, how rich is this design landscape? In this work, we characterize the designs and deformations of all possible"generalized Miura Origami" (rigidly and flat foldable origami crease patterns that are topologically equivalent to an array of squares). The key result is a rigidity theorem which provides that the design and deformation of any generalized Miura Origami is completely determined by its geometry and Mountain/Valley folds on the boundary. Based on this result, we develop an efficient algorithm to compute all possible designs and deformations. We also include several examples, which highlight diverse range of complex shape achievable through the systematic design of crease patterns.

Paul Plucinsky, Fan Feng, Richard James
University of Minnesota
plucinsp@gmail.com, fengx258@umn.edu, james@aem.umn.edu

MS24

Designing with Grids of Inextensible Rods

Many manufactured materials are built from (nearly) inextensible, but flexible, rods formed into a grid that then behaves as a shell-like structure. Everyday examples range from fabrics made of 1000s of interwoven yarns; to kitchen strainers made of 100s of plastically deforming wires; to architectural gridshells and tents made of 10s of elastic rods. In this talk, we will emphasize the geometric similarity between these systems, by harnessing a continuum model for woven fabric introduced by Pafnuty Chebyshev in 1878. We briefly present the theory of Chebyshev nets, aligning theoretical limitations with intuition from practical experience. We will then discuss two recent collaborative efforts on (i) an adaptation of Chebyshev nets for computational design and fabrication of wire mesh sculptures and (ii) the applicability of Chebyshev nets to rationalize the counter-intuitive behavior observed in precision experiments with elastic gridshells. In turn, our results suggest precise mathematical questions on shapes of Chebyshev nets that may be within reach.

Andrew Sageman-Furnas
Institut für Mathematik
aosafu@math.tu-berlin.de

MS24

Dualities in the Linear Isometries and Self-stresses of Shells

An elastic shell can be discretized into a framework of triangular faces joined by hinges. The continuum Gaussian curvature of the shell has an analogue as the deficit (or excess) angle at each vertex and the mean curvature is analogous to the fold angle of each hinge. In this context, I will discuss a duality between self-stresses and linear isometries in triangulated shells. This duality is the discrete equivalent of the so-called static-geometric analogy, which relates self-stresses on a continuum shell to the linear isometries of the shell. This duality extends to discrete shells with nontrivial topologies in which holes in the shell are exchanged with rigid blocks. While many of these dualities have been previously observed, the connections between these have some important ramifications to the possible deformations of structures with complex geometries.

Christian Santangelo
UMass Amherst
csantang@physics.umass.edu

Bryan G. Chen
University of Massachussetts
bryanchen@umass.edu

David Zeb Rocklin
University of Michigan
drocklin@umich.edu

Louis Theran
Freie Universitat Berlin
lst6@st-andrews.ac.uk

MS25

Michell Trusses in Two Dimensions As a Gamma-Limit of Optimal Design Problems in Linear Elasticity

We reconsider the minimization of the compliance of a two dimensional elastic body with traction boundary conditions for a given weight. It is well known how to rewrite this optimal design problem as a nonlinear variational problem. We take the limit of vanishing weight by sending a suitable Lagrange multiplier to infinity in the variational formulation. We show that the limit, in the sense of Gamma-convergence, is a certain Michell truss problem. This proves a conjecture by Kohn and Allaire.

Heiner Olbermann
University of Liepzig
heiner.olbermann@math.uni-leipzig.de

MS25

Existence of Solitary Waves in One Dimensional Peridynamics

We give a rigorous proof of existence for solitary waves of a peridynamics model in one space dimension proposed by Silling. We adapt the framework developed by Friesecke and Wattis for the Fermi-Pasta-Ulam-Tsingou lattice equations to treat a truncated problem which cuts off short-range interactions, then pass to the limit.

Son Van, Robert Pego
Carnegie Mellon University
sonv@andrew.cmu.edu, rpego@cmu.edu

MS25

Low-Energy Martensitic Inclusions in Shape Memory Alloys

Shape memory alloys are special materials that undergo a martensitic phase transition, i.e., a diffusionless first order solid-solid phase transformation. It has been found and confirmed experimentally that the width of the associated thermal hysteresis is related to the minimal energy that is necessary to build a martensitic nucleus in a surrounding austenitic matrix. Mathematically, this energy barrier is typically modeled by nonconvex elasticity functionals which might be singularly perturbed. In this talk, I will report some recent analytical progess on the resulting variational problems, in particular on stress-free martensitic inclusions and low-hysteresis alloys. Parts of this talk

are based on joint works with S. Conti, M. Klar, A. Rland and C. Zillinger.

Barbara Zwicknagl
University of Würzburg
barbara.zwicknagl@mathematik.uni-wuerzburg.de

MS26

Torque-Dipolar Micro-Swimmers: Modeling, Circling Behavior and Large-Scale Simulations

We present a new model for micro-swimmers that takes into account the counter-rotation of the body and flagella, as seen in motile bacteria or spermatozoa. The disturbance fluid flow of one such swimmer now contains a torque-dipole singularity in addition to the well-known force-dipolar singularity. We show that this head-and-flagella counter-rotation gives rise to clock-wise circling at no-slip walls just as observed in experiments of bacteria on surfaces. We discuss the scattering behavior of spermatozoa in a forest of cylindrical pillars, confirmed also by new experiments. Last, we show large scale and fast simulations of millions of such swimmers that interact with each-other through direct collisions as well as coupled hydrodynamics.

Enkeleida Lushi, Wen Yan
Flatiron Institute
Simons Foundation
elushi@flatironinstitute.org, wyan@flatironinstitute.org

Vasily Kantsler
University of Warwick
Skolkovo Institute of Technology
v.kantsler@warwick.ac.uk

Michael J. Shelley
New York University
Courant Inst of Math Sciences
shelley@cims.nyu.edu

MS26

Three-Dimensional Multicomponent Vesicles – Methods and Dynamics

Recent work has demonstrated the interesting dynamics possible when considering multicomponent vesicles. Up to now, the dynamics of two dimensional vesicles have been studied. In this work, the dynamics of fully three-dimensional, multicomponent vesicles will be investigated. Building upon a volume and surface area conserving Navier-Stokes projection method, the appropriate forcing terms are derived from the energy of a multicomponent membrane. The evolution of the surface components is done via a conserving, surface Cahn-Hilliard model. The results show a rich variety of dynamics, from stationary phases to pinch-off, can occur when considering multicomponent vesicles.

Prerna Gera, David Salac
University at Buffalo - SUNY
prernage@buffalo.edu, davidsal@buffalo.edu

MS26

Towards a Continuum Mechanics of Active Matter

Active particles swim by converting energy into self-propulsion and collectively they form active matter. To describe the collective motion of active particles, thermodynamics-like models are successful but are not sufficient when the detailed dynamics, structure, and deformation are of interest, for example, in sedimentation or micro-rheology problems. A continuum mechanical theory is proposed based on the minimal Active Brownian Particles (ABP) model. On the macroscopic length scale, the surface force is found to be the swim stress, and the body force includes the average swim force as an internal contribution. On the microscopic scale, the behavior of active particles is analyzed as a micromechanical explanation for the continuum mechanics. Based on mechanical balance, the behavior of ABPs can be predicted with a Navier-Stokes-like equation. The continuum mechanics theory for ABPs can be used to understand the general active matter, for example, chemically active Janus particles.

Wen Yan
Flatiron Institute
Simons Foundation
wyan@flatironinstitute.org

MS27

Selective Gels: Controlling Mobility Through Programmable Binding

The ability to create a selective gel that can filter particles based on their interactions is a major goal of nanotechnology, but the physical principles that such a material could exploit are difficult to understand when the particles are larger than the mesh size of the gel. Since non-interacting particles are unable to move through such a gel, binding interactions must lead to enhanced, not decreased, motion. We present an equilibrium mechanism for this where specific binding sites on the particle promote the temporary reorganization of the internal structure of the gel, which allows the particle to pass through.

Carl Goodrich
Harvard University
goodrich@g.harvard.edu

MS27

Folding Mechanisms at Finite Temperature

Folding mechanisms are zero elastic energy motions essential to the deployment of origami, linkages, reconfigurable metamaterials, and robotic structures, and can be middle steps in the self-assembly of complex structures. In this talk, we discuss the fate of folding mechanisms when such structures are miniaturized so that thermal fluctuations cannot be neglected. First, we identify geometric and topological design strategies aimed at minimizing undesired thermal energy barriers that generically obstruct kinematic mechanisms at the microscale. Our findings are illustrated in the context of a quasi one-dimensional linkage structure that harbors a topologically protected mechanism. However, thermal fluctuations can also be exploited to deliberately lock a reconfigurable metamaterial into a fully expanded configuration, a process reminiscent of order by disorder transitions in magnetic systems. We demonstrate that this effect leads certain topological mechanical structures to exhibit an abrupt change in the pressure – a bulk signature of the underlying topological invariant at finite temperature. We conclude with a discussion of potential applications of our work to self assembly.

Xiaoming Mao

University of Michigan
maox@umich.edu

MS27

Self-assembly of Irregular Patchy Particles into Regular Structures

We show that ordered 2D structures can be self-assembled from irregular patchy particles with specific interactions. By means of dynamic and equilibrium computer simulations, and analytic theory, we identify hitherto unknown solid structures with unit cells of up to 40 particles. Due to the interaction specificity these complex structures are kinetically accessible and thermodynamically stable in regions of parameter space accessible to experiment. The emergence of such complex structures, whose symmetry properties are not obviously related to those of its constituent particles, highlights the potential for creating new structures from simple variants of existing nanoparticles.

Zdenek Preisler
Lawrence Berkeley National Laboratory
zpreisler@lbl.gov

MS27

How to Build a Diamond?

I will review recent advances in programmable self-assembly of superlattices. This progress is facilitated by the use of what we call "chromatic interactions", such as specific binding between complementary DNA. One structure that is notoriously challenging for self-assembly, and often viewed as a Holy Grail of the field, is a diamond lattice. I will therefore use diamond as a model system to illustrate general principles and specific approaches to programmable self-assembly. Some of those approaches are already implemented in experiments, while others are theoretical prescriptions.

Alexei Tkachenko
Brookhaven National Lab
oleksiyt@bnl.gov

MS28

Towards Active Ink in 3D Printers: Modeling and Experiments

3D printing is of great technological importance because it provides facile methods for fabricating advanced materials and shortens the path from prototype to product. Typically, in 3D printing, inks are sequentially deposited on the substrate by inkjet printer heads. We propose a new concept of active ink. Unlike standard ink, the active ink contains a small fraction of active rod-like particles capable of transducing chemical energy stored in liquid ink into directed mechanical motion. Our previous studies showed that the material and rheological properties of such active suspensions are fundamentally different from their inactive counterparts. The distribution of active particles significantly affects the material properties of the printed object. We have developed novel PDE models of low computational complexity and carried out experiments with suspensions of active bimetallic nanorods to understand the non-trivial focusing of these rods in trapezoid nozzles, commonly used in 3D printers. Our models and accompanied experiments suggest new nozzle geometries that will reduce upstream swimming and boundary accumulation typically exhibited by active particles, and thus significantly enhance the performance of 3D printers. We anticipate that our work will allow us to: (a) facilitate 3D printing, (b) tune the mechanical, magnetic, and optical properties of printed objects, and (c) support experiments by novel mathematical modeling techniques.

Leonid Berlyand
Penn State University
Eberly College of Science
lvb2@psu.edu

Igor Aronson
Penn State
isa12@psu.edu

Anna Balazs
Chemical Engineering Department
University of Pittsburgh, Pittsburgh, PA
balazs1@engr.pitt.edu

Ayusman Sen
Penn State
asen@psu.edu

MS28

Designing Microstructure for Engineering Toughness

Recent advances in material synthesis enable us to control material microstructure with unprecedented detail. This talk explores whether this ability can be exploited to create materials with unprecedented properties. Of particular interest is toughness, or the ability of a material to resist fracture. Fracture is a free discontinuity problem and the overall toughness of a heterogeneous medium is characterized not by averaging but pinning at critical defects. This talks describes a framework for understanding overall fracture toughness, and selected examples where the microstructure can be engineered for superior toughness.

Kaushik Bhattacharya
Howell N. Tyson Sr. Professor of Mechanics
California Institute of Technology
bhatta@caltech.edu

MS28

Chromonic Liquid Crystals and Living Systems

Chromonic liquid crystals consist of plank-like molecules that, when placed in water, form a hierarchical structure in which individual molecules self-assemble into complex supramolecular aggregates bound by weak non-covalent bonds. As the concentration increases, a phase transition from the isotropic phase to the nematic takes place, which turns into the hexagonal or columnar phase at even higher concentration. The latter presents two-dimensional crystal ordering. With the addition of concentrating agents, these systems form clusters whose shapes are topologically equivalent to a torus. One remarkable feature of these aggregates is their geometric resemblance to the shapes presented by DNA at high concentration, as in the case of bacteriophage viruses, although such clusters differ by several orders of magnitude. However, defects found on both systems have very different mathematical and physical features. We develop models of chromonic liquid crystals, analyze relevant free boundary problems, and present discretization tools for domain-shape optimization. We compare the latter results with those of previous works on DNA aggregates in solution as well as in encapsidation. We

discuss how our models apply to the design of biosensors and nanofluidic devices activated by bacteria swimming in chromonic nematic liquid crystals.

Maria-Carme Calderer
University of Minnesota
calde014@umn.edu

MS28

Structural Optimization and 3D Printing

Additive manufacturing (also known as 3D printing) permits unprecedented flexibility in structural design. The availability of this technology raises new questions in structural optimization, including: (a) What effective Hooke's laws can be achieved by printable periodic microstructures that avoid stress concentrations? (b) How should the microstructure vary macroscopically, in a design problem with specific mechanical goals and constraints? (c) How can macroscopic variation of the microstructure be accommodated while maintaining manufacturability? I'll discuss progress on these (and related) questions by J. Panetta, Q. Zhou, D. Zorin, and others, done through a DMREF-funded program "Adaptive fine-scale structure design: from theory to fabrication.'

Robert V. Kohn
Courant Institute of Mathematical Sciences
New York University
kohn@cims.nyu.edu

MS29

Elastic Instability and Secondary Flow in Cross-Slot Flow of Wormlike Micellar Solutions

Recently, there has been intense experimental investigations about the development of an asymmetric instability in the flow of wormlike micellar solutions in a cross-slot. In addition, a lip vortex upstream of the corners has been observed in the same experiments. To date, numerical investigations into the elastic instability have focused on polymeric models. Near the hyperbolic stagnation point in the cross-slot, the polymer chains stretch resulting in extensional thickening that feeds back on the flow, and may cause the symmetric flow to become asymmetric. Unlike polymer chains, wormlike micelles (WLMs) break if stretched too far. This chain breakage results in a decrease in the extensional viscosity. Despite this difference with polymers, the elastic instability is still observed. In this work, we focus on simulations of the VCM constitutive model (Vasquez, McKinley and Cook (2007)), a two species, microstructural network model, which incorporates breakage and reforming of two micellar chains. The model predicts the typical WLM rheological trends of shear thinning and extensional thinning. Using the open-source CFD library OpenFOAM, we show that the VCM model predicts the formation of an asymmetric elastic instability. In addition, the VCM model predicts the formation of recirculation zones just upstream of where the inlet and outlet channels meet. In this talk, we focus on the role breakage and reforming play on the instability and secondary flow.

Michael Cromer
Rochester Institute of Technology
mec2sma@rit.edu

MS29

Emergence and Persistence of Flow Inhomogeneities in the Yielding and Fluidization of Dense Soft Solids

Dense soft solids such as emulsions, foams or colloidal pastes, yield and eventually flow under an imposed shear deformation, a feature important for materials from wet cement to food, paint or pharmaceutical products. Controlling the flow properties upon yielding is tough, since the evolution towards the steady-state is often accompanied by strong spatial inhomogeneities, where only part of the material flows while the rest stays jammed. Such phenomenon is called shear banding and has been known for many decades to geologists and engineers, but the question of what favors the stress accumulation and the persistence of flow inhomogeneities upon yielding is fundamentally unanswered. In 3D large scale computer simulations of a model non-Brownian jammed suspension we analyze the time required for the onset of homogeneous flow, the normal stresses and the particle packing at different shear rates with and without confinement, finding that the stress overshoot and flow inhomogeneities are controlled by the presence of overconstrained microscopic domains in the initially solid samples. Being able to identify such domains in our model by prevalently icosahedrally packed regions, we show that they allow for stress accumulation during the stress overshoot and that their structural reorganization controls the emergence and the persistence of the shear banding.

Vishwas V Vasisht
Universite' Grenoble Alpes
vv120@georgetown.edu

Gabrielle Roberts
Yale University
gabrielle.roberts@yale.edu

Emanuela Del Gado
Georgetown University
ed610@georgetown.edu

MS29

Suspensions of Non-Brownian Particles in a Shear Thickening Matrix

A cornstarch suspension is a particulate system that exhibits shear thickening, i.e., viscosity appears to increase when the shear rate increases. In a shear thickening behavior, the rise in viscosity may happen in a continuous or discontinuous fashion leading to the so called Continuous Shear Thickening (CST) or Discontinuous Shear Thickening (DST) behaviors. By adding large non-Brownian spheres to a CST cornstarch suspension, we show that transition from the CST to DST may occur. This transition is explained by two possible mechanisms. The first is the excluded volume effect due to existence of large particles in the shear thickening matrix. This leads us to calculate the effective cornstarch volume fraction. We show that the effective cornstarch volume fraction is the one on which, the DST or CST prediction should be based. The second mechanism is the geometrical confinement effect applied on the cornstarch grains when they are forced to flow within the large spheres.

Sarah Hormozi
Department of Mechanical Engineering, University of British
Columbia
hormozi@ohio.edu

Yasaman Madraki
Ohio University
fm721714@ohio.edu

Guillaume Ovarlez
CNRS, Bordeaux University
guillaume.ovarlez@u-bordeaux.fr

MS29

Complex Dynamics of Wormlike Micelles in Shear and Extensional Flows

We report experiments on wormlike micellar solution in a modified Taylor-Couette geometry and under uniaxial extension. In simple shear flow, we report a shear thinning like behavior, an elastic recoil with negative velocities, and a significant wall-slip at the surface of outer cylinder for shear rates below, within and above the shear banding regime, respectively. We also show that extensional rheology is sensitive to structural changes from linear to branched and/or linear to shorter wormlike micelles.

Hadi Mohammadigoushki
Florida State University
hadi.moham@fsu.edu

MS30

Exchange Correlation Potentials from Electron Densities Using a Complete Basis

The ability to accurately invert the Kohn-Sham (KS) eigenvalue equation to obtain the exchange-correlation (xc) potential, $v_{xc}(\mathbf{r})$, that yields a given density, $\rho(\mathbf{r})$, is key to our understanding and development of accurate xc functionals. To this end, we cast the inverse problem as a PDE-constrained optimization - with $v_{xc}(\mathbf{r})$ as the control variable and the KS eigenvalue problem as the PDE-constraint. We employ limited-memory BFGS (L-BFGS) to solve the resultant non-linear optimization problem. We note that previous attempts at inverting the KS equation have suffered from non-uniqueness or spurious oscillations in $v_{xc}(\mathbf{r})$, both of which have been attributed to the incompleteness of the Gaussian basis that was employed in those calculations. We overcome these issues by using spectral finite-elements - a complete basis - to discretize the problem. We demonstrate the accuracy and robustness of the proposed approach for cases where the densities are generated from known xc functionals (LDA, GGA). Further, we also consider densities obtained from wavefunction-based methods (e.g., full configuration interaction).

Bikash Kanungo
University of Michigan
bikash@umich.edu

Vikram Gavini
Mechanical Engineering, University of Michigan
vikramg@umich.edu

MS30

Multi-Fidelity High-Throughput Screening of Electrochemical Stability of Battery Electrolytes

In high-throughput screening, a large chemical space is explored to discover materials with desired properties. For electrolytes with applications in batteries, electrochemical stability at the operating voltage of electrodes and the ability to form a stable passivation layer on electrode surfaces are critical. Quantum chemistry (QC) models are capable of accurate prediction of electrochemical properties relevant to electrolyte design given a sufficient level of theory. However, high-fidelity QC models also have a high computational cost. Therefore, in order to expedite high-throughput screening of potential electrolytes, lower fidelity methods, such as density functional theory or semi-empirical methods, are often used for property prediction. We will discuss recent work on the use of multi-fidelity surrogate models in high-throughput screening of battery electrolytes. Multi- fidelity surrogate models provide a framework to combine the predictions of material properties obtained from multiple models. In multi-fidelity high-throughput screening, a lower-fidelity model is used to rapidly explore the chemical space in combination with far fewer evaluations of an expensive high-fidelity model. The multi-fidelity surrogate model serves to discover the correlation structure between the two models from available data and to correct low-fidelity model predictions. Subsequently, the multi-fidelity surrogate model is used to guide the search for electrolytes with desired properties.

Jaroslaw Knap, Kenneth Leiter
U.S. Army Research Laboratory
jaroslaw.knap.civ@mail.mil,
kenneth.w.leiter2.civ@mail.mil

Xin-Cindy Wang
University of Colorado
xwang3@uccs.edu

Claire Eisner, Oleg Borodin
U.S. Army Research Laboratory
claire.g.eisner.ctr@mail.mil, oleg.a.borodin.civ@mail.mil

MS30

Probing Multiscale Materials Physics through Informatics

Material Informatics is transforming the existing paradigm of accelerated materials discovery, namely from one that involves the generation of, and searching among, massive chemical libraries via high throughput computation and/or experiments, to one of targeted materials discovery based on discovering the best pathways for that and for future discoveries. This will be accomplished by applying a combination of mathematical tools that include the analysis of the structure of high dimensional data through the tools of topological data analysis and a unique probabilistic framework for linking uncertainty in high dimensional data and information. We explore the different approaches that such data analytics offers to gain further insight into multiscale materials physics.

Krishna Rajan
University at Buffalo, The State University of New York
krajan3@buffalo.edu

MS30

Statistical Learning for Small Data Materials Challenges: Solid Lithium-ion Conductors for Batteries

Many problems in material science are accompanied by relatively small data sets that pose challenges for statistical approaches. Collecting significantly more data is frequently not feasible. I will discuss our efforts to augment small data sets with approximate physics-based models to perform holistic computational structure screening of >12,000 lithium-ion battery materials. We double the number of

known solid materials that exhibit high Li conductivity at room T by developing a novel large-scale computational approach for identifying solid state electrolytes that is capable of screening all known Li containing solids. To be useful for batteries, high performance solid state electrolytes must satisfy many requirements at once, an optimization that is difficult to perform experimentally or with ab-initio techniques. We first screen 12,831 Li containing crystalline solids for those with high structural and chemical stability, low electronic conductivity, and low cost. We then develop a data-driven ionic conductivity classification model for identifying which candidate structures are likely to exhibit fast lithium conduction based on experimental measurements. The screening reduces the list of candidate materials from 12,831 down to 21 structures that show promise as electrolytes and are 3 times more likely to be good ion conductors than randomly chosen structures. I will discuss our approach to feature selection and careful model validation for small data.

Austin Sendek, Ekin Cubuk, Qian Yang, Yi Cui,
Evan Reed
Stanford University
-, -, -, -, evanreed@stanford.edu

MS31

On the Edge Energy of Graphene

Surface/edge energy is typically modeled as a continuous function of orientation, $\gamma(\mathbf{n})$. We put forward a simple geometric argument that suggests this picture is inadequate for crystals with a non-Bravais lattice structure. In the case of the idealized graphene/hexagonal lattice, our arguments indicate that the edge energy can be viewed as both discontinuous and multi-valued for a subset of orientations that are commensurate with the crystal structure.

Tim Krumwiede
Brigham Young University
timwiede@gmail.com

Tim Schulze
University of Tennessee, USA
shulze@math.utk.edu.

MS31

Growth and Dissolution of Confined Crystals

Confinement constraints growth in many natural environments. In biomineralization, confinement is known to play a key role to control the shape and phase of nano-crystals that constitute, e.g. skeletons or dentine. This is also relevant for geology and building materials where crystals growing in confinement within pores and cracks can influence the forces exerted by these crystals on rocks during growth. Finally, confinement is also relevant for technological applications such as nanomotors where crystal growth is used to produce motion or forces. We have developed a thin film model describing the dynamics of growth or dissolution at a crystal interface, including diffusion, hydrodynamics, and interface kinetics. In collaboration with experiments at the Univ. of Oslo, we have shown that when a growing crystal is placed in the vicinity of a wall, a cavity forms in the crystal within the contact region. The cavity then usually expands and gives rise to growth rims. Using our thin film model, we show that at the nanoscale, this transition becomes discontinuous due to van der Waals interactions, or can disappear due to hydrodynamics. We also consider the opposite problem of pressure solution, where an interface dissolves due to a load exerted on the crystal. We show that the crystal interface can be flat or pointy depending on the type of interactions. In addition, we find that touching contact is never reached in steady-state.

Olivier Pierre-Louis
CNRS / Université C. Bernard Lyon 1
olivier.pierre-louis@univ-lyon1.fr

Luca Gagliardi
UCBL Lyon 1
luca.gagliardi@ens-lyon.fr

MS31

Crystals and Liquid Crystals on Curved Surfaces

We consider crystalline and liquid crystalline materials on surfaces, derive the corresponding scalar-, vector- and tensor-valued surface partial differential equations by means of a thin-film limit, discuss numerical approaches and demonstrate the delicate interplay between topology, geometry and positional and orientational defects.

Axel Voigt
TU Dresden
axel.voigt@tu-dresden.de

MS31

Chiral Morphometrics of Faceting Crystal Interfaces

The morphology of chiral nano-faceted interfaces that emerge from the spinodal decomposition of thermodynamically unstable interface of a crystal is controlled by the interface's initial orientation, the orientation of the emerging stable facets and the relative edge-energies between them. We introduce a novel chiral surface energy, and an associated computational framework, to explore the morphometric landscape associated with these control parameters. We present a complete theoretically characterisation of the emergent facet dynamics, and present empirical data exhibiting dynamic scaling regimes, as well as novel two-scale terrace-step morphologies that go beyond the dynamic scaling hypothesis.

Stephen Watson
Department of Mathematics, University of Glasgow
Stephen.Watson@glasgow.ac.uk

MS32

Dimension Reduction for the Landau-de Gennes Model: the Vanishing Nematic Correlation Length Limit

We present results regarding nematic liquid crystalline films within the framework of the Landau-de Gennes theory in the limit when both the thickness of the film and the nematic correlation length are vanishingly small compared to the lateral extent of the film. We discuss a Gamma-convergence result for a sequence of singularly perturbed functionals with a potential vanishing on a high-dimensional set and a Dirichlet condition imposed on admissible functions. In addition, we demonstrate the existence of local minimizers of the Landau-de Gennes energy, in the spirit of a theorem due to Kohn and Sternberg, despite the lack of compactness arising from the high-dimensional structure of the wells. The limiting energy

consists of leading order perimeter terms, similar to Allen-Cahn models, and lower order terms arising from vortex structures reminiscent of Ginzburg-Landau models.

Michael Novack
Indiana University
mrnovack@indiana.edu

MS32

Regularity of the Eikonal Equation with Two Vanishing Entropies

We study regularity of solutions to the Eikonal equation $|\nabla u| = 1$ a.e. in a bounded simply-connected two dimensional domain. Solutions to this equation have very little regularity in general. However, with the help of two vanishing entropies, we are able to obtain strong regularity results for solutions of the Eikonal equation. The motivation of our problem comes from a classical problem in Calculus of Variations, called the Aviles-Giga functional in connection with the theory of smectic liquid crystals and thin film blisters. Our result for the first time uses only two entropies to characterize regularity properties in this direction.

Andrew Lorent
Department of Mathematical Sciences
University of Cincinnati
lorentaw@ucmail.uc.edu

Guanying Peng
Department of Mathematics
The University of Arizona
gypeng@math.arizona.edu

MS32

Nematic Liquid Crystal Structures in Slabs

We examine minimizers for the Landau - de Gennes energy in a slab
$\Omega \times (-\delta, \delta)$ where the cross section Ω is a bounded simply connected domain in $\mathbf{R}^2$. The minimizers are to satisfy tangential boundary conditions on the top and bottom faces and prescribed boundary conditions on the lateral surface. The defect structures, textures and estimates on the energies of minimizers are determined. In particular it is shown how these features depend on the relative size of the Landau - de Gennes order parameter ε and the slab thickness δ.

Daniel Phillips
Department of Mathematics, Purdue University
phillips@purdue.edu

Patrica Bauman
Purdue University
bauman@math.purdue.edu

MS32

A Finite Element Method for the Generalized Ericksen Model of Liquid Crystals

We consider the generalized Ericksen model of liquid crystals, which is an energy with 8 independent "elastic' constants that depends on two order parameters $\mathbf{n}$ (director) and s (variable degree of orientation). In addition, we present a new finite element discretization for this energy, that can handle the degenerate elliptic part without regularization, with the following properties: it is stable and it Γ-converges to the continuous energy. Moreover, it does not require the mesh to be weakly acute (which was an important assumption in our previous work). A minimization scheme for computing discrete minimizers will also be discussed. Furthermore, we include other effects such as weak anchoring (normal and tangential), as well as fully coupled electro-statics with flexo-electric and order-electric effects. We also present several simulations (in 2-D and 3-D) illustrating the effects of the different elastic constants and electric field parameters.

Shawn W. Walker
Louisiana State University
Department of Mathematics and CCT
walker@math.lsu.edu

MS33

The Effect of Rate-Dependence on Necking Localization: Analysis Based on One-Dimensional Model

We derive a one-dimensional model describing localization in a cylindrical bar made of a visco-plastic material. The model is obtained by dimension reduction using a two-scale expansion, starting from the 3D constitutive equations that are used to charaterize metals undergoing hot forming. Our model captures the influence of both the rate-dependence and of the second gradient of the mean axial displacement, and it is consistent with previous works addressing each of these effects separately. Numerical simulations of the one-diemensional model provides the evolving shape of the neck, and reveals that rate-dependence can result in a significant necking retardation.

Basile Audoly
Moore Distinguished Scholar
baudoly@gmail.com

John Hutchinson
Harvard School of Engineering
jhutchin@fas.harvard.edu

MS33

Capillarity-induced Folding of Wrinkled Skin

We investigate what happens when a liquid droplet is placed on a wrinkled surface that is obtained via the wrinkling instability of compressed stiff skin on a soft substrate. Two different scenarios were observed. Liquid remains in a droplet when the contact angle between the liquid and the skin is larger than some critical angle, which depends on the aspect ratio of wrinkles, i.e. the ratio between the height amplitude and the wavelength of wrinkles. However, if the contact angle is smaller than the critical angle, then the liquid from droplet starts entering wrinkled channels. Interestingly, we observed that liquid didn't enter all wrinkled channels, but it formed periodically spaced liquid filaments, when both the contact angle and the critical angle were small. This is because at the onset of the wrinkling instability, system is extremely sensitive to additional surface forces. Once the first liquid filament is formed, capillary forces from the liquid squeeze that wrinkle to a tight fold and they also flatten neighboring wrinkles. The reduced aspect ratio of neighboring wrinkles decreases the critical angle and prevents formation of new liquid filaments in nearby wrinkles. The next liquid filament can thus form only some distance away, where the flattening effect is diminished. Finally, we exploited this effect for the fabrication of periodic array of DNA nanowires by us-

ing the liquid solution with DNA molecules.

Andrej Kosmrlj
Princeton University
andrej@princeton.edu

So Nagashima
Osaka University
so.nagashima@ams.eng.osaka-u.ac.jp

Howard Stone
Princeton University
hastone@princeton.edu

Myoung-Woon Moon
Korea Institute of Science and Technology
mwmoon@kist.re.kr

MS33

Dynamics of Confined Membranes

MS Thin Structures: Defects, Pattern and Bifurcation ORAL Lipid membranes are the main ingredient of cell walls, and stacks of lipid membranes play an important role as protective coatings in biolubrication systems, and in the stratum corneum. Usually these biological systems are crowded, and membranes are confined between other membranes, or between other biological substrates. We discuss the role of confinement within a lubrication model for an inextensible membrane between two attractive walls. This simple model inspired by cell membrane adhesion [O. T. Fackler et al, J. Cell Biol.(2008);R. Bruinsma, et al, PRE (2000); M. Asfaw, et al, EPL(2006); K. Sengupta et al, PRL(2010)], gives rise to dynamics controlled by a nonlocal tension. We find three dynamical regimes which depend on the available membrane area. Small area membranes form finite-size flat and frozen adhesion domains. Large area membranes form a dense labyrinthine wrinkle phase, which also freezes. However, for intermediate membrane areas, we find coarsening with a coexistence of adhesion domains and wrinkles. For small and intermediate membrane area, the nonlocal tension tends spontaneously to one of the two special values corresponding to the linear and nonlinear instability thresholds of flat fronts in the Swift-Hohenberg equation. We show that adhesion domain boundaries exhibit motion by curvature with oscillatory interactions and a time-dependent prefactor controlled by the nonlocal tension.

Olivier Pierre-Louis
CNRS / Université C. Bernard Lyon 1
olivier.pierre-louis@univ-lyon1.fr

MS33

Phase-Field Models and Connectedness

We propose a phase-field approach to the problem of minimising the Willmore energy in the class of connected surfaces with prescribed area which are confined to a small container based on De Giorgi's diffuse Willmore functional. Our main contribution is a penalization term which ensures connectedness in the sharp interface limit. The penalization of disconnectedness is based on a geodesic distance chosen to be small between two points that lie on the same connected component of the transition layer of the phase field. Along the way we obtain improved convergence properties for the phase fields. We present numerical evidence of the effectiveness of our method in three dimensions.

Stephan Wojtowytsch
Carnegie Mellon University
swojtowy@andrew.cmu.edu

MS34

Minimizing Patterns for a Nonlocal Isoperimetric Problem with Confinement

We consider a variant of Gamow's liquid drop model, with a general repulsive Riesz kernel and a long-range attractive background potential with weight Z. The addition of the background potential acts as a regularization for the liquid drop model in that it restores the existence of minimizers for arbitrary mass. We consider the regime of small Z and characterize the structure of minimizers in the limit $Z \to 0$ by means of a sharp asymptotic expansion of the energy. In the process of studying this limit we characterize all minimizing sequences for the Gamow model in terms of "generalized minimizers'.

Stan Alama, Lia Bronsard
McMaster University
Department of Mathematics and Statistics
alama@mcmaster.ca, bronsard@mcmaster.ca

Rustum Choksi
Department of Mathematics
McGill University
rchoksi@math.mcgill.ca

Ihsan Topaloglu
Department of Mathematics and Applied Mathematics
Virginia Commonwealth University
iatopaloglu@vcu.edu

MS34

Discrete-to-Continuum Modeling of Supported Graphene and Lattice Mismatch

Recently, a rich collection of moire patterns has been observed in graphene deposited over flat crystalline substrates. The primary source of these patterns is the lattice constant mismatch between graphene and the substrate. I will discuss a model for the formation of these patterns and related networks of wrinkles in supported graphene and other 2D materials. The Ginzburg-Landau-type model is based on a formal discrete-to-continuum procedure that, in particular, provides a continuum description of registry effects due to the atomistic van der Waals interactions. I will also present numerical results by which we qualitatively compare predictions of our models to discrete simulations.

Dmitry Golovaty
The University of Akron
Department of Mathematics
dmitry@uakron.edu

MS34

A Game-theoretical Interpretation of the Robin Boundary Conditions

In this talk, we will discuss a stochastic process whose value coincides with the solution to the classical Poisson's equation under the Robin boundary condition. Although the related variational problem is convex and lo-

cal, the method allows for the extensions to more complex convection-diffusion problems.

Marta Lewicka
Department of Mathematics
University of Pittsburgh
lewicka@pitt.edu

MS34

On Defects in Nematic-Isotropic Phase Boundaries

We study a 2D toy model to understand defects along nematic-isotropic phase boundaries in liquid crystals. This is joint work with Dmitry Golovaty, Mike Novack and Peter Sternberg.

Raghav Venkatraman
Indiana University, USA
rvenkatr@umail.iu.edu

Peter Sternberg
Indiana University
Department of Mathematics
sternber@indiana.edu

Dmitry Golovaty
The University of Akron
Department of Mathematics
dmitry@uakron.edu

Michael Novack
Indiana University
mrnovack@indiana.edu

MS35

Incommensurability in 2D Multilayer Materials: Non-Commutative Geometry to the Rescue of Numerical Computation

The recent discovery of a whole family of two-dimensional crystalline materials such as graphene, hexagonal boron nitride (h-BN) and many others leads to study the properties of their combinations, particularly by stacking a number of layers vertically. Such structures are generally non-periodic, with interesting geometric properties such as moir effects. I will first recall the usual description for electronic structure and conduction phenomena in periodic as well as disordered systems, using quantum models of tight-binding type. I will show how a unified framework, formulated by Bellissard et al. in the context of noncommutative geometry to model disordered systems, extends to non-periodic systems with multiple layers and allows to write an explicit formula for their macroscopic electrical conductivity. This abstract framework surprisingly leads to a new type of numerical scheme going beyond traditional methods.

Paul Cazeaux
Department of Mathematics
University of Kansas
pcazeaux@ku.edu

Eric Cances
Ecole des Ponts and INRIA, France
cances@cermics.enpc.fr

Mitchell Luskin
School of Mathematics
University of Minnesota
luskin@umn.edu

MS35

Discrete-to-Continuum Modeling of Weakly Interacting Incommensurate Chains

In this talk, we present a formal discrete-to-continuum procedure to derive a continuum variational model for two chains of atoms with slightly incommensurate lattices. The chains represent a cross-section of a three-dimensional system consisting of a graphene sheet suspended over a substrate. The continuum model recovers both qualitatively and quantitatively the behavior observed in the corresponding discrete model. We show that numerical solutions for both models demonstrate the presence of large commensurate regions separated by localized incommensurate domain walls.

Malena I. Espanol
Department of Mathematics
The University of Akron
mespanol@uakron.edu

Dmitry Golovaty
The University of Akron
Department of Mathematics
dmitry@uakron.edu

Patrick Wilber
University of Akron
jw50@uakron.edu

MS35

Relaxation of Incommensurate 2D Layers in Configuration Space

2D layers are vertical stacks of a few crystalline monolayers which are typically incommensurate because of the rotation of one layer with respect to another or because of incommensurate lattice parameters. Due to the weak van der Waals nature of the interactions between layers, each layer essentially keeps the crystalline structure it possesses as an isolated monolayer. The resulting assembly is in general an aperiodic system with long-range order, creating large scale Moiré patterns. In this case, an ordered, locally collective relaxation motion of atoms takes place as the layers maximize the area of energetically favorable stacking. We present a systematic model of the relaxation of such heterostructures by a rigorous depiction and parameterization of the particular geometry of unrelaxed ideal multilayered structures, which will serve as a reference configuration in the elastic modeling of the relaxation phenomenon. Previous approaches approximate incommensurate structures by periodic structures (supercells) and compute the relaxation in real space. Our approach directly models the incommensurate structure by computing the relaxation in configuration space, thus permitting the more accurate and efficient computation of larger scale relaxation patterns than possible by real space methods.

Mitchell Luskin
School of Mathematics
University of Minnesota
luskin@math.umn.edu

Paul Cazeaux
Department of Mathematics
University of Kansas
pcazeaux@ku.edu

Daniel Massatt
University of Minnesota
massa067@umn.edu

MS36

Viruses and Geometry: New Insights into Virus Structure, Assembly, Evolution and Therapy

Viruses are remarkable examples of order at the nanoscale. The capsids of many viruses, enclosing and protecting their genomes, are organised in lattice-like arrangements with overall icosahedral symmetry. Mathematical techniques from group, graph and tiling theory can therefore be used to characterise their architectures. In this talk, I will introduce our mathematical approach to the modelling of viral capsids, and demonstrate its applications to the modelling of virus assembly. In particular, I will present our Hamiltonian path approach to the modelling of genome packing in RNA viruses that underpins the discovery of an RNA-encoded assembly instruction manual in a wide range of viruses, including Picornaviruses, Hepatitis C and Hepatitis B virus. I will then demonstrate how these models can be used to develop a new approach to vaccine design and define implicit fitness functions that shed new light on viral evolution and anti-viral drug therapy.

Reidun Twarock
Departments of Mathematics and Biology
University of York
rt507@york.ac.uk

Richard Bingham
University of York
r.j.bingham@york.ac.uk

MS36

Modeling Aggregation Processes of Lennard-Jones Particles Via Stochastic Networks

I will discuss modeling an isothermal aggregation process of atoms interacting according to the Lennard-Jones pair potential by mapping the energy landscapes of each cluster size N onto stochastic networks and connecting these networks into a single joint network. The parameters of the system are the attachment rate and the temperature. The resulting network is analyzed and the most persistent atomic configurations for each cluster size are determined.

Maria K. Cameron
University of Maryland
cameron@math.umd.edu

MS36

Robust Nonequilibrium Pathways to Microcompartment Assembly

Bacterial microcompartments, organelle-like, proteinaceous structures found in photosynthetic bacteria, assemble to encapsulate enzymes crucial for carbon fixation. Geometric similarities between microcompartment shells and viral capsids have inspired models of the assembly process that posit that the microcompartment represents a stable, equilibrium arrangement of its constituent proteins. This assumption does not hold, however, for shells that lack intrinsic curvature. I will discuss a microscopic model of the assembly process that is fundamentally nonequilibrium but, nevertheless, can robustly and reliably produce microcompartment structures. The essence of the dynamics of this process can be understood from a minimal mathematical model that resolves the kinetics of the protein shell and its fluctuating, internal cargo. These results highlight experimentally controllable parameters for modulating the size and shape of bacterial microcompartments in the lab.

Grant Rotskoff
Courant Institute of Mathematical Sciences
New York University
rotskoff@cims.nyu.edu

MS36

Calculating the Symmetry Number of Flexible Sphere Clusters

In this talk I will present a theoretical and computational framework to compute the symmetry number of a flexible sphere cluster in $\mathbb{R}^3$. I will define the topological group of the cluster and analyze its properties, and introduce a numerical algorithm to efficiently compute its elements. This is a joint work with Miranda Holmes-Cerfon.

Emilio Zappa
Courant Institute of Mathematical Sciences
New York University
ez21@nyu.edu

MS37

Mathematics of Grain Growth: Microstructure Evolution with Experimentally-Derived Interface Properties

Predicting exactly how microstructures evolve during thermal annealing is one of the longstanding problems in materials science. While it is known how the average grain size will change with annealing, very little is known about the evolution of the grain boundary character distribution, the texture, and the grain shape. In collaboration with experimentalists, we aim to develop quantitative models of microstructure evolution with a particular focus on accounting appropriately for anisotropy. Joint with Gregory Rohrer (CMU) and Robert Suter (CMU).

Kaushik Dayal
Carnegie Mellon University
Kaushik.Dayal@gmail.com

MS37

Solving Nanostructure Inverse Problems via Data Mining

We will present some recent work on reformulations of nanostructure inverse problems (NIPs) with noisy and insufficient observation data (such as the atomic pair distribution function obtained from x-ray scattering) using various data mining techniques.

Qiang Du
Columbia University
Department of Applied Physics and Applied Mathematics
qd2125@columbia.edu

Ran Gu
Columbia University
rg3142@columbia.edu

Simon Billinge

Columbia University and Brookhaven National Laboratory
sb2896@columbia.edu

MS37

An Overview of the NSF DMREF Program and Conversation with NSF Program Officers

The interdisciplinary NSF program "Designing Materials to Revolutionize and Engineer our Future" (DMREF) is the primary program by which NSF participates in the national "Materials Genome Initiative." The DMREF program involves ten different NSF divisions, including the Division of Mathematical Sciences (DMS), and is led by the Division of Materials Research (DMR). We will discuss some aspects of this program, including its features and emphases, how it is managed at NSF, the review process for submitted proposals, and some data on awards. The presentation will conclude with a question-and-answer period with NSF Program Officers in attendance from DMS, DMR, and the Division of Civil, Mechanical, and Manufacturing Innovation (CMMI).

Eugene C. Gartland, Jr.
Kent State University
gartland@math.kent.edu

MS37

Origins of Hysteresis in Phase Transformations and Magnetism

Owing to the development of a quantitative mathematical theory of hysteresis, transforming materials with record low hysteresis are now being synthesized worldwide. We present a brief review of the state-of-the art, and then turn attention to magnetic materials. Are the same ideas used in phase transformations applicable to magnetic hysteresis? The answer is no, but the way of thinking is promising. Clearly, magnetostriction, often neglected, is important. Linear stability analysis of the single domain state on the shoulder of the hysteresis loop is misleading. Recent work on the origins of soft magnetism in permalloy suggests a way forward.

Richard James
Department of Aerospace Engineering and Mechanics
University of Minnesota
james@umn.edu

MS38

Title Not Available At Time Of Publication

The rheology of active suspensions is critical to understanding biological systems composed of many swimmers in complex media, including mammalian fertility and biofuel production. Shear viscosity of active suspensions in Newtonian media has been studied experimentally and numerically, suggesting a decrease in bulk viscosity at large volume fractions of swimmers. However, rheological measurements of active suspensions are complicated by several facets. First, they are typically low viscosity suspensions ill-suited for measurement in commercially-available rheometers due to minimum torque limitations at small Peclet number, where advection does not dominate the local motion of swimmers. Second, active suspensions are not amenable to traditional passive microrheology techniques due to the fact they are inherently out of equilibirum. Finally, techniques which overcome these first two hurdles, such as highly sensitive steady shear viscosity measurements in Couette cell geometries, are unable to fully describe the non-Newtonian behavior of active suspensions. To overcome these technical challenges, we have developed a simple microfluidic rheometer, which applies an oscillating pressure gradient as low as O(1) Pa in a microfluidic channel. We then use fluorescent microscopy and particle tracking techniques to measure the instantaneous strain and strain rate in the fluid, allowing us to compute the storage and loss moduli of our active suspensions with high precision.

Paulo E. Arratia
Mechanical Engineering and Applied Mechanics
University of Pennsylvania, Philadelphia.
parratia@seas.upenn.edu

David Ganon, Sebastien Acharige, Brendan Blackwell
University of Pennsylvania
david.gagnon@georgetown.edu, akosgo@seas.upenn.edu, bcb@seas.upenn.edu

MS38

(Active) Particles in Complex Fluids

There is a rich history in the literature on the effects of particles in Newtonian flows but when the suspending fluid is also complex, as it is in many applications from down-hole scenarios in the oilfield to cells in the human body, the rheology of these suspensions is far less understood. Particles can interact with nonlinear non-Newtonian stresses in these complex suspensions to significantly alter flows, for example, particles suspended in a Newtonian fluid will increase the apparent viscosity of the fluid due to the additional dissipation caused by the disruption of streamlines; however, if instead the suspending fluid is shear-thinning, the higher strain-rates induced by the particles will also produce a competing apparent reduction of the viscosity. We discuss here a recently derived an exact analytical expression for how these effects combine for a dilute suspension of particles in a weakly shear-thinning fluid and other interesting suspension dynamics in shear-thinning fluids. Furthermore, the motion of 'active' particles in fluids has received considerable attention, with interest ranging from phoretic propulsion to biological locomotion, but studies on active bodies immersed in complex fluids are relatively scarce. In this talk we present theory for active particles in a complex fluids, and then discuss the effects of viscoelasticity and shear-thinning rheology in the context of biological locomotion and the propulsion of colloidal Janus particles.

Gwynn Elfring
University of British Columbia
gelfring@mech.ubc.ca

MS38

A Rigorous Error Analysis Framework for Slender Body Theory

Slender body theory facilitates computational simulations of thin fibers immersed in a viscous fluid by approximating each fiber as a one-dimensional curve of point forces. We develop a PDE framework for analyzing the error introduced by approximating a truly three-dimensional object in Stokes flow by a one-dimensional curve. In particular, given a 1D force specified along the fiber centerline, we define a notion of 'true' solution to the full 3D slender body problem and obtain an error estimate for the slender body

approximation in terms of the fiber radius.

Laurel Ohm
University of Minnesota
ohmxx039@umn.edu

Yoichiro Mori
School of Mathematics
University of Minnesota
ymori@umn.edu

Daniel Spirn
University of Minnesota
spirn@umn.edu

MS38

Mesoscale Modeling and Simulation of Transiently Networked Fluids

Complex Fluids can be modeled and studiedat either the macroscopic or mesoscopic level. In order to understand the effects of the embedded elements in the fluids, which are responsible for the non-Newtonian responses, for example inhomogeneities in simple shear or non-exponential relaxation, mesoscopic modeling using stochastic differential equations has the advantage over macroscopic modeling of capturing the local properties of the embedded structure elements and their effects onthe macroscopic behavior of theflow. In this talk stochastic mesoscale models of transiently networked fluids are presented in which the network elements are modeled as connectedbead-spring dumbbells. The topology of this mesoscale network is tracked in the simulation, that is the location and the connections of each element are tracked at any given time. Simulation results describing both transient and steady state predictions are presented. Networks with varying numbers of allowed connected elements (at each junction) are investigated as well as networks with varying energy functions governing the attachment/detachment kinetics. The eventual goal of the work is to offer a better understanding of transiently networked systems such as telechelic polymer solutions or mucins.

Lin Zhou
Mathematics Department, New York City College of Techonology
Brooklyn, NY 11201, USA
lzhou@citytech.cuny.edu

L. Pamela Cook
University of Delaware
Department of Mathematical Sciences
cook@udel.edu

MS39

Temperature and Driving Force Dependence of Grain Boundary Dynamics

Grain boundary (GB) migration is controlled by the motion of line defects/disconnections. For any GB misorientation, crystallography determines the set of possible disconnection Burgers vectors and step heights. GB dynamics depend on which or which combination of these sets operate. After introducing the link between dynamics and disconnections, we present a theoretical approach to understanding why different driving forces lead to different GB dynamics. Based upon a disconnection nucleation model, we extend these ideas to predict GB dynamics as functions of both temperature and driving force and compare these predictions with molecular dynamics results. We demonstrate that GB dynamics are well described by an Onsager formalism and present analytical results for a few simple cases. Next, we apply this approach within a kinetic Monte Carlo formalism.

David J. Srolovitz, Jian Han, Kongtao Chen, Spencer Thomas
University of Pennsylvania
srol@seas.upenn.edu, jianhan@seas.upenn.edu, kongtao@seas.upenn.edu, thospe@seas.upenn.edu

MS39

Continuum Models of Grain Boundary Motion with Atomistic Stress Coupling

I was fortunate to know and work with John Cahn for over 40 years. One such interaction resulted in our introducing and developing a continuum model for coupling of grain boundary motion to relative tangential grain motion (Cahn & Taylor, A unified approach to motion of grain boundaries, relative tangential translation along grain boundaries, and grain rotation, Acta Mat. 2004), perhaps combined with sliding and surface diffusion along the interface (Taylor & Cahn, Shape accommodation of a rotating embedded crystal via a new variational formulation, Interfaces and Free Boundaries, 2007). The variational method that we developed in order to include various effects is quite general and will be presented. We began by trying to understand a 3D molecular dynamics simulation by Srini Srinivasan, of one cylindrical grain embedded inside another grain. This grain was observed to rotate as it shrank (decreasing its interfacial free energy), but it rotated to increase the initially small misorientation. Later simulations by others, especially Yuri Mishin and colleagues, greatly increased our understanding of the phenomenon. Simulations by David Srolovitz and others have demonstrated not only that there is almost always a tangential stress when an interface moves by one crystal growing into another, especially in the presence of triple junctions, but also that discrete line defects in the interiors of the crystals are often created.

Jean Taylor
New York University
CIMS
jtaylor@cims.nyu.edu

MS39

Motion of Grain Boundaries Based on Disconnections

Disconnection is a type of line defects in the Grain boundary (GB) interface that can be characterized by both a Burgers vector and step height. The motion of the set of disconnections along the GB controls the GB migration. We present a continuum model in two dimensions to describe motion of high angle GBs based on the underlying disconnections structure and mechanism. In this model, GB migration may be driven by stresses, GB energy difference within the material, as well as the surface tension along the interface. We firstly apply this model to the simulations of bicrystalline structures to understand the motion of a single GB under different types of boundary conditions. Then we apply this model to polycrystalline structures where the motion of the triple junctions is discussed.

Chaozhen Wei

State University of New York at Buffalo
iasczwei@ust.hk

Luchan Zhang
National University of Singapore
matzlu@nus.edu.sg

Jian Han, Spencer Thomas
University of Pennsylvania
jianhan@seas.upenn.edu, thospe@seas.upenn.edu

Yang Xiang
Hong Kong University of Science and Technology
maxiang@ust.hk

David J. Srolovitz
University of Pennsylvania
srol@seas.upenn.edu

MS39

Motion of Grain Boundaries Incorporating Dislocation Structure

We present a continuum model for the dynamics of low angle grain boundaries in two dimensions incorporating both the motion of grain boundaries and the dislocation structure evolution on the grain boundaries. This model is derived from the discrete dislocation dynamics model. The long-range elastic interaction between dislocations is included in the continuum model, which ensures that the dislocation structure on a grain boundary is consistent with the Frank's formula. These evolutions of the grain boundary and its dislocation structure are able to describe both normal motion and tangential translation of the grain boundary and grain rotation due to both coupling and sliding. Since the continuum model is based upon dislocation structure, it naturally accounts for the grain boundary shape change during the motion and rotation of the grain boundary by motion and reaction of the constituent dislocations. Using the derived continuum grain boundary dynamic model, simulations are performed for the dynamics of circular and non-circular two dimensional grain boundaries, and the results are validated by discrete dislocation dynamics simulations.

Luchan Zhang
National University of Singapore
matzlu@nus.edu.sg

Yang Xiang
Hong Kong University of Science and Technology
maxiang@ust.hk

MS40

Estimates of Microscale Features from Macroscale Measurements

Surrogates based on polynomial chaos, collocation, and reduced order models have been used successfully to solve a broad range of forward stochastic problems. These methods have been extended to solve stochastic inverse problems. Generally, the Bayesian framework is used for solution, the operator defining the input/output relation is deterministic, measurements are polluted by random noise, and source parameters are unknown. We focus on inverse problems in which the operator is stochastic and partially known since, *e.g.*, the random fields characterizing a material microstructure are known up to some parameters. Moreover, some of the unknown parameters of the random fields in the definition of these operators are not observable. Our objective is to identify the unobservable microscale parameters from macroscale measurements. We illustrate the approach by a simple one-dimensional stochastic transport equation in which the conductivity random field is known up to its spatial correlation and a more realistic example dealing with a polycrystalline microstructure.

John M. Emery
Sandia National Laboratories
jmemery@sandia.gov

Mircea Grigoriu
Cornell University
mdg12@cornell.edu

MS40

Modeling Material Variability with Uncertainty Quantification and Machine Learning Techniques

Material variability originating from heterogeneous microstructural features can have significant effects on behavior and creates uncertainty around performance. Engineering models typically do not incorporate microstructural variability explicitly, rather functional forms are chosen based on intuition and parameters are selected to reflect mean behavior. Conversely, mesoscale models that capture the microstructural physics, are impractical to utilize at the engineering scale. To address the challenge of designing with variable materials, we have developed a method based on the uncertainty formulation of Sargsyan, Najm, and Ghanem (2015) to calibrate distributions of material parameters from high-throughput experimental data. With this method, material variability is directly associated with commonly-used material parameters using a chosen nominal model. One of the benefits of this approach is that expert knowledge can be extended to interpret the effect of (hidden) microstructure on variable mechanical response. In a complementary effort, we are developing machine learning techniques to handle the large volume of data from high-throughput methods. Here we adapt common machine learning models, such as neural networks, to obey the same exact properties and symmetries as traditional constitutive models while representing features in the data in a flexible, bias-less manner.

Reese Jones
Co-author
rjones@sandia.gov

Coleman Alleman, Mohammad Khalil, Ari Frankel, Francesco Rizzi, Jeremy Templeton, Jakob Ostien
Sandia National Laboratories
callema@sandia.gov, mkhalil@sandia.gov, alfrank@sandia.gov, fnrizzi@sandia.gov, jatempl@sandia.gov, jtostie@sandia.gov

MS40

Active Learning of Constitutive Relations from Mesoscopic Dynamics for Macroscopic Modeling of Soft Matter

We simulate complex fluids by means of an on-the-fly coupling of the bulk rheology to the underlying microstructure dynamics. In particular, a macroscopic continuum model of polymeric fluids is constructed without a pre-specified constitutive relation, but instead it is actively learned from mesoscopic simulations where the dynamics of polymer

chains is explicitly computed. To couple the macroscopic rheology of polymeric fluids and the microscale dynamics of polymer chains, the continuum approach (based on the finite volume method) provides the transient flow field as inputs for the (mesoscopic) dissipative particle dynamics (DPD), and in turn DPD returns an effective constitutive relation to close the continuum equations. In this multiscale modeling procedure, we employ an active learning strategy based on Gaussian process regression (GPR) to minimize the number of expensive DPD simulations, where adaptively selected DPD simulations are performed only as necessary. Compared to traditional multiscale approaches, applying an active learning scheme to multiscale modeling of non-Newtonian fluids can significantly increase the computational efficiency. Although the method demonstrated here obtains only a local viscosity from the mesoscopic model, it can be extended to other multiscale models of complex fluids whose macro-rheology is unknown.

Zhen Li
Division of Applied Mathematics
Brown University
Zhen_Li@brown.edu

George Em Karniadakis
Brown University
george_karniadakis@brown.edu

MS40

Fostering Machine Learning Through Coordination Descriptors, Site Fingerprints, and Structure Similarity Measures

Structure characterization and classification is often based on coordination information from the crystal structure [Zimmermann et al. Front. Mater. 4, 34, 2017]. Therefore, reliable and robust procedures to evaluate the coordination patterns are important for machine learning. We present new local structure order parameters that are specifically designed to rapidly detect rotationally invariant and asymmetric environments. We apply the new local environment descriptors to define site fingerprints and measure similarity between structures. We use the new tools then as proxy variables for hydrothermal stability of zeolites [Zimmermann and Haranczyk, Cryst. Growth Des. 16, 3043, 2016] and to identify similar structures in a large materials database. We have computed all 2.45 billion structure similarity distances between each pair of the $\approx$ 70,000 materials that are currently present in the Materials Project database and integrated the data into the openly accessible Materials Project website.

Nils Zimmermann, Anubhav Jain
Lawrence Berkeley National Laboratory
nerz@lbl.gov, ajain@lbl.gov

MS41

Modeling of Non-Equilibrium Nanocluster Growth Shapes in Surface Systems

Self-assembly of metallic nanoclusters or islands during deposition on surfaces often leads to non-equilibrium shapes as relaxation processes for aggregated atoms incorporated in the clusters are limited on the time scale of nanocluster growth [Surf. Sci. Rep. 61 (2006) 1]. For traditional island formation on top of surfaces, extensive analysis and elucidation of this behavior is available. Shapes depend on the details of periphery diffusion (e.g., not just along straight step edges, but also around kinks or corners for 2D clusters). This behavior can be captured precisely by atomistic models, where recent developments enable ab-initio level description of both system thermodynamics and periphery diffusion kinetics [J. Phys. Chem. C 120 (2016) 21617]. We note that it is still challenging for coarse-grained continuum modeling to capture these details. However, this talk will also consider recent studies of unconventional island formation in the gallery below the top surface of layered materials. Access to the gallery is provided by isolated defect portals in the top layer. A theory for the nucleation and growth of such islands has been developed determining, e.g., the typical distance from the portals for nucleation, and island growth shapes [Phys. Rev. Materials 1 (2017) 053403]. For some systems of interest, non-equilibrium island growth reflects the directional nature of the flux aggregating atoms which primarily originates at a nearby portal.

Jim Evans
Ames Laboratory USDOE and Iowa State University
evans@ameslab.gov

Ann Lii-Rosales, Patricia Thiel
Iowa State University
ylii@iastate.edu, thiel@ameslab.gov

Yong Han
IOwa State University
yhan.ameslab@gmail.com

MS41

Analytical Aspects of Slope Selection in Epitaxial Mound Growth

Slope selection in homoepitaxial growth of mounds is modeled using a BCF-type model for step motion, incorporating the Ehrlich-Schwoebel (ES) barrier, deposition, downward funneling, and step creation/annihilation. A perturbative technique is used to analytically determine the long-term behavior of the model for large ES barriers. Implications for a rigorous continuum limit of the step model are considered.

Ian Johnson, Dionisios Margetis
University of Maryland, College Park
ijohnso6@umd.edu, dio@math.umd.edu

MS41

A Level Set Method for Mound Formation and Slope Selection

In this talk we will discuss a level set method for thin film growth and its application to the formation and growth of mounds. In particular, we will discuss our numerical implementation for a step edge barrier (that leads to mound formation), and competing mechanisms for downward transport, such as downward funneling and transient mobility. We will compare the results to detailed kinetic Monte Carlo simulations that demonstrate that the scaling exponents for surface roughness and feature size change continuously as a function of the model parameters.

Christian Ratsch
University of California, Los Angeles
cratsch@math.ucla.edu

MS41

A Rejection Scheme for Off-Lattice Kinetic Monte

Carlo Simulation

We introduce a new kinetic Monte Carlo (KMC) algorithm for off-lattice simulation. In off-lattice KMC one needs to calculate the rates for all possible moves from the current state by searching the energy landscape for index-1 saddle points surrounding the current basin of attraction. We introduce a rejection scheme where the true rates are replaced by rate estimates. This is done by first associating each saddle point with the atom that would move the most if that transition were to take place, then constructing an estimate for the total rate associated with each atom by using a nearest-neighbor bond count. These estimates allow one to select a set of possible transitions, one of which is accepted or rejected based on a localized saddle point search focused on a particular atom. In principle, this allows a performance boost that scales with the number of particles in the system. We test the method on a growing two-species nano-cluster, and find we can reduce computation time by 90% for clusters that contain around 55 particles, and 96% for clusters that contain around 65 particles.

Hamza M. Ruzayqat
University of Tennessee, Knoxville
University of Tennessee, Knoxville
ruzayqat@math.utk.edu

Tim Schulze
University of Tennessee
Department of Mathematics
schulze@math.utk.edu

MS42

Behavior of Eigenvalues for the Constrained Landau-De Gennes Energy Including All Anisotropic Terms

We prove regularity of minimizers for the consrained Landau-de Gennes energy including all anisotropic elastic terms with constants L_1, L_2, L_3, L_4, L_5. As a result, we prove that minimizers have their eigenvalues in the physically realistic interval $(-1/3, 2/3)$.

Patricia Bauman
Purdue University
bauman@math.purdue.edu

Daniel Phillips
Department of Mathematics, Purdue University
phillips@purdue.edu

MS42

Droplet Phase in a Nonlocal Isoperimetric Problem under Confinement

We address small volume-fraction asymptotic properties of a nonlocal isoperimetric functional with a confinement term, derived as the sharp interface limit of a variational model for self-assembly of diblock copolymers under confinement by nanoparticle inclusion. We introduce a small parameter η to represent the size of the domains of the minority phase, and study the resulting droplet regime as $\eta \to 0$. By considering confinement densities which are spatially variable and attain a nondegenerate maximum, we present a two-stage asymptotic analysis wherein a separation of length scales is captured due to competition between the nonlocal repulsive and confining attractive effects in the energy. A key role is played by a parameter M which gives the total volume of the droplets at order η^3 and its relation to existence and non-existence of Gamow's Liquid Drop model on R^3. For large values of M, the minority phase splits into several droplets at an intermediate scale $\eta^{1/3}$, while for small M minimizers form a single droplet converging to the maximum of the confinement density. This is joint work with Stan Alama, Rustum Choksi and Ihsan Topaloglu.

Stan Alama, Lia Bronsard
McMaster University
Department of Mathematics and Statistics
alama@mcmaster.ca, bronsard@mcmaster.ca

Rustum Choksi
Department of Mathematics
McGill University
rchoksi@math.mcgill.ca

Ihsan Topaloglu
Department of Mathematics and Applied Mathematics
Virginia Commonwealth University
iatopaloglu@vcu.edu

MS42

Nonlinear Rheology of Nematic Liquid Crystals in Oscillatory Shear in a Magnetic Field

We model the effects of applying an oscillatory shear flow to a nematic liquid crystal in the presence of a magnetic field. If the liquid crystal anchoring conditions and the magnetic field are both aligned parallel or orthogonal to the plates, there is no qualitative difference from the linear rheological response without the magnetic field. However, applying a magnetic field in the shearing plane that is neither parallel nor orthogonal to the plates generates a nonlinear rheological response even for oscillatory shear that would normally be considered small amplitude. Furthermore, the liquid crystal alignment with the oblique magnetic field creates an asymmetry in the shear stress with respect to the forward and backward motion of the plates so that even harmonics are present in the shear stress beyond start up, and in some cases causes a chaotic response in the orientation.

Eric P. Choate, Jacob Britton
Department of Mathematics and Statistics
Radford University
echoate2@radford.edu, jbritton2@radford.edu

MS42

Gradient Flow for a Relaxed Model of Bent-Core Liquid Crystals

Columnar phases of liquid crystals, if made of bent-core molecules, exhibit spontaneous polarization. For the particular B_{1Rev} phase, this polarization can be easily reoriented by an external electric field without damaging the structure of the phase. Further, in the tilted B_{1Rev} phase, the molecules can either rotate around the molecular axis or around the tilt cone. To understand how the dynamics of the switching mechanism are affected by the system parameters, we consider a relaxed Landau-De Gennes-type free energy. We construct a discretized-in-time gradient flow through energy minimization and prove existence and uniqueness of the continuous gradient flow.

Lidia Mrad
Department of Mathematics

University of Arizona
lmrad@math.arizona.edu

Tiziana Giorgi
Department of Mathematical Sciences
New Mexico State University
tgiorgi@math.nmsu.edu

Sookyung Joo
Old Dominion University
sjoo@odu.edu

MS43

On the Role of Curvature in Non-Euclidean Thin Elastic Bodies

A major topic in elasticity is the study of thin elastic bodies, e.g. plates, shells and rods. In incompatible elasticity, when the metric of the thin elastic body is non-Euclidean (and smooth), the elastic energy of a plate or a shell of thickness h scales like h^2 or h^4, depending on the metric, and for rods it always scales like h^4. In this talk I will present a general result for thin bodies of arbitrary dimension and co-dimension, that relates the elastic energy scaling to the Riemannian curvature of the body along its mid-surface. This includes the scalings of plates, shells and rods as special cases.

Cy Maor
Department of Mathematics
University of Toronto
cmaor@math.toronto.edu

Asaf Shachar
Hebrew University
asaf.shachar@mail.huji.ac.il

MS43

Elastodynamics on Manifolds

We discuss the dynamics of continua on differentiable manifolds. We present a covariant derivation of equations of motion, viewing motion as a curve in the infinite-dimensional Banach manifold of embeddings of a body manifold in a space manifold. Our main application is the motion of residually-stressed elastic bodies; residual stress results from a geometric incompatibility between body and space manifolds. We then study a particular example of elastic vibrations of a two- dimensional curved annulus embedded in a sphere. Based on a joint work with Raz Kupferman and Reuven Segev.

Elihu Olami
Hebrew University
elikolami@gmail.com

MS43

On the Geometry of Leaves, Flowers and Sea Slugs

I will outline ideas that connect pattern formation in non-Euclidean elastic sheets to problems in integrable systems and to topological invariants of *quadmeshes*, a type of planar graphs. The key to understanding these relationships is a novel type of geometric singularity – *ramification points for the Gauss normal map*. I will discuss these singularities and their role in (i) regularity, rigidity, and flexibility for solutions of hyperbolic Monge-Ampere equations; (ii) the observed morphology of various types of soft matter; and (iii) extrinsic geometric flows and dynamical problems in non-Euclidean sheets.

Shankar C. Venkataramani
University of Arizona
Department of Mathematics
shankar@math.arizona.edu

Toby Shearman
University of Arizona
tshearman@math.arizona.edu

Kenneth K. Yamamoto
Program in Applied Mathematics, University of Arizona
kyamamoto@math.arizona.edu

John Gemmer
Wake Forest University
Department of Mathematics and Statistics
gemmerj@wfu.edu

MS43

Nonlinear Mechanics of Surface Growth

We present a nonlinear theory of surface growth (accretion). In this theory the material manifold (stress-free configuration) of an accreting body is a time-dependent Riemannian manifold with a time-independent metric that at each point depends on the state of deformation at that point at its time of attachment to the body. We discuss several examples of surface growth and calculate the residual stresses in a nonlinear elastic body induced from accretion.

Arash Yavari, Fabio Sozio
Georgia Institute of Technology
arash.yavari@ce.gatech.edu, fsozio3@gatech.edu

MS44

Free Boundary Models of Cell Motility

We consider free boundary PDE models of motility of eukaryotic cells on a substrate. Our goal is to capture mathematically the key biological phenomena such as steady motion with no external stimuli, spontaneous breaking of symmetry, and rotation. This model consists of an elliptic equation describing the flow of the cytoskeleton gel coupled with a convection-diffusion PDE for the density of myosin motors. This PDE system is of Keller-Segel type but in a free boundary setting with nonlocal condition that involves boundary curvature. Analysis of this system allows for a reduction to a Liouville type equation which arises in various applications ranging from geometry to chemotaxis. This equation contains an additional term that presents a challenge in analysis. In the analysis of the above models our focus is on establishing the traveling wave solutions that are the signature of the cell motility. We also study breaking of symmetry by proving existence of non- radial steady states. Bifurcation of traveling waves from steady states is established via the Schauder's fixed point theorem for the phase field model and the Leray-Schauder degree theory for the free boundary problem model.

Leonid Berlyand
Penn State University
Eberly College of Science

lvb2@psu.edu

MS44

Nonlocal Interactions in the Slow Diffusion Limit

For a range of physical and biological processesfrom dynamics of granular media to biological swarmingthe evolution of a large number of interacting agents is modeled according to the competing effects of pairwise attraction and (possibly degenerate) diffusion. We prove that, in the slow diffusion limit, the degenerate diffusion becomes a hard height constraint on the density of the population, as arises in models of pedestrian crown motion. We then apply this to develop numerical insight for open conjectures in geometric optimization.

Katy Craig
University of California, Santa Barbara
kcraig@math.ucsb.edu

MS44

Ferroelectric SmA Phase for Bent-Core Liquid Crystals

Ferroelectric liquid crystals made of achiral molecules have been studied extensively in the past decade, since synthesizing chiral molecules is expensive, and the bent-shaped molecules' efficient packing may result in ferroelectric properties. Unlike for materials composed of rod-like molecules, the layers in the SmA-like phase of bent-core molecules can be polar, resulting in a ferroelectric phase. We will discuss a free energy functional used to model one smectic layer, represented by a thin planar cells, and study the effect on the polarization of the different parameters of the problem, such as thickness of the cell, strength of the surface anchoring, and intensity of an applied electric field.

Tiziana Giorgi
Department of Mathematical Sciences
New Mexico State University
tgiorgi@math.nmsu.edu

Sookyung Joo
Old Dominion University
sjoo@odu.edu

MS44

Conic Programming of a Variational Problem Arising from the Large Deviations Limit of the Boltzmann Distribution

We examine the problem of minimizing a class of non-local, non-convex functionals, that arise from modeling large systems of pairwise interacting particles. Although finding and verifying local minima to these functionals is relatively straightforward, computing and verifying global minima is much more difficult. Global minima are important as they characterize the most likely observable states for the associated particle systems interacting in the presence of thermal noise. We discuss how minimizing the energy functionals can be viewed as testing whether an associated bilinear form is co-positive. We then examine sufficient conditions for global optimality obtained through a convex relaxation of the cone of co-positive functionals. The sufficient conditions are (i) sometimes sharp (for instance, in the case when minimizers are a lattice); and (ii) provide an optimal decomposition of the functional (into the sum of a convex and non-negative functional) that can be used to characterize the emerging shapes of self-assembled structures.

David Shirokoff
New Jersey Institute of Technology
david.g.shirokoff@njit.edu

MS45

Objective Twisted Light Waves in Chiral Liquid Crystal Elastomers

We examine the propagation of twisted light waves (a solution to Maxwell's equation recently constructed by Friesecke, James and co-workers) in thin films of twisted liquid crystal elastomer, and examine various regimes of wavelength to specimen thickness. Joint with Dick James, Rob Lipton, and M. Ravi Shankar.

Kaushik Dayal
Carnegie Mellon University
Kaushik.Dayal@gmail.com

MS45

Optical Programming and Switching of Curvature in Liquid Crystal Elastomers

Abstract Not Available At Time Of Publication.

Ben Kowalski
Wright Patterson Labs
enjamin.kowalski.ctr@us.af.mil

MS45

Simulation of An Optical Amplitude Modulator Involving Metamaterials

The hyperbolic phonon-polaritons within the Reststrahlen band of hBN is of great interest for applications in nanophotonics as they are capable of propagating light signals with low losses over large distances. However, due to the phononic nature of the polaritons in hBN, amplitude modulation of its signal proves to be difficult and has been underexplored. We proposed [Maier et al., ACS Photonics 2017] a broadband efficient amplitude modulator for hyperbolic rays in hBN. The modulating region comprises a few tens of nanometers wide gap carved within the hBN slab and covered by a graphene layer, where electrostatically gated graphene serves as a mediator that facilitates the coupling between phonon-polaritons on each side of the gap through plasmonic modes within graphene. In this talk we present a number of computational results based on an adaptive, higher-order finite element approach for the simulation of SPPs on 2D materials and layered structures. Aspects of the numerical treatment such as absorbing perfectly matched layers, local refinement and a-posteriori error control will be discussed as well.

Matthias Maier
University of Minnesota Twin Cities
msmaier@umn.edu

MS45

Patterning Shape Change with Molecular Order in Semicrystalline Networks and Elastomers

Materials capable of undergoing programmable, reversible changes in shape may enable a wide variety of devices from active substrates for cell culture to morphing engineering structures. Here, liquid crystal order will be

used as a versatile tool for material processing to control the photoresponsive behavior of a wide range of polymeric materials from high toughness, semicrystalline polymer networks to low-modulus elastomers. We first describe semicrystalline polymers with patterned stimulus-response, where the phase behavior of thiol-acrylate polymer networks is engineered such that processing occurs in the nematic state, which enables control of shape-changing behavior. After polymerization, the networks crystallize, allowing for robust mechanical properties while remaining photoresponsive. The resulting films have similar toughness to engineering thermoplastics at room temperature (up to 50 MPa) and generate large photoinduced stress (up to 1 MPa). Finally, we will discuss direct ink write printing as a new way to control molecular orientation, and therefore the stimulus-response, in a variety of responsive liquid crystal materials. This processing approach enables 3D structures capable of undergoing unprecedented reversible shape change including porous materials that shrink volumetrically and curved shells that rapidly snap between configurations on exposure to light.

Taylor Ware
University of Texas, Dallas
taylor.ware@utdallas.edu

Hyun Kim, Cedric Ambulo
The University of Texas at Dallas
kimhyun@utdallas.edu, cedric.ambulo@utdallas.edu

MS46

Linear Response Eigenvalue Problem Solved by Extended Locally Optimal Preconditioned Conjugate Gradient Methods

Linear response eigenvalue problems, also known as Bethe-Salpeter eigenvalue problems, arise from excitation states calculation of many-particle systems in computational materials science. In this talk, we will review some recent progress in solving LR eigenvalue problems with focus on two main improvements of a local optimal block preconditioned 4-d conjugate gradient method, namely a shifting deflation technique and enhanced search subspace. This is a joint work with Ren-Cang Li of Texas at Arlington and Wenwei Lin of Taiwan Chiao Tung University.

Zhaojun Bai
Departments of Computer Science and Mathematics
University of California, Davis
bai@cs.ucdavis.edu

MS46

A Unified Approach to Wannier Interpolation

The so-called Wannier localization problem in quantum physics is analogous to finding a localized representation of a subspace associated with a nonlinear eigenvalue problem, and plays an important role in Hartree-Fock and Kohn-Sham density functional theory calculations. While this problem is well studied for insulating systems and good algorithms exist, considerably less is known for metallic systems with entangled eigenvalues. We propose a new, unified method to solve the Wannier localization problem that works in both the isolated and entangled setting. Our method is robust and efficient, and can optionally be paired with an optimization procedure to further improve the locality of the resulting orbitals.

Anil Damle
Cornell University
Department of Computer Science
asd239@cornell.edu

MS46

Frequency-sparse Control of Quantum Systems

We propose a new class of cost functionals for the optimal control of quantum systems which produces controls which are sparse in frequency and smooth in time. This is achieved by penalizing not the control field but a suitable time-frequency representation of it, and employing norms which are of L^1 or measure form with respect to the frequency but smooth with respect to time. We prove rigorously and demostrate numerically that the optimal controls, unlike those obtained with the usual L^2 or H^1 costs, sharply concentrate on just a few frequencies, even in the infinite-dimensional case of laser-controlled chemical reactions modelled by Schrödinger dynamics on multiple potential energy surfaces. Joint work with Felix Henneke (FU Berlin) and Karl Kunisch (University of Graz), to appear in Math. Control and Related Fields (2018)

Gero Friesecke
Centre for Mathematical Sciences
Technische Universität München, Germany
gf@ma.tum.de

MS46

Fast Numericaql Algorithms for Structure Relaxation

We examine and compare several algorithms for performing structure relaxation in the context of Kohn-Sham density function theory, i.e. minimizing the total energy of a nanosystem with respect to atomic positions. We discuss a number of issues that affect the convergence of the optimization algorithms such as search direction determination, line search strategies, and the accuracy of the gradient which is determined from a KS-DFT calculation.

Chao Yang
Lawrence Berkeley National Lab
cyang@lbl.gov

Subhajit Banerjee
University of California at Davis
jitbanerjee@ucdavis.edu

Amartya S. Banerjee
Lawrence Berkeley National Laboratory
asb@lbl.gov

Lin Lin
University of California, Berkeley
Lawrence Berkeley National Laboratory
linlin@math.berkeley.edu

MS47

Parametrization of Tight-Binding Models for 2D Heterostructures from Density Functional Theory Calculations

In this talk, I will present a method for parameterizing tight-binding Hamiltonians for 2D heterostructures. I will first recall the definition and properties of Wannier functions of periodic monolayers, which are the building blocks of the method. Second, I will show that greedy algo-

rithms can be used to efficiently compress Wannier functions of monolayers originating from DFT calculations, into a sum of a limited number of symmetry-adapted Gaussian orbitals. Lastly, I will explain how to use the so-obtained compressed Wannier functions (as well as some auxiliary quantities) to construct tight-binding Hamiltonians for incommensurate 2D heterostructures. This approach can easily be combined with the computational non-commutative geometry methods presented by Paul Cazeaux in another talk, aiming at computing electronic and optical properties of incommensurate 2D heterostructures.

Eric Cances
École des Ponts and INRIA, France
cances@cermics.enpc.fr

MS47

Electronic Localization and Superlattices in Stacked 2D Materials

Using a multiscale modeling approach starting from Density Functional Theory (DFT), we calculate the electronic properties of disordered 2D multi-layered structures. In the presence of lattice mismatch, twist, or strain, we find similar electronic features throughout many different heterostructures. Perhaps the most interesting of these features are single-particle electron states which are highly confined in space. We present a physical model that explains the origin of such electronic structure, and discuss some of the many-body phenomenon that they can host. In the case of a pristine 2D layer the many-body effects are usually ignorable, but they dominate the electronic structure in certain multi-layer structures.

Stephen Carr
Department of Physics
Harvard University
stephencarr@g.harvard.edu

MS47

Electronic Structure of Incommensurate Materials Using Momentum Space

To make the investigation of electronic structure of incommensurate heterostructures computationally tractable, effective alternatives to Bloch theory must be developed. In previous work, we developed and analyzed a real space scheme that exploits spatial ergodicity and nearsightedness. Here we present an analogous scheme formulated in momentum space, which we prove has significant computational advantages in specific incommensurate systems of physical interest, e.g., bilayers of a specified class of materials with small rotation angles. We use our theoretical analysis to obtain estimates for improved rates of convergence with respect to total CPU time for our momentum space method that are confirmed in computational experiments.

Daniel Massatt
University of Minnesota
massa067@umn.edu

MS47

Numerical Construction of Wannier Functions for Topological Insulators

Numerical construction of localised Wannier functions is done through minimisation of a localisation functional, so results are dependent on the quality of the initial guess (given by physical intuition). In recent work, Cancs, Levitt, Panati and Stoltz proposed a systematic approach to giving an appropriate initial guess, that could be used when no prior physical intuition is available. This method, however, fails on topological insulators, in which additional symmetries prevent the existence of localised and symmetric Wannier functions. However, one can theoretically still construct non-symmetric but still localised Wannier functions. We propose here a new method for constructing reasonable initial guesses that works even when there are topological obstructions. We test the approach on the Kane-Mele model.

Sami Siraj-Dine
CERMICS, Université Paris Est
sami.siraj-dine@enpc.fr

Antoine Levitt
Inria and Ecole des Ponts ParisTech
antoine.levitt@inria.fr

David Gontier
Ceremade, Université Paris Dauphine, France
gontier@ceremade.dauphine.fr

MS48

Inverse Problems of Elasticity on n Cavities and Inclusions

Two inverse problem of elasticity are considered. The first one is a two-dimensional problem of plane elasticity that concerns n equal-strength cavities in a plane subjected to constant loading at infinity and in the cavities' boundary. By reducing the governing boundary value problem to the Riemann-Hilbert problem on a symmetric Riemann surface of genus $n-1$ a family of conformal mappings from a parametric slit domain onto the n-connected elastic domain is constructed. The conformal mappings are presented in terms of hyperelliptic integrals, and the zeros of the first derivative of the mappings are analyzed. It is shown that for any $n \geq 1$ there always exists a set of the loading parameters for which these zeros generate inadmissible poles of the solution. The second problem is the inverse problem of antiplane elasticity on determination of the profiles of n uniformly stressed inclusions. The inclusions are in ideal contact with the surrounding matrix, the stress field inside the inclusions is uniform, and at infinity the body is subjected to antiplane uniform shear. The exterior of the inclusions, an n-connected domain, is treated as the image by a conformal map of an n-connected slit domain with the slits lying in the same line.The inverse problem is solved by quadratures by reducing it to two Riemann-Hilbert problems on a Riemann surface of genus $n-1$. Samples of two and three symmetric and non-symmetric uniformly stressed inclusions are reported.

Yuri A. Antipov
Louisiana State University
Department of Mathematics
antipov@math.lsu.edu

MS48

Explicit Finite Volume Method for Evolving Discontinuities in Elastic Solids with Discontinuity-Driven Mesh Alignment

We developed a highly accurate, efficient, and robust adaptive-mesh computational method for hyperbolic sys-

tems of conservation laws, with particular reference to problems with evolving discontinuities. The main idea is to combine the flexibility afforded by a dynamically moving mesh with the increased accuracy and efficiency of a discontinuity tracking algorithm, while preserving the stability of the scheme. Key features of proposed method are accuracy and stability, which will be ensured by ability of the adaptive technique to preserve the modified mesh as close to the original fixed one as possible.

Mihhail Berezovski
Department of Mathematics
Embry-Riddle Aeronautical University
mihhail.berezovski@erau.edu

MS48

Properties of a TwoDimensional Periodic Medium at Low Frequencies

We consider transverse propagation of waves through a two-dimensional composite material containing a periodic rectangular array of circular cylinders. The wave propagation is described by a two-dimensional Helmholtz equation. In our approach we assume the wave frequency to be small so that the equation can be viewed as a perturbation of the Laplace equation. We show that the eigenfrequency is an even analytic function of the perturbation parameter and provide its series expansion. A system of recurrence equations is derived for determination of the coefficients of the series and a frequency correction term to the effective dielectric tensor is determined.

Yuri Godin
University of North Carolina at Charlotte
ygodin@uncc.edu

MS48

On the Augmented Biot-JKD Poroelastic Wave Equations

The time-domain Biot-JKD(Johnson-Koplik-Dashen) poroelastic wave equations contains a memory term that addresses the fact that the (pore fluid)-(solid matrix) interaction is frequency-dependent in the frequency domain. The form of the Laplace transform of the memory kernel needs to satisfy certain analytic conditions in order for the memory kernel to be causal in the time domain. We utilize this constraint and the function theory it associates with to derive a pole-residue approximation of the frequency-domain JKD memory-kernel, which is known as JKD tortuosity. In time-domain, these approximations are Prony sums with various relaxation times. We present two different ways for constructing the approximation, both of which are deeply rooted in approximation theory for Stieltjes functions with special attention to its asymptotic behavior as frequency becomes large. As a results of this approximation, the time-domain Biot-JKD equations can be dealt with efficiently by an augmented system of equations that contains no memory terms. Solution of the augmented system of equations by Discontinous Galerkin method will also be presented.

M. Yvonne Ou
University of Delaware
mou@udel.edu

Hugo J. Woerdeman
Drexel University
hugo @ math.drexel.edu

Jiangming Xie
Chongqing University
xiejm@cqu.edu.cn

Liwei Xu
University of Electronic Science and Technology of China
xul@uestc.edu.cn

MS49

Dislocation Network Structures in 2D Bilayer System

We present a multiscale model to describe the interlayer defects in bilayer materials. The model incorporates both the elasticity of each layer and the first-principle calculation informed interaction between two layers, i.e., the 3-dimensional generalized stacking-fault energy based upon the disregistry between two layers. The force balance between these two contributions determines the structure. We apply this approach to determine the structure and energetics of twisted bilayer material. In tBLG, two distinct, modified Moir structures are observed. The breathing mode, stable at large twist angle, has small amplitude (opposite sign) buckling of the two layers. The bending mode is characterized by large amplitude (same sign) buckling of the layers. The latter gives rise to a distorted Moir pattern consisting of a twisted dislocation structure. The relaxation of the Moir structure reduces the symmetry and increases the period of the tBLG. Our model agrees well with the atomistic results. An analytical description is developed based on the obtained structural features. We also study the buckling twisted heterogeneous bilayer material.

Shuyang Dai
Wuhan University
shuyang_dai@whu.edu.cn

MS49

Algorithms for Fully Anisotropic, Continuum Models of Grain Boundary Motion

I will describe an algorithm that enables specifying n-choose-2 possibly distinct, normal dependent mobilities, and n-choose-2 possibly distinct, normal dependent surface tensions for a grain network of n grains in two or three dimensions. This is a new version of threshold dynamics that can treat the fully anisotropic version of Mullins' model of grain boundary motion. These algorithms generate the desired interfacial motion by alternating convolutions with a kernel and simple pointwise thresholding. The algorithm builds on previous work with Felix Otto on the variational formulation of these schemes. The novelty I will report is how to bake the desired anisotropic surface tension and desired anisotropic mobility of an interface into the convolution kernel used in the algorithm. Joint work with Matt Jacobs and Pengbo Zhang.

Selim Esedoglu
University of Michigan
esedoglu@umich.edu

MS49

A Concurrent Atomistic-continuum Study of Sequential Slip Transfer of Curved Dislocations Across Grain Boundaries

Sequential slip transfer across grain boundaries (GB) plays an important role in grain size-dependent plastic deforma-

tion in polycrystalline metals. In spite of extensive studies in modeling individual phases and grains, well accepted criteria of slip transfer across GBs and models of predicting irreversible GB structure evolution are still lacking. Slip transfer is inherently multiscale since both the atomic scale structure of the interface and the long-range fields of dislocation pile-ups come into play. In this work, large-scale concurrent atomistic-continuum (CAC) simulations [Xu et al., Int. J. Plast. 72 (2015) 91] are performed to address the slip transfer of dislocation pile-ups across S3 coherent twin boundary in Cu and Al [Xu et al., npj Comput. Mater. 2 (2016) 15016], as well as S11 symmetric tilt grain boundary in Ni [Xu et al., JOM 69 (2017) 814]. Results suggest the viability of the CAC method to describe the interface reactions with fully-resolved atomistics while preserving the net Burgers vector and associated long-range stress fields of curved dislocations. In addition, we explore the role of specific twist GB structures and dislocation character in interface absorption-desorption reactions, including the evolution of the structure of the interface.

Shuozhi Xu
University of California, Santa Barbara
shuozhixu@ucsb.edu

MS49

A New Model for Interface Motion by Interface Diffusion

We shall first present a new phase-field model for interface motion by interface diffusion formulated by Alber and myself, which may be applied to Sindering, powder metallurgy, etc. Then a new concept of weak derivatives is proposed, and weak solutions to an initial-boundary value problem of this model are defined. Next an approximate problem for the IBVP is constructed. Finally making use of a classical theorem (the Egorov theorem) we prove the existence of weak solutions to the IBVP.

Peicheng Zhu
University of Basque Country, Spain
pczhu@t.shu.edu.cn

MS50

Mathematical Aspects of Modeling the Rheology of Complex Material

Recent work using small angle neutron scattering under flow has identified the existence of a microstructure that is dependent on flow conditions in soft colloidal systems. Additionally, over the last twenty years, a large number of empirically based thixotropic rheological models has been developed that involve, albeit phenomenologically, a single scalar structural parameter, lambda. These models involve the combination of a lambda-dependent decomposition of the shear stress to an elastic and a viscous contribution with a relaxation-based evolution equation for lambda. The rich behavior of the soft colloidal systems is primarily due to the interaction of the structure and the hydrodynamic force and this can be particularly enhanced applied through in transient flow, and/or large amplitude oscillatory shear flow. To successfully model thixo-elastic-viscoplastic complex material systems each modelling technique employs between 2 4 ODEs, and several algebraic equations, meaning that any optimization strategy must involve robust, and accurate ODE solvers. Due to the stiffness of the models, the ODE solvers must seamlessly be able to incorporate implicit ODE solution techniques. In addition we will discuss several other viscoelastic models like the de Souza Mendes and Thompson and the Blackwell and Ewoldt model using a modified Jeffreys model with a structural, thixotropic parameter, whose evolution is modeled with an ODE in time.

Matthew J. Armstrong
United States Military Academy
matthew.armstrong@usma.edu

Antony N. Beris
University of Delaware
Newark, DE
beris@udel.edu

Jeffrey S. Horner
University of Delaware
jshorner@udel.edu

Geoffrey Bull
United States Military Academy
geoffrey.bull@usma.edu

MS50

Gel Swelling and Maintenance of the Gastric Mucus Layer

The gastric mucus layer is widely recognized to serve a protective function in the human stomach, shielding the epithelium and the gastric mucosa from the extremely low pH and digestive enzymes present in the stomach lumen. How this gel layer and the extreme pH gradient across it are maintained is not fully understood. Mucus secretion and swelling at the stomach wall are balanced by enzymatic degradation of the gel network at the lumen. All of these processes, as well as the rheology of the mucus itself are mediated by local pH, which is non-uniform throughout the layer. Here, we present a model of gastric mucus based on a two-phase gel framework, combined with a Nernst-Planck treatment of ionic diffusion. Ionic binding and unbinding with the gel phase are also considered. The model allows us to directly address the kinetics of ion mediated mucus swelling immediately after secretion.

Owen L. Lewis, James P. Keener, Aaron L. Fogelson
University of Utah
olewis@math.utah.edu, keener@math.utah.edu, fogelson@math.utah.edu

MS50

Active Hydrodynamics of Interphase Chromatin: Coarse-Grained Modeling and Simulations

While the sequence of the human genome has been known for two decades, its 3D dynamic organization inside the cell nucleus has remained elusive. Experiments by Displacement Correlation Spectroscopy (DCS) reveal the existence of slow coherent chromatin motions occurring on micron-second scales, which are ATP-dependent but have yet to be explained. Using a coarse-grained computational model for the chromatin as a flexible polymer chain acted upon by active force dipoles representing the action of ATP-powered enzymes, we explore the microscopic mechanisms for the emergence of coherent dynamics via hydrodynamic interactions. Extensile dipolar activity is found to drive large-scale chromatin motions akin to experimental observations through microstructural reconfigurations of the chromatin chain by long-ranged nucleoplasmic flows.

David Saintillan

Department of Mechanical Science and Engineering
University of Illinois at Urbana-Champaign
dsaintillan@eng.ucsd.edu

Achal Mahajan
Mechanical and Aerospace Engineering
UCSD
acmahaja@eng.ucsd.edu

Alexandra Zidovska
Center for Soft Matter Research
New York University
az45@nyu.edu

Michael J. Shelley
New York University
Courant Inst of Math Sciences
shelley@cims.nyu.edu

MS50

Gel-Gel Transition of Interphase Chromosomes

Regions of highly repetitive DNA, such as those found in the nucleolus, show a self-organization that is marked by spatial segregation and frequent self-interaction. The mechanisms that underlie the sequestration of these subdomains are largely unknown. Using a stochastic, bead-spring representation of chromatin in budding yeast, we find enrichment of protein-mediated, dynamic chromosomal cross-links recapitulates the segregation, morphology, and self-interaction of the nucleolus. Rates and enrichment of dynamic crosslinking have profound consequences on domain morphology. Our model demonstrates the nucleolus is phase separated from other chromatin in the nucleus, and predicts that multiple rDNA loci will form a single nucleolus independent of their location within the genome.

Paula A. Vasquez
University of South Carolina
paula@math.sc.edu

Kerry Bloom
University of North Carolina
kerry_bloom@unc.edu

Greg Forest
UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL
forest@unc.edu

Cailtin Hult
University of North Carolina at Chapel Hill
chult@live.unc.edu

David Adalsteinsson
Department of Mathematics
University of North Carolina, Chapel Hill
david@math.unc.edu

Josh Lawrimore
Biology Department
University of North Carolina at Chapel Hill
lawrimor@email.unc.edu

MS51

Degenerate Functionalized Cahn-Hilliard Functional and Defects in Amphiphilic Structures

We introduce a modified functionalized Cahn-Hilliard (FCH) functional to model the free energy of amphiphilic mixtures. We prove that the modified FCH functional admits geometrically localized minimizers, which correspond to lipid bilayers, filamentous pores, or micelles. In addition, we identify the leading order profile of the bilayers under the assumption that the geometrically localized minimizers have bounded variations along the tangential directions. We will also describe how to handle defects caused by the presence of nanoparticles or molecules.

Shibin Dai
University of Alabama
sdai4@ua.edu

MS51

Latent Singularity in Crystal Growth: Application of Gradient Flow Theory in Metric Space

We consider a class of step flow models from mesoscopic view and their continuum limit to 4th order degenerate parabolic equations. Using the regularized method we obtain a global weak solution to the slope equation, which is sign-preserved almost everywhere. However, in order to study the global strong solution with latent singularity, which occurs whenever the solution approaches zero, we formulate the problem as the gradient flow of a suitably-defined convex functional in a non-reflexive Banach space and establish a framework to handle a class of degenerate parabolic equations, including exponential model for epitaxial growth, described by gradient flow in metric space.

Jian-Guo Liu
Duke University
jliu@math.duke.edu

MS51

Evolution Equations from Epitaxial Growth

Epitaxial growth is a process in which a thin film is grown above a much thicker substrate. In the simplest case, no deposition is considered, and all the interactions are assumed to be purely elastic. However, since the film may potentially have different rigidity constant from the substate, such growth leads to a nonuniform film thickness. The equations governing epitaxial growth are high order (generally fourth order), nonlocal, and highly nonlinear. In this talk I will present several results about the regularity of solutions to several equations arising from epitaxial growth, obtained in a series of joint works with I. Fonseca Y. Gao, G. Leoni J.-G. Liu and X. Xu.

Xin Yang Lu
Department of Mathematics and Statistics
McGill University
xlu8@lakeheadu.ca

MS51

Step Bunching in Epitaxial Growth with Elasticity Effects

In epitaxial growth on vicinal surfaces, elasticity effects which give rise to step bunching instability are widely believed to be important in the fabrication of nanostructures. However, due to the nonlocal effects and the interaction between different length scales, difficulties appear in analysis

of the related models. In this talk, we start with analyzing a discrete model for epitaxial growth with elasticity. Our results include the minimum energy scaling law, the appearance of bunch structure and sharp bounds for the bunch size as well as the slope of the optimal profile. After that, we will extend these results to the step systems with general Lennard-Jones type interactions. This systematic study will reveal the mechanism of bunching/non-bunching regimes for epitaxial growth with elasticity.

Yang Xiang
Hong Kong University of Science and Technology
maxiang@ust.hk

Tao Luo
Purdue University
luo196@purdue.edu

Aaron Nung Kwan Yip
Purdue University
Department of Mathematics
yip@math.purdue.edu

MS52

Phase Diagrams From First Principles Using Nested Sampling

Nested sampling is a relatively recently introduced algorithm that enables the efficient computation of global partition functions in the presence of phase transitions. I will show its application to (i) the determination of pressure-temperature-composition phase diagrams from first principles, without a priori knowledge of the solid phases; (ii) transition path sampling, where it enables the computation of rates at all temperatures simultaneously from a single simulation, and, if time permits (iii) a highly non-Gaussian mechanical inverse problem, the determination of mechanical properties from noisy strain measurements.

Gabor Csanyi
University of Cambridge
gc121@cam.ac.uk

MS52

Absorbing Boundary Conditions for Molecular Dynamics Simulations

In the direct simulations using molecular dynamics or quantum-mechanical models, one is often confronted with a system with a large number of degrees of freedom. We will present a formulation of absorbing boundary conditions so that the computation can be confined to a much smaller subdomain. In particular, we will represent the boundary conditions as a Dirichlet-to-Neumann map by using lattice Green's function. To further reduce the computational cost, we introduce auxiliary variables and eliminate the memory effects. The approximations are constructed to also ensure the stability.

Xiantao Li
Pennsylvania State University
xxl12@psu.edu

MS52

High Order and Energy Stable Numerical Methods to Solve the Phase Field Equations

In this talk, I will introduce Convex Splitting Runge-Kutta methods to solve the gradient flow considering the energy stability, which provide a simple unified framework. The core idea is the combination of convex splitting methods and multi-stage implicit-explicit Runge-Kutta methods. The proposed methods are high-order accurate in time. In addition, the energy stability is completely proved when we consider the special design of implicit-explicit Runge-Kutta tables, called a resemble condition. We present numerical experiments with the phase field equation which is a typical example for the gradient flow to show the numerical accuracy, stability, and efficiency of the proposed methods.

Jaemin Shin
Ewha Womans University
Institute of Mathematical Sciences
jmshin@ewha.ac.kr

Hyun Geun Lee
Department of Mathematics
Kwangwoon University
leeh1@kw.ac.kr

June-Yub Lee
Department of Mathematics
Ewha Womans University
jyllee@ewha.ac.kr

MS52

A Variational String Method for MaxFlux Transition Paths

Considered is the problem of determining a representative path or paths for conformation transitions of molecular systems, with special attention to cases where it is advantageous to seek a path in a much lower dimensional space of collective variables. Consideration is restricted to an approach that avoid generating an ensemble of trajectories and that instead optimize some functional that measures path quality. Especially appropriate, because it is physically sensible, is a line integral termed the resistance functional, introduced in 1983, whose minimum is a path of maximum flux. The focus of the presentation is to build on past experience to design and test a better numerical method: How should one handle arbitrariness of curve parameterization? ignore it? restrain it? constrain it? At what stage in the design of the method should one discretize the resistance functional? And what about errors that might arise from exponentially large variation in the integrand of the resistance functional? What iterative process is most effective for optimization?

Robert Skeel
Purdue University
skeel@cs.purdue.edu

Ruijun Zhao
Minnesota State University, Mankato
ruijun.zhao@mnsu.edu

Matthew Wolff
Purdue Research Park
wolffm2002@yahoo.com

Carol Wolff
Purdue University

cbp@purdue.edu

MS53

On Ring Defects in Nematic Liquid Crystals

We consider energy minimizing configurations of a nematic liquid crystal, as described by the Landau-de Gennes model. We focus on an important model problem concerns a nematic surrounding a spherical colloid particle, with normal anchoring at the surface. For topological reasons, the nematic director must exhibit a defect (singularity), which may take the form of a point or line defect. We consider two physical regimes in which "Saturn-ring" configurations will be energetically favorable: the case of colloids of small radius, and the case of strong applied magnetic fields.

Stan Alama, Lia Bronsard
McMaster University
Department of Mathematics and Statistics
alama@mcmaster.ca, bronsard@mcmaster.ca

Xavier Lamy
Universite Paul Sabatier, Toulouse
xavier.lamy@math.univ-toulouse.fr

MS53

A Ginzburg-Landau Problem With Highly Anisotropic Elastic Terms: Critical Points of the Gamma-Limit

This talk supplements Peter Sternberg's presentation of the general results on Gamma-convergence and on criticality conditions for the Gamma-limit for a Ginzburg-Landau functional with highly anisotropic elastic terms. I will discuss the analytical and computational work on specific examples including the strip under periodic boundary conditions and the disc under a variety of conditions carrying degree. I will demonstrate that the critical points of the Gamma-limit are characterized by the presence of domain walls and vortices. This is joint work with Peter Sternberg and Raghav Venkatraman (Indiana).

Dmitry Golovaty
The University of Akron
Department of Mathematics
dmitry@uakron.edu

Peter Sternberg
Indiana University
Department of Mathematics
sternber@indiana.edu

Raghav Venkatraman
Indiana University, USA
rvenkatr@umail.iu.edu

MS53

Boundary Vortice of Polarization Modulated Orthogonal Smectic Liquid Crystals

We consider polarization-modulated orthogonal smectic liquid crystals which exhibits a bistable response to applied electric field. The opposite anchoring at the stripe boundaries and in-polarization form topological singularities. The free energy of the polarization with electric self-interaction term on one stripe reduces to the Ginzburg-Landau functional with boundary penalty term. We describe the boundary vortices of the reduced functional and obtain convergence results of minimizers. We also perform numerical simulations to illustrate the results of our analysis. This is a joint work with T. Giorgi and C. J. García-Cervera.

Sookyung Joo
Old Dominion University
sjoo@odu.edu

Carlos Garcia-Cervera
Mathematics, UCSB
cgarcia@math.ucsb.edu

Tiziana Giorgi
Department of Mathematical Sciences
New Mexico State University
tgiorgi@math.nmsu.edu

MS54

Machine Learning of Phase-field Simulated Domain Structure of Ferroelectrics

Physical properties of materials are determined by materials microstructures. However, experimental determination of the microstructure and processing conditions needed for a targeted physical property can be a non-trivial and expensive task. Over the past three decades phase-field simulations have been effective in providing the microstructure evolution during solidification and a variety of solid-state phase transformations. On the other hand, machine learning tools have been gradually making inroads in materials science demonstrating tremendous potential in establishing the processing-microstructure-property relationship in materials. In this presentation, it will be shown that a combination of two different tools namely, phase-field simulations and Deep neural networks, a machine learning tool, can be an alternative pathway to determine the processing-microstructure-property linkage in materials. Phase-field generated microstructures will be used to build a microstructure database needed to train a neural network. Bulk polycrystalline ferroelectric lead titanate will be used as a model system. It will be shown that our approach can predict the processing conditions and microstructure/domain structure required for a targeted coercive field, a critical physical property of ferroelectrics. Finally, the universality of this approach in designing materials microstructures beyond ferroelectric materials will also be discussed.

Samrat Choudhury, Issac Curtis
University of Idaho, USA
samrat@uidaho.edu, curt6972@vandals.uidaho.edu

Vishnu Boddeti
Michigan State University, USA
vishnu@msu.edu

MS54

Large Scale Phase-Field Simulations of Solidification Morphologies

During the directional solidification of metallic alloys various morphologies evolve in the microstructure. These morphologies influence directly the material properties. Depending on the alloy, the composition of the melt and the process conditions, characteristic structures arise. For the development of tailored materials with defined properties a deep understanding of the microstructure evolu-

tion and underlying process is required. With a thermodynamic consistent phase-field model based on a grand potential approach different morphologies are investigated in large-scale three-dimensional domains. Starting from on a ternary phase diagram, the common microstructures resulting from binary and ternary eutectic growth as well as from the evolution of multiple dendrites are studied. Based on these results, the interaction between dendrites and eutectics during their coupled growth is investigated. For the eutectic structures also the adjustment processes of the rods and lamellae during dynamic velocity changes are analyzed. Therefore multiple velocity decreases and increases are performed during a single simulation. By increasing the solidification velocity over the stability range, the formation of eutectic colonies is systematical investigated. All investigated morphologies show a good qualitative accordance with experimental micrographs as well as a quantitative accordance to analytic approaches.

Johannes Hötzer
Hochschule Karlsruhe Technik und Wirtschaft
Institute of Materials and Processes
johannes.hoetzer@kit.edu

Michael Kellner, Marco Seiz, Kaveh Daraghi Noubary
Institute for Applied Materials
Karlsruhe Institute of Technology
michael.kellner@kit.edu, marco.seiz,
kaveh.noubary@kit.edu

Britta Nestler
Karlsruhe Institute of Technology (KIT)
Institute of Applied Materials (IAM-ZBS)
britta.nestler@kit.edu

MS54

Putting Just Enough Physics into Phase Field Models of Grain Boundaries

This talk will study several closely connected density functional theories that employ both short and long range, rotationally invariant, multi-point particle correlations. Collectively, these models give rise to a class of structural phase field crystal (XPFC) models. These XPFC models allow for numerous microstructural phenomena to be studied simultaneously in materials processes. Results from recent studies conducted using XPFC modelling will be presented and compared to experiments and molecular dynamics. These include multi-step nucleation in solidification, dislocation-assisted nucleation in solid state precipitation in alloys, cavitation in nano-confined liquid during rapid cooling, and electromigration and void formation metallic interconnects. We end by discussing coarse graining methods for deriving practical phase field theories from phase field crystal models.

Bálint Korbuly
ignore Research Centre for Physics
Budapest, Hungary
korbuly.balint@wigner.mta.hu

Mathis Plapp
Ecole Polytechnique
mathis.plapp@polytechnique.fr

Hervé Henry
École Polytechnique, CNRS
Palaiseau, France
hh@pmc.polytechnique.fr

James Warren
NIST
Metallurgy Division
james.warren@nist.gov

László Gránásy
Wigner Research Centre for Physics, Hungary
grana@szfki.hu

Tamas Pusztai
Wigner Research Centre for Phyics
Budapest, Hungary
pusztai.tamas@wigner.mta.hu

MS55

Isometric Immersions, Energy Minimization, and Self-Similar Patterns in Non-Euclidean Sheets

The edges of torn elastic sheets and growing leaves often display hierarchical self-similar like buckling patterns. On the one hand, such complex, self similar patterns are usually associated with a competition between two distinct energy scales, e.g. elastic sheets with boundary conditions that preclude the possibility of relieving in plane strains, or at alloy-alloy interfaces between distinct crystal structures. On the other hand, within the non-Euclidean plate theory this complex morphology can be understood as low bending energy isometric immersions of hyperbolic Riemannian metrics. In particular, many growth patterns generate residual in-plane strains which can be entirely relieved by the sheet forming part of a surface of revolution or a helix. In this talk we will show that this complex morphology (i) arises from isometric immersions (ii) is driven by a competition between the two principal curvatures, rather than between bending and stretching. We identify the key role of branch-point (or monkey-saddle) singularities, in complex wrinkling patterns within the class of finite bending energy isometric immersions. Using these defects we will give an explicit construction of strain-free embeddings of hyperbolic surfaces that are fractal like and have lower elastic energy than their smooth counterparts.

John Gemmer
Wake Forest University
Department of Mathematics and Statistics
gemmerj@wfu.edu

Shankar C. Venkataramani
University of Arizona
Department of Mathematics
shankar@math.arizona.edu

Eran Sharon
Racah Institute of Physics
The Hebrew University
erans@mail.huji.ac.il

Toby Shearman
University of Arizona
tshearman@math.arizona.edu

MS55

Elastic Instabilities in Floating Shells

Non-Euclidean shells, when confined, can deform to a broad assortment of large scale shapes and smaller scale wrinkling or folding patterns quite unlike what is produced by their flat counterparts. In this talk we discuss the mor-

phological landscape of curved shells deposited on a geometrically flat, fluid substrate. The curved shells need to accommodate the excess length and depending on the elastic and geometric properties of the shell, form wrinkles, dimples, and folds. In this talk we examine these elastic instabilities and the interplay between geometry and the mechanics that produces them. Finally we discuss the potential of geometry and intrinsic curvature as a new tool for the controlled fabrication of patterns on thin surfaces.

Eleni Katifori
University of Pennsylvania
katifori@sas.upenn.edu

Octavio Albarran
Max Planck Institute of Dynamics and Self Organization
o.e.albarran.a@gmail.com

Desislava Todorova
University of Pennsylvania
d.v.todorova@gmail.com

Lucas Goehring
Max Planck Institute of Dynamics and Self Organization
lucas.goehring@ntu.ac.uk

MS55

The Bending Energy of Buckled Edge-Dislocations

The study of elastic membranes carrying topological defects has a longstanding history, going back at least to the 1950s. When allowed to buckle in three-dimensional space, membranes with defects can totally relieve their in-plane strain, remaining with a bending energy, whose rigidity modulus is small compared to the stretching modulus. It was suggested in the 1980s that a disc endowed with a single edge dislocation can totally relieve its stretching energy on the expense of a bending energy, whose magnitude is independent of the size of the system. In this lecture, I will show that this is not true: the minimum bending energy associated with strain-free configurations diverges logarithmically with the size of the system.

Raz Kupferman
Institute of Mathematics,
The Hebrew University
raz@math.huji.ac.il

MS55

Anomalously Soft Non-Euclidean Springs

In this work we study the mechanical properties of a frustrated elastic ribbon spring – the non-Euclidean minimal spring. This spring belongs to the family of non-Euclidean plates: it has no spontaneous curvature, but its lateral intrinsic geometry is described by a non-Euclidean reference metric. The reference metric of the minimal spring is hyperbolic, and can be embedded as a minimal surface. We argue that the existence of a continuous set of such isometric minimal surfaces with different extensions leads to a complete degeneracy of the bulk elastic energy of the minimal spring under elongation. This degeneracy is removed only by boundary layer effects. As a result, the mechanical properties of the minimal spring are unusual: the spring is ultra-soft with rigidity that depends on the thickness, t, as $t^{\frac{7}{2}}$, and does not explicitly depend on the ribbon's width. These predictions are confirmed by a numerical study of a constrained spring. This work is the first to address the unusual mechanical properties of constrained non-Euclidean elastic objects. We also present a novel experimental system that is capable of constructing such objects, along with many other non-Euclidean plates.

Ido Levin
Racah Institute of Physics
The Hebrew University of Jerusalem
ido.levin@mail.huji.ac.il

Eran Sharon
Racah Institute of Physics
The Hebrew University
erans@mail.huji.ac.il

MS56

Spectral Approach to the Microstructural Evolution

Evolution of a microstructure of a polycrystalline material due to grain boundaries relaxation is captured by the spectral measure of a related operator. We suggest a two-phase model of a polycrystalline composite in which an elastic phase corresponds to the polycrystal grains and a viscoelastic frequency-dependent phase arising at the grain boundaries describes effects due to relaxation, dislocations, and points defects. The evolution of the spectral measure of a related operator provides an efficient way to model the evolution of the microstructure of the polycrystal.

Elena Cherkaev
University of Utah
Department of Mathematics
elena@math.utah.edu

MS56

Towards Characterization of All 3 Times 3 Extremal Quasiconvex Quadratic Forms

The problem of constructing optimal bounds for the effective parameters of composites is known to be complex. The classical bounds (Hashin-Shtrikman, Cherkaev-Gibiansky, Murat-Tartar, Milton, etc.), mainly achieved by the translation method using Null-Lagrangians, fail to be optimal and are unachievable in some cases. Milton has suggested that using extremal quasiconvex quadratic forms would provide the sought tightest bounds, but unfortunately such forms had been studies very little and no such example was known prior to our work. In this talk I will present our study of such forms that has led to some partial characterizations, reducing the complexity of the problem. This is joint work with Graeme Milton.

Davit Harutyunyan
University of Utah
harutyunyan@ucsb.edu

MS56

Centroidal Voronoi Tessellations: Minimizers and Dynamics

Centroidal Voronoi Tessellations (CVT) are tessellations using Voronoi regions of their centroids. CVTs are useful in data compression, optimal quadrature, optimal quantization, clustering, and optimal mesh generation. Many patterns seen in nature are also closely approximated by a CVT. CVTs are obtained as minimizers of the second mo-

ment energy over Voronoi cells, which is highly nonlocal and nonconvex. In this talk we will present some recent results about minimizers, and a introduce a dynamic version of the CVT problem.

Xin Yang Lu
Department of Mathematics and Statistics
McGill University
xlu8@lakeheadu.ca

MS56

From Atomistic Model to Peierls-Nabarro Model

The Peierls-Nabarro (PN) model for dislocations is a hybrid model that incorporates the atomistic information of the dislocation core structure into the continuum theory. In this talk, we present the connection between a fully atomistic model and a PN model with γ-surface for the dislocation in a bilayer system (e.g. bilayer graphene). Under some stability condition, we prove that the displacement field of the atomistic model is asymptotically close to that of the dislocation solution of the PN model. Our work can be considered as a generalization of the analysis of the convergence from atomistic model to Cauchy-Born rule for crystals without defects in the literature. This is a joint work with Prof. Pingbing Ming and Prof. Yang Xiang.

Tao Luo
Purdue University
luo196@purdue.edu

MS57

Pushing the Envelope of Large Scale First Principles Simulations of Non-Insulating Systems

I will describe a novel iterative strategy for Kohn Sham Density Functional Theory calculations aimed at large systems, that applies to metals and insulators alike. This technique avoids diagonalization of the Kohn-Sham Hamiltonian on every self-consistent field (SCF) iteration, and instead, employs a two-level Chebyshev polynomial filter based complementary subspace strategy to: 1) compute a set of vectors that span the occupied subspace of the Hamiltonian; 2) reduce subspace diagonalization to just partially occupied states; and 3) obtain those states in an efficient manner via an inner Chebyshev-filter iteration. These steps reduce the cost of large metallic calculations significantly, while eliminating the subspace diagonalization cost for insulating systems altogether. Unlike linear-scaling methods however, this approach does not invoke additional approximations related to nearsightedness. I will describe the implementation of this strategy within the framework of the Discontinuous Galerkin (DG) electronic structure method and demonstrate that this results in a computational scheme that can effectively tackle systems containing tens of thousands of electrons, with chemical accuracy, within a few minutes of wall clock time per SCF iteration on large-scale computing platforms. I will end with a discussion of possible future applications of this computational strategy, particularly its use in the study of materials defects using abinitio molecular dynamics.

Amartya S. Banerjee
Lawrence Berkeley National Laboratory
asb@lbl.gov

Lin Lin
University of California, Berkeley
Lawrence Berkeley National Laboratory
linlin@math.berkeley.edu

Phanish Suryanaryana
Georgia Institute of Technology
phanish.suryanarayana@ce.gatech.edu

Chao Yang
Lawrence Berkeley National Lab
cyang@lbl.gov

John Pask
Lawrence Livemore National Lab
pask1@llnl.gov

MS57

Solving Large-Scale DFT Problems in O(N) Operations with Localized Orbitals and Principal Submatrix Solvers

Using a Finite Difference discretization of the Kohn-Sham equations, a localized orbitals representation of the electronic structure can be obtained that approximates the exact solution with a good accuracy. These localized orbitals can be interpreted as an auxiliary basis set, and a complete solution also involves computing the single particle density matrix in that basis. In this talk we will focus on O(N) approaches to compute that matrix. Although the size of this matrix is much smaller and less sparse compared to a Gaussian basis set, there are a lot of similarities in the numerical solvers that can be used for this problem. Starting from our recent work for the special case where the number of localized orbitals equal the number of occupied orbitals, we will describe how our local principal submatrix solver approach can be extended to more general problems, including unoccupied or partially occupied orbitals. We will also discuss how we can leverage recent developments in numerical algorithms and their implementations on modern architectures to accelerate the density matrix solver. This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.

Jean-Luc Fattebert
Lawrence Livermore National Lab.
fattebertj@ornl.gov

Daniel Osei-Kuffuor
Lawrence Livermore National Laboratory
oseikuffuor1@llnl.gov

Christian Negre
Los Alamos National Laboratory
cnegre@lanl.gov

Jamaludin Mohd-Yusof
CCS-2, Computational Physics and Methods
Los Alamos National Laboratory
jamal@lanl.gov

Susan Mniszewski
Los Alamos National Laboratory
smm@lanl.gov

MS57

Error Estimates for Diffusion Monte Carlo Algo-

rithms with Finite Time Step

Diffusion Monte Carlo (DMC) is a stochastic algorithm used to compute the ground state energy of Schrodinger operators. It relies on Feynman–Kac semigroups, which also appear in large deviations theory and nonlinear filtering. In practical situations, these processes need to be discretized in time. I will present in this talk recent results on the time discretization of such semigroups, in particular error estimates on their ergodic properties. This work [G. Ferre & G. Stoltz, ArXiv:1712.04013], provides criteria to construct efficient integration schemes for the DMC dynamics, as well as a mathematical justification of numerical results already observed in the Diffusion Monte Carlo community. If time allows, I will present new results on the long time stability of Feynman–Kac semigroups, a work in collaboration with M. Rousset and G. Stoltz.

Grégoire Ferré
CERMICS, Ecole Nationale des Ponts et Chaussées
gregoire.ferre@enpc.fr

Gabriel Stoltz
ENPC, Paris
gabriel.stoltz@enpc.fr

Mathias Rousset
INRIA Rennes
IRMA, Université Rennes I
mathias.rousset@inria.fr

MS57

Discrete Discontinuous Basis Projection Method for Large-scale Electronic Structure Calculations

We present an approach to accelerate real-space electronic structure methods several fold, without loss of accuracy, by reducing the dimension of the discrete eigenproblem that must be solved. To accomplish this, we construct an efficient, systematically improvable, discontinuous basis spanning the occupied subspace and project the real-space Hamiltonian onto the span. In calculations on a range of systems, we find that accurate energies and forces are obtained with 8–25 basis functions per atom, reducing the dimension of the associated real-space eigenproblems by 1–3 orders of magnitude.

Phanish Suryanarayana
Georgia Institute of Technology
phanish.suryanarayana@ce.gatech.edu

MS58

X-Rays and the Determination of Atomic Structure a New Twist?

My talk will explore - at the level of modelling and simulation - the possiblity of novel X-ray methods for the determination of the atomic structure of highly regular but not periodic molecules. The details were worked out for helical structures. These include carbon nanotubes, the necks and tails of many viruses, and some common proteins (actin, collagen). As regards helical structures, we found exact solutions to Maxwells equations (twisted X-rays) which yield discrete Bragg-type diffraction patterns, in the same way in which plane waves used in current X-ray crystallography yield discrete patterns for crystals. Mathematically, once one has the waveform, the discreteness (or extreme sparsity) of the diffraction pattern follows from the Poisson summation formula on abelian groups. We demonstrated the possiblity of structure determination by recovering the structure of the Pf1 virus (Protein data bank entry 1pfi) from its simulated diffraction data under twisted X-rays. An interesting feature of the required waves is that they carry orbital angular momentum (OAM); unfortunately OAM waves can at present only be realized experimentally down to the regime of soft-Xray wavelengths, not hard-Xray wavelengths needed for atomic resolution.? Joint work with Richard James (University of Minnesota) and Dominik Juestel (Helmholtz Center Munich), SIAM J. Appl. Math. 76 (3), 2016, and Acta Cryst. A72, 190, 2016.

Gero Friesecke
Centre for Mathematical Sciences
Technische Universität München, Germany
gf@ma.tum.de

Richard James
University of Minnesota
james@aem.umn.edu

Dominik Juestel
Helmholtz Center Munich
juestel@ma.tum.de

MS58

Generating X Waves at Microwave Frequencies

Devices that radiate transverse magnetic Bessel beams (localized waves) in the radiative near field are reported. The cone angle of the emitted radiation remains constant over a wide frequency range, allowing localized pulses (X waves) to be generated under a broadband excitation. Two radiating devices are introduced. One device is based on a ray optics design approach, while the other is based on a quasi-conformal transformation optics technique. The talk describes the procedures used to design the devices, and the theoretical and simulated performance of the devices. Frequency and time domain measurements are also reported for an experimental prototype. Agreement between theory, simulation and measurement demonstrates the devices ability to emit broadband X Waves at microwave frequencies.

Nicholas Chiotellis
University of Michigan
Ann Arbor
nchiot@umich.edu

Victor Mendez, Scott M. Rudolph
U.S. Naval Research Laboratory
victor.mendez@nrl.navy.mil, scott.rudolph@nrl.navy.mil

Anthony Grbic
University of Michigan Ann Arbor
agrbic@umich.edu

MS58

Metamaterial Control of the Direction of Light at Different Frequencies

We examine electric and magnetic fields inside metamaterials made from sub wavelength high contrast media. We introduce an analytic representation theory for fields inside optical metamaterials based on the spectra of Neumann Poincare operators. We apply this framework to construct microstructured media for controlling the direction of in-

formation propagation across different frequency bands.

Robert P. Lipton
Department of Mathematics
Louisiana State University
lipton@math.lsu.edu

MS58

Propagation and Scattering of Surface Waves and Line Waves on Metasurfaces

We will discuss propagation and scattering of surface waves on metasurfaces, including the behavior of transverse magnetic and transverse electric polarizations, which require inductive or capacitive surfaces respectively. We will then examine the effects of anisotropy, which allow direction and polarization dependent propagation and scattering effects. Recently we have developed a new concept known as line waves which are the one-dimensional analog of surface waves, confined to the interface between two complementary two-dimensional impedance surfaces. They support one-way propagation of two orthogonal modes, and they do not require any external magnetic field. They link time inversion to spatial inversion, thus forming a kind of chiral mode. They also have the unique property of a field singularity at the interface, which is not present in higher dimensional interface modes. We will examine the relationship between photonic topological insulators and chiral modes. These new material systems promise one-way propagation without scattering due to unique band structure properties. In electromagnetic systems, this sometimes requires classical time reversal symmetry breaking features, such as magnetic materials or time modulation. However, static and nonmagnetic photonic topological insulators have been demonstrated by taking advantage of certain geometrical tricks. These materials and methods for evaluating them will be illustrated through several examples.

Daniel F. Sievenpiper, Diaaaldin Bisharat, Shreya Singh, Xianghong Kong
University of California, San Diego
dsievenpiper@eng.ucsd.edu, dbisharat@eng.ucsd.edu, shs154@eng.ucsd.edu, klovek@sjtu.edu.cn

MS59

Nonlinear Plasmons in Graphene

The rapid development of high-power sources in the mid- and far-infrared frequency range where graphene plasmons exist opens up a new field of nonlinear graphene plasmonics. Two types of nonlinear graphene plasmonic devices have been recently proposed. In the first one only an external dielectric Kerr medium is assumed to interact nonlinearly with the light source while graphene is used for its linear optical properties. The second type only exploits the Kerr nonlinearity of graphene. Recent theoretical and experimental studies of graphenes optical properties have shown that the nonlinear coefficient of graphene is at least as large as the one of a typical dielectric Kerr medium. So, both graphene and surrounding medium can exhibit nonlinear properties during the interaction with a strong light source. We studied graphene plasmons influenced by Kerr nonlinearities of both graphene and dielectric media. We analytically obtained plasmon dispersion relation using Maxwells equations and assuming that the backscattering in dielectric media is negligible. This assumption is valid in a broad frequency range including far-infrared. Our approach addresses the limitations of previous works where the approximation of slowly varying amplitudes is used which does not work in the frequency range where graphene plasmons exist. We found that the dispersion relation of graphene plasmons can be shifted with the source intensity increasing the contrast of plasmonic mode.

Vera Andreeva
Department of Mathematics
University of Minnesota
andr0616@umn.edu

Dionisios Margetis
University of Maryland, College Park
dio@math.umd.edu

Mitchell Luskin
School of Mathematics
University of Minnesota
luskin@math.umn.edu

MS59

Adaptive Finite-Element Simulation of Optical Phenomena on Layered Heterostructures

Plasmonic crystals, a class of particularly interesting metamaterials, consist of stacked metallic layers arranged periodically with subwavelength distance, and embedded in a dielectric host. These structures have made it possible to observe aberrant behavior like no refraction, referred to as epsilon-near-zero (ENZ), and negative refraction. This level of control of the path and dispersion of light is of fundamental interest and can lead to exciting applications. In particular, plasmonic metamaterials offer significant flexibility in tuning permittivity or permeability values. In this talk we present an adaptive, higher-order finite element approach for the simulation of optical phenomena on layered structures. The aproach is based on a homogenization theory of layered heterostructures. Corresponding analytical results elucidate the solution structure.

Matthias Maier
University of Minnesota Twin Cities
msmaier@umn.edu

MS59

Surface Plasmons on Curved Sheets: Dispersion and Renormalization

Surface plasmon-polaritons (SPPs) are evanescent electromagnetic waves that can be excited along 2D conducting materials with appropriate conductivity. In this talk, we show analytically how the slowly varying geometry of atomically thick sheets of conducting materials, e.g., graphene, can influence the dispersion of SPPs. We point out that the dispersion relation attains a form identical to that of a flat substrate but with an effective, curvature- and wavenumber-dependent, conductivity. This effective description unveils the different effect of convex and concave bends of the sheet on the SPP dispersion.

Dionisios Margetis
University of Maryland, College Park
dio@math.umd.edu

MS59

Numerical Methods for Computing Edge States

We present algorithms for computing the edge states of semi-infinite two dimensional materials, which incorporate

the correct boundary conditions on the infinite end so as to avoid the spurious modes that are created when the material is simply truncated. We test the algorithms on the SSH model and on zigzag and armchair edges of graphene.

Kyle Thicke
Department of Mathematics
Duke University
kyle.thicke@duke.edu

Alexander Watson
Duke University
Department of Mathematics
abwatson@math.duke.edu

Jianfeng Lu
Mathematics Department
Duke University
jianfeng@math.duke.edu

Qinyi Zhu
Nankai University
qinyi_zhu@mail.nankai.edu.cn

MS60

On the Stefan Problem with Internal Heat Generation in Cylindrical Geometry

We study time-dependent motion of the solid-liquid interface during melting and solidification of a material with constant internal heat generation in cylindrical coordinates. We derive a nonlinear, first-order ordinary differential equation for the interface that involves Fourier-Bessel series. The model is valid for all Stefan numbers. One of the primary applications of this problem is for a nuclear fuel rod during meltdown. The numerical solutions of the initial value problem are compared with the solutions of a previously derived model that was based on the quasi-steady approximation, which is valid only for Stefan numbers less than one. The agreement between the two models is excellent in the low Stefan number regime. For higher Stefan numbers, where the quasi-steady model is not accurate, the new model differs from the approximate model since it incorporates the time-dependent terms for small times, and as the system approaches steady-state, the curves converge. At higher Stefan numbers, the system approaches steady-state faster than for lower Stefan numbers. During the transient process for both melting and solidification, the temperature profiles become parabolic.

Lyudmyla Barannyk
University of Idaho
Department of Mathematics
barannyk@uidaho.edu

John Crepeau, Patrick Paulus
University of Idaho
crepeau@uidaho.edu, paul2217@vandals.uidaho.edu

MS60

Soret Effects in Electrokinetically-Driven Heat Exchangers for Electronics Applications

We extended classical asymptotic approaches to allow for the spatial pattern wavenumber to vary on the macroscale variables and to find how changes in microstructure geometry affect macroscopic properties and transport. We consider here the thermal transport of a weakly dielectric coolant through nonuniformly spaced laminates, under an applied electric field, as a simple model for heat sinks in electronics. Power is continuously being generated by the laminates, and the local rates of heat and ion transport depend on the local electric potential, local ion concentrations, and local thermal gradients in the coolant. We find a coupled system of pdes that describe the local microscale temperature and deviations from the Darcy pressure. Microscale values of all of these quantities are known in terms of the solutions to these effective equations.

Silvia Jiménez Bolaños
Louisiana State University
sjimenez@math.lsu.edu

Burt S. Tilley
Worcester Polytechnic Institute
Mathematical Sciences Department
tilley@wpi.edu

Bogdan M. Vernescu
Worcester Polytechnic Inst
Dept of Mathematical Sciences
vernescu@wpi.edu

MS60

Efficient Numerical Treatment of HighContrast Composite Materials

This talk concerns a robust numerical treatment of an elliptic PDE with high contrast coefficients. A finite-element discretization of such an equation yields a linear system whose conditioning worsens as the variations in the values of PDE coefficients become large. We introduce a procedure by which a discrete system obtained from a linear finite element discretization of the given continuum problem is converted into an equivalent linear system of the saddle point type. A robust preconditioner for the Lancsoz iterative method to solve this saddle point problem is proposed. We demonstrate that the number of iterations is independent of the contrast and the discretization scale.

Yuliya Gorb
Department of Mathematics
University of Houston
gorb@math.uh.edu

MS60

Modeling Reversible Protein Aggregation on Dna and Its Impact on Dna Compaction

The role of DNA is not limited only to carrying and protecting the genetic code. DNA may also play a very active role in its own functions. There is increasing experimental evidence that conformational and dynamic changes of the double strand may direct protein aggregations that are responsible for fundamental functions of DNA. Using simple stochastic models, I will show that the coalescence of protein-induced DNA bubbles can mediate allosteric interactions that drive such protein aggregation. We will also discuss how this new type of allostery could regulate (a) the packaging of DNA and (b) the assembly of the transcription machinery and (c) the spiral configuration of some protein filaments on DNA.

Nikolaos Voulgarakis
Washington State University, Pullman
nvoul@math.wsu.edu

Traverso Julian, V Manoranjan
Washington State University
joseph.traverso@wsu.edu, mano@wsu.edu

Kim Rasmussen, Alan Bishop
Los Alamos National Laboratory
kor@lanl.gov, arb@lanl.gov

MS61

Simulation of Dislocation Climb and Applications to Point Defect Sink Efficiency of Grain Boundaries

We derive a Green's function formulation for the climb of curved dislocations and multiple dislocations in three-dimensions. In this new formulation, the dislocation climb velocity is determined from the PeachKoehler force on dislocations through vacancy diffusion in a non-local manner. The long-range contribution to the dislocation climb velocity is associated with vacancy diffusion rather than from the climb component of the well-known, long-range elastic effects captured in the PeachKoehler force. Analytical and numerical examples show that the widely used local climb formula, based on straight infinite dislocations, is not generally applicable, except for a small set of special cases. We also present a numerical discretization method of this Green's function formulation appropriate for implementation in discrete dislocation dynamics simulations. Based on this dislocation climb formulation, point defect sink efficiency of low angle grain boundaries is examined.

Yang Xiang
Hong Kong University of Science and Technology
maxiang@ust.hk

MS61

Automatic Information Learning for Atomistic Structures

Recent developments in imaging techniques enable researchers to visualize materials at the atomic resolution to better understand the microscopic structures of materials. This talk focuses on the automatic and quantitative characterization of potentially complicated microscopic crystal images, providing feedback to tweak theories and improve synthesis in materials science. As such, we introduce an efficient toolbox, SynCrystal, based on phase-space analysis and optimization for automatic information learning for atomistic structures, including crystal image segmentation, classification, defect detection, rotation and deformation estimation.

Haizhao Yang
National University of Singapore
matyh@nus.edu.sg

Jianfeng Lu
Mathematics Department
Duke University
jianfeng@math.duke.edu

Benedikt Wirth
Universität Münster
benedikt.wirth@uni-muenster.de

Lexing Ying
Stanford University
Department of Mathematics
lexing@stanford.edu

MS61

Effect of Distribution of Oxygen Partial Pressure on the Mechanisms of Degradation of Solid Oxide Fuel/Electrolyser Cells

In long term operation, it is known that the transportation of oxide ion in the electrolyte may cause oxygen pressure to build up in closed pores and cavities inside the electrolyte. It then acts like an applied stress to drive cavities or pores along the grain boundaries grow and connect with each other, which may cause degradation and delamination of the electrolyte. Moreover, the oxygen potential may also influence the oxidization or the decomposition of the chemical component in the electrolyte. We investigate the distribution of oxygen partial pressure in the electrolyte by mathematical models for different materials, different structures and different operating modes of the fuel cell. It is found that there is a ubiquitous oxygen potential transition rooted in the p-type/n-type transition of electronic conductivity inside mixed conducting oxides, which characterizes the distribution of oxygen partial pressure in the electrolyte. The sharp transition of oxygen partial pressure may lead to interface instability under some operating conditions. We find that this transition is sensitive to the material properties of the electrolyte (such as conductivity of the oxide ion, diffusivity of electrons and holes) and the operating conditions of the cell (such as the current density, operating temperature and environmental oxygen partial pressure).

Qian Zhang
Northwestern University
qian.zhang_jennifer@northwestern.edu

MS62

A Sweeping Process Framework to Model and Stabilize the Evolution of Elastoplastic Systems

A network of elastoplastic springs (termed *elastoplastic system*) is a possible discretization of an elastoplastic material. We developed [arXiv:1708.03084] an analytic framework to design T-periodic loadings which make stresses of springs of the elastoplastic system converging to a unique periodic regime. The solution of such an evolution problem is a pair of vector-functions $(e(t), p(t))$, where $e_i(t)$ and $p_i(t)$ are the elastic and plastic elongations of spring i. After we rigorously convert the problem into a differential inclusion with a t-dependent polyhedral constraint $C(t)$ (called *sweeping process* as originally introduced by Moreau [CIME book series, vol. 63, 1974, 171–322]) it becomes natural to expect (based on a result by Krejci [Gattotoscho, 1996]) that the solution $(e(t), p(t))$ always converges to a T-periodic function. We discovered a large class of elastoplastic systems where the Krejci's limit doesn't depend on the initial condition $(e(t_0), p(t_0))$ and so all the trajectories asymptotically stabilize to the same T-periodic regime. The result can be used to spot elastoplastic materials with localized periodic solutions (leading to shear bands). We offer explicit formulas to convert any 1D-network of elastoplastic springs into a sweeping process and discuss extensions to 2D and 3D. MatLab constrained quadratic optimization package is used for visualizations. This research was supported by NSF CMMI-1436856.

Ivan Gudoshnikov
Department of Mathematical Sciences
University of Texas at Dallas

ixg140430@utdallas.edu

Oleg Makarenkov
University of Texas at Dallas
makarenkov@utdallas.edu

MS62

Motion of Dislocations

We present an overview of some recent results on variational models for the motion of dislocations.

Giovanni Leoni
Carnegie Mellon University
giovanni@andrew.cmu.edu

MS62

Dislocation Climb Models: from Atomistic Schemes to Dislocation Dynamics

Dislocation climb mechanism plays an important role in the plastic deformation of crystal materials at high temperature. I will present a mesoscopic dislocation dynamics model for vacancy-assisted dislocation climb by upscaling from a stochastic model on the atomistic scale. This model incorporates microscopic mechanisms of (i) bulk diffusion of vacancies, (ii) vacancy exchange dynamics between bulk and dislocation core, (iii) vacancy pipe diffusion along the dislocation core, and (iv) vacancy attachment-detachment kinetics at jogs leading to the motion of jogs. This mesoscopic model consists of the vacancy bulk diffusion equation and a dislocation climb velocity formula. This climb velocity formula is able to quantitatively describe the translation of prismatic loops at low temperatures when the bulk diffusion is negligible. Simulations performed show evolution, translation, coalescence of prismatic loops and the interaction between a prismatic loop and an infinite edge dislocation are in excellent agreement with available experimental and atomistic results.

Xiaohua Niu
Jimei University
xniu@connect.ust.hk

MS62

A Crystal Surface Model Featuring the P-Laplacian Operator

The manufacturing of crystal films lies at the heart of modern nanotechnology. How to accurately predict the motion of a crystal surface is of fundamental importance. Many continuum models have been developed for this purpose, including a number of PDE models, which are often obtained as the continuum limit of a family of kinetic Monte Carlo models of crystal surface relaxation that includes both the solid-on-solid and discrete Gaussian models. In this talk, we offer an analytical perspective into some of these models. To be specific, we investigate the existence of a weak solution to the boundary value problem for the equation $-\Delta e^{-\mathrm{div}(|\nabla u|^{p-2}\nabla u)}+au=f$, where $p>1, a>0$ are given numbers and f is a given function. This problem is derived from a crystal surface model proposed by J.L. Marzuola and J. Weare (2013 Physical Review, E 88, 032403). The mathematical challenge is due to the fact that the principal term in our equation is an exponential function of a p-Laplacian. Our investigations reveal that the key to our existence assertion is how to control the set where $-\mathrm{div}\left(|\nabla u|^{p-2}\nabla u\right)$ is $\pm\infty$.

Xiangsheng Xu
Mississippi State University
xxu@ra.msstate.edu

MS63

Convergence of Stochastic Integrators for Homogeneous Nonequilibrium Flow

We study numerical schemes for molecular simulations of particle systems with steady average flow, such as shear or elongational flow. In particular, we analyze numerical integration of the nonequilibrium Langevin dynamics (NELD) coupled to appropriate nonequilibrium boundary conditions. The interplay between the deforming boundary conditions and the numerical schemes leads to a loss of convergence for a naive implementation, but higher-order convergent schemes are still possible. We also discuss the accuracy of the invariant measure being sampled.

Matthew Dobson, Abdel Kader Geraldo
University of Massachusetts Amherst
dobson@math.umass.edu, ageraldo@umass.edu

MS63

A Perturbative Approach to Control Variates in Molecular Dynamics

We propose a general variance reduction strategy for diffusion processes. Our approach does not require the knowledge of the measure that is sampled, which may indeed be unknown as for nonequilibrium dynamics in statistical physics. We show by a perturbative argument that a control variate computed for a simplified version of the model can provide an efficient control variate for the actual problem at hand. We illustrate our method with numerical experiments and show how the control variate is built in practice.

Julien Roussel
Cermics, ENPC
julien.roussel@enpc.fr

Gabriel Stoltz
ENPC, Paris
gabriel.stoltz@enpc.fr

MS63

Assessing Numerical Methods for Molecular and Particle Simulation

We discuss the design of state-of-the-art numerical methods for molecular dynamics, focusing on the demands of soft matter simulation, where the purposes include sampling and dynamics calculations both in and out of equilibrium. We discuss the characteristics of different algorithms, including their essential conservation properties, the convergence of averages, and the accuracy of numerical discretizations. Formulations of the equations of motion which are suited to both equilibrium and nonequilibrium simulation include Langevin dynamics, dissipative particle dynamics (DPD), and the more recently proposed "pairwise adaptive Langevin' (PAdL) method, which, like DPD but unlike Langevin dynamics, conserves momentum and better matches the relaxation rate of orientational degrees of freedom. PAdL is easy to code and suitable for a variety of problems in nonequilibrium soft matter mod-

eling; our simulations of polymer melts indicate that this method can also provide dramatic improvements in computational efficiency. Moreover we show that PAdL gives excellent control of the relaxation rate to equilibrium. In the nonequilibrium setting, we further demonstrate that while PAdL allows the recovery of accurate shear viscosities at higher shear rates than are possible using the DPD method at identical timestep, it also outperforms Langevin dynamics in terms of stability and accuracy at higher shear rates.

Xiaocheng Shang
Brown University
x.shang@mat.ethz.ch

Martin Kroger
ETH Zurich
mk@mat.ethz.ch

Benedict Leimkuhler
University of Edinburgh
b.leimkuhler@ed.ac.uk

MS63

Stability and Convergence of the String Method

We give an analysis of the stability and convergence of the improved string method of E, Ren, and Vanden-Eijnden to a minimum energy path. In the simplest setting of an index one saddle point connecting two linearly stable local minima, we show that the string method initialized in a neighborhood of a minimum energy path converges to an arbitrarily small neighborhood of the minimum energy path as the number of images is increased.

Brian Van Koten
The University of Chicago
vankoten@galton.uchicago.edu

Mitchell Luskin
School of Mathematics
University of Minnesota
luskin@umn.edu

MS64

The Spectrum of a Schrdinger Operator in a Wire-Like Domain with a Purely Imaginary Degenerate Potential in the Semiclassical Limit

Consider a two-dimensional domain shaped like a wire, not necessarily of uniform cross section. Let V denote an electric potential driven by a voltage drop between the conducting surfaces of the wire. We consider the operator $\mathcal{A}_h = -h^2\Delta + iV$ in the semi-classical limit $h \to 0$. We obtain both the asymptotic behaviour of the left margin of the spectrum, as well as resolvent estimates on the left side of this margin. We extend here previous results obtained for potentials for which the set where the current (or ∇V) is normal to the boundary is discrete, in contrast with the present case where V is constant along the conducting surfaces.

Yaniv Almog
Lousiana State University
Department of Mathematics
almog@math.lsu.edu

Bernard Helffer
University of Paris, Orsay
bernard.helffer@math.u-psud.fr

MS64

A GInzburg-Landau Type Problem for Nematics with Highly Anisotropic Elastic Term

I will discuss a model for thin film nematics whose salient feature is that one elastic constant is much larger than the others. The goal is to understand how this extreme anisotropy in elastic constants affects the morphology of singular structures emerging in the limit where the width of domain walls and the core of vortices approaches zero. This model problem sits in a regime between two well-studied energies: the BBH (Brezis/Bethuel/Helein) energy and the Aviles-Giga energy. As such, it shares features of both models, including the presence of vortex structures and walls. Our work on this problem includes an establishment of the Gamma-limit and a rigorous and computational study of minimizers of this limiting problem. In my talk, I will introduce the model and discuss the general results on Gamma-convergence and on criticality conditions for the Gamma-limit. In a talk on the same project, Dmitry Golovaty will then discuss our analytical and computational work on specific examples including the strip under periodic boundary conditions and the disc under a variety of conditions carrying degree. This is joint work with Dmitry Golovaty (Akron) and Raghav Venkatraman (Indiana).

Peter Sternberg
Indiana University
Department of Mathematics
sternber@indiana.edu

Dmitry Golovaty
The University of Akron
Department of Mathematics
dmitry@uakron.edu

Raghav Venkatraman
Indiana University, USA
rvenkatr@umail.iu.edu

MS64

Equilibrium and Hydrodynamics of Biaxial Nematic Liquid Crystals

In this talk, I will introduce the biaxial nematic liquid crystal model proposed by Govers-Vertogen, and Leslie back in 1980's. Then I will describe our recent results on the partial regularity of equilibrium solutions of such a model in dimension three, and the existence and uniqueness result of global almost smooth solutions for a simplified version of hydrodynamics of such a model in dimension two.

Changyou Wang
Purdue University
wang2482@purdue.edu

Junyu Lin
South China University of Technology
Guangzhou, Guangdong, P. R. China
scjylin@scut.edu.cn

MS65

Morphological Self-assembly in Vapor-deposited

Binary Films

Experiments have demonstrated a rich variety of self-organized nanoscale concentration modulations in physical vapor deposited films of phase-separating binary alloys. However, no comprehensive model capable of predicting the entire spectrum of these self-organized nanostructures as a function of material and processing parameters has yet been developed. We adopt a 3D phase-field approach to numerically investigate the role of substrate temperature, lattice misfit, deposition rates, and phase fraction on the morphological self-structuring in representative binary vapor-deposited alloys. We propose new strategies for synthesizing hybrid films based on insights gained from numerical studies.

Kumar Ankit
Arizona State University
kumar.ankit@asu.edu

MS65

Improving Direct Physical Properties Prediction of Heterogeneous Materials from Imaging Data via Convolutional Neural Network and a Morphology-Aware Generative Model

Direct prediction of material properties from microstructures through statistical models has shown to be a potential approach to accelerating computational material design with large design spaces. However, statistical modeling of highly nonlinear mappings defined on high-dimensional microstructure spaces is known to be data-demanding. Thus, the added value of such predictive models diminishes in common cases where material samples (in forms of 2D or 3D microstructures) become costly to acquire either experimentally or computationally. To this end, we propose a generative machine learning model that creates an arbitrary amount of artificial material samples with negligible computation cost, when trained on only a limited amount of authentic samples. The key contribution of this work is the introduction of a morphology constraint to the training of the generative model, that enforces the resultant artificial material samples to have the same morphology distribution as the authentic ones. We show empirically that the proposed model creates artificial samples that better match with the authentic ones in material property distributions than those generated from a state-of-the-art Markov Random Field model, and thus is more effective at improving the prediction performance of a predictive structure-property model.

Ruijin Cang
Mechanical Engineering
Arizona State University
cruijin@asu.edu

Yi Ren, Yang Jiao
Arizona State University
yren32@asu.edu, yang.jiao.2@asu.edu

MS65

Interfacial Statistics and Effective Physico-mechaical Properties of Random Heterogeneous Materials with Nonspherical Particles

The physical and morphological properties of particles and interfaces can seriously impact the whole physico-mechanical properties of random heterogeneous materials like granular materials, particle-reinforced composites, and porous materials, to name but a few. In this talk, we first propose a theoretical framework to symmetrically present the interfacial volume fraction using the stereological theory and the nearest-surface distribution functions. To verify the theoretical generalization, we simulate three-phase heterogeneous materials by employing hard-core-soft-shell structures composed of hard non-spherical particles, soft interfaces, and matrix. We numerically derive the interfacial volume fraction by a Monte Carlo integration scheme. Then, we devise a robust coupling model of DEM-FEM to numerically investigate the effective elastic modulus and conductivity of such three-phase heterogeneous materials. On the other hand, we also develop different micromechanical models including the multiple-inclusion model and the n-phase differential effective approximation to theoretically calculate the effective elastic modulus and conductivity of multiphase heterogeneous materials by incorporating the volume fraction of interfaces proposed above. We show that our numerical and theoretical models lead to predictions of the effective physico-mechanical properties of multiphase heterogeneous materials to a reasonable accuracy by comparing with available experimental data.

Wenxiang Xu
Hohai University, China
xwxfat@gmail.com

MS66

Geometric Incompatibilities and Bending of Ultra-Thin Films

Molecular beam epitaxy (MBE) is a layer-by-layer crystal growth process on a template substrate and provide very high precision of the material composition and layer thickness. Changes in composition affect the lattice parameter and thus induce pre-stress in the multi-layered films. From a macroscopic point of view, when released from the substrate, a planar domain of the pre-stressed material will change its shape in order to reduce the elastic energy due to the pre-stress. Our goal is : (a) to characterize shapes that can be obtained by stress relaxation from a given multi-layered ultra-thin film and (b) to illustrate by experiments these results. A classical result in plate theory predicts that small domains will relax toward spherical caps, a fact well confirmed by the experiment. However, this result does not hold neither at large strains nor in the simplest situation of small strains and large rotations. The main reason for this is the geometric incompatibility. In order to obtain some insight on the later problem we shall first address the simplest question concerning the relaxation of planar domains with one characteristic length much smaller than the other (ribbons). In this case we can relate the curvature of the planar ribbon to that of the relaxed object and confront the results to the experimental evidence. For domains with same order of magnitude lateral dimensions we present experimental results and discuss branch selection of relaxed configurations.

Alexandre Danescu
Ecole Centale Lyon
alexandre.danescu@yahoo.com

Philippe Regreny, Pierre Cremillieu, Jean-Louis Leclercq
Lyon Institute of Nanotechnology - UMR 5270
Ecole Centrale de Lyon
philippe.regreny@ec-lyon.fr, pierre.cremillieu@ec-lyon.fr,

jean-louis.leclercq@ec-lyon.fr

MS66

The Shape of Positively Curved Ribbons

The shape of elastic ribbons in thermal environment is fluctuating, is a question of great interest and importance in many self-assembled nano-ribbons. In many such cases these structures are likely to be geometrically incompatible (i.e- they are residually stressed), a fact that complicates the problem even more. Such ribbons exhibit unusual characteristics as shape bifurcations, and abnormal mechanical properties, which manifest in unique and nontrivial statistics. Using a recently derived quasi-one-dimensional theory [Grossman et al., PRL 116.25 (2016): 258105.], we study systems with positive spontaneous extrinsic curvature which are likely to arise in asymmetric systems (such as uneven bi-layers). We find these ribbons undergo a conformational transition at a critical width. Above it (wider ribbons), have anomalously soft zero-modes, which give rise to unique conformational thermodynamic phase even at the limit of infinitely small temperatures. We find the phase diagram of such ribbons and identify three phases- the Ideal Chain (IC) in high (enough) temperatures; the Random Structured (RS) phase at low temperatures and large widths, similar to IC yet a low scales ($\sim \frac{1}{T}$) the effective segments have a range of possible shapes (and are not straight); and the Plane Ergodic (PE) phase at low temperatures and small widths, where at small scales the ribbon gyrate at almost planar configuration.

Doron Grossman
Racah Institute of Physics, Hebrew University
Jerusalem 91904
doron.grossman@mail.huji.ac.il

Eran Sharon
Racah Institute of Physics
The Hebrew University
erans@mail.huji.ac.il

Eytan Katzav
Racah Institute oHebrew University,
Jerusalem 91904, Israel
eytan.katzav@mail.huji.ac.il

MS66

Dimension Reduction for Thin Films with Transversally Varying Prestrain: The Oscillatory and the Non-oscillatory Case

We compute the Gamma-limit of the non-Euclidean elasticity on thin films, with prestrain that varies across the specimen in both the midplate and the thin (transversal) directions. We also cover the case of the oscillatory prestrain and exhibit its relation to the non-oscillatory case via identifying the effective metric. Our analysis pertains to the Kirchhoff and the von-Karman energetical regimes.

Marta Lewicka
University of Pittsburgh
lewicka@pitt.edu

MS66

The Cost of Crushing: Curvature-Driven Wrinkling of Thin Elastic Shells

How much energy does it cost to flatten an intrinsically curved thin elastic shell? Motivated by recent experiments involving the placing of thin spherical caps onto a flat liquid bath, we study this question in the framework of Gamma-convergence to develop a rigorous method for evaluating the cost of crushing to leading order in the shell's thickness and other small parameters. Two commonly observed motifs are regions of uni-directional wrinkling with clear long-range order, and other disordered regions in which no single direction of wrinkling is preferred. In developing a limiting model, our goal is to explain the appearance and lack thereof of such "wrinkling domains"; however, we do not allow ourselves to assume that these are the only possibilities. The basic mathematical objects of study are short maps from a surface to the plane, describing the macroscopic deformation of the mid-shell. To such short maps we assign an energy proportional to the area covered in the plane, so that a sort of surface tension effect determines the cost of stamping and, oftentimes, the wrinkling domains. Somewhat surprisingly, we find that only part of this cost comes from the bare surface tension of the exposed liquid-vapor interface, while a second part comes from the cost of superimposing low amplitude, high frequency perturbations on top of the limiting short maps. Resolving this limiting model in many cases, we offer new explicit predictions and comparisons with experiment.

Ian Tobasco
Courant Institute of Mathematical Sciences
New York University
itobasco@umich.edu

MS67

Topological Modeling of Granular Material

In this talk we consider a planar model of granular material in which the particles are heterogeneous communities of jammed disks (following Basset, et. al.). This model produces randomly shaped particles. We use the method of swatch and cloth developed by Schweinhart, Mason, and MacPherson to compare the distribution of local topological structure of this model to that of material consisting of randomly sized disks to determine under what conditions the first model can be replaced by the second.

David Damiano, Allison Sullivan
College of the Holy Cross
ddamiano@holycross.edu, arsull19@g.holycross.edu,

Emily Winn
Brown University
emily_winn@brown.edu

MS67

Topological Data Analysis in Materials Science

In this talk, I will explain our recent activity of topological data analysis on materials science. Our main tool is the persistent homology, which is an emerging mathematical concept for characterizing shapes of data. In particular, it provides a tool called the persistence diagram that extracts multiscale topological features such as rings and cavities in atomic configurations and digital high dimensional images. I present a unified method using persistence diagrams for studying the geometry embedded in those data. Furthermore, I will also show a new framework of materials informatics by combining machine learning methods with

persistence diagrams.

Yasuaki Hiraoka
Kyushu University
hiraoka.yasuaki.6z@kyoto-u.ac.jp

MS67

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Risi Kondor
University of Chicago
risi@cs.uchicago.edu

MS67

Local Feature Classification Using the Gromov-Wasserstein Distance

Contemporary molecular dynamics simulations often contain many millions of atoms, and automated classification of local atomic environments is increasingly necessary to process the data generated by these simulations. Previous approaches, such as the centrosymmtery parameter and common neighbor analysis, can fail to distinguish between certain solid phases or lack important mathematical properties such as stability with respect to small perturbations. We propose the 1-Gromov-Wassertein distance as an alternative method to classify local atomic environments. We use this distance to identify defects in a simulation of a polycrystalline material, and compare its ability to distinguish distinct phases to several methods previously proposed in the literature. This is joint work with Jeremy Mason.

Benjamin D. Schweinhart
Ohio State University
Department of Mathematics
schweinhart.2@osu.edu

Jeremy K. Mason
University of California, Davis
jkmason@ucdavis.edu

MS68

Next Generation of Fully Self-Consistent Thermodynamic Models of Solutions: Challenges, Applications and Perspectives

Thermodynamic models typically used in the CALPHAD approach to describe the energetics of solid solutions are often represented by mean of the Compound Energy Formalism (CEF). The CEF accounts for ideal configurational entropy of mixing contributions per sublattice by introducing random-mixing expressions, i.e. without considering short range order. Other non-configurational excess contributions, in the form of temperature and composition dependent polynomials, can also be added to the Gibbs free energy of these solid solutions to finely tune their energetic behavior. As a consequence, the CEF is highly flexible and allows to fit precisely thermodynamic and phase diagram data. The CEF is not designed to describe order/disorder transitions such as the L12 face centered cubic disordered solution observed for example in the Au-Cu system. This phase transition is driven by non-ideal configurational entropy of mixing contributions that need to be mimicked with complex excess functions. Moreover, the impact of the internal atomic structure as well as the effect of interatomic distances on the strength of the chemical interactions are not explicitly accounted for in the CEF. Vibrational entropy contributions are also not integrated in the CEF which limits its predictive abilities. For these reasons, we explore in this presentation the implementation and minimization challenges associated to the next generation of physics-based self-consistent thermodynamic models.

Jean-Philippe Harvey
Ecole Polytechnique de Montreal
Canada
jean-philippe.harvey@polymtl.ca

MS68

Chemical Equilibrium: Numerical Challenges for Efficient and Stable Calculations in Computationally Intensive Applications

Chemical equilibrium calculations are vital for a wide range of industrial and environmental applications. In these applications, the number of equilibrium calculations can vary from a few (e.g., to calculate the solubility of minerals and gases) to dozens of thousands (e.g., for the calculation of phase diagrams), and millions to billions (e.g., in reactive transport simulations). In the first part of this talk, a robust and efficient interior-point algorithm is presented for calculating chemical equilibrium by minimizing Gibbs energy using exact Hessian matrices of the Gibbs molar energy function. In the second part of the talk, an on-demand machine learning algorithm is presented to speed up the evaluation of thousands to billions of equilibrium calculations. The algorithm works by identifying among all previously solved chemical equilibrium problems, the one that is closest to the new problem. After this, the machine learning algorithm is able to quickly predict the new equilibrium state, or determine that a full calculation should be performed instead, which constitutes an on-demand training event that will permit many future calculations to be quickly estimated. We show that reactive transport simulations can be performed orders of magnitude faster using the proposed smart equilibrium algorithm. The talk ends with a discussion on the potential use of this on-demand machine learning algorithm for speeding up the calculation of phase diagrams.

Allan M. M Leal
ETH Zurich
Department of Earth Sciences
allan.leal@erdw.ethz.ch

William R. Smith
University of Guelph, Canada
Department of Mathematics and Statistics
bilsmith@uoguelph.ca

Dmitrii A. Kulik
Paul Scherrer Institut, Switzerland
Laboratory for Waste Management
dmitrii.kulik@psi.ch

Martin O. Saar
ETH Zurich
Department of Earth Sciences
msaar@ethz.ch

MS68

Continuum Mechanics and CALPHAD: A Mathe-

matically Challenging Liasion

Computational thermodynamics plays an integral role in facilitating engineering design of a wide array of materials and processes, such as nuclear fuels, additive manufacturing, and geological applications. Recent trends are focused towards larger and more sophisticated representations of complex systems and the integration of thermodynamic calculations into continuum mechanics codes in order to enhance their predictive capabilities. The increasing computational complexity of thermodynamics models amplifies existing, and introduces new, numerical and algorithmic challenges. Specifically, how one effectively reconciles differences in space and time between thermodynamics (i.e., 0D; equilibrium) and continuum mechanics (i.e., 1-3D; steady-state or time-dependent) remains to be solved. Furthermore, the manner in which one effectively utilizes the results of thermodynamic calculations in a continuum mechanics is an on-going area of work. Recent advancements in algorithm development will be presented in addition to the welcoming an open discussion within the community on the matter.

Markus Piro
Univ. Ontario Inst. Tech.
markus.piro@uoit.ca

Srdjan Simunovic
Computer Science and Mathemati
Oak Ridge National Laboratory
simunovics@ornl.gov

Bernie Fitzpatrick
Univ. Ontario Inst. Tech.
bernie.fitzpatrick@uoit.ca

MS68

Third Generation CALPHAD Databases by Automated Statistical Regression Analysis

The aim of the third generation of CALPHAD databases is to develop an accurate physically-based description of Gibbs energies of pure elements from 0K up to high temperatures that can guarantee a robust prediction of thermodynamic properties of binary, ternary and high-order systems within a wide temperature range. Recently, one of the successful attempts in this direction has been performed by Roslyakova et al. [I. Roslyakova, B. Sundman, H. Dette, L. Zhang, I. Steinbach, Modeling of Gibbs energies of pure elements down to 0 K using segmented regression, Calphad 55 (Part 2) (2016) 165180]. A novel thermodynamic modeling strategy of stable, metastable and liquid phases is proposed based on segmented regression approach and it considers several physical effects, which could be activated in low and high temperatures depending on the properties of the studied elements and systems. The segmented regression model has been applied for several pure elements, Cr, Al, Fe, Ni, Nb, Mo, Ta, W, Cu, Mg, Bi, Te, Ir, Ag, Re, Ge and calculation of phase diagrams for several binary and ternary systems from 0K. This modeling approach demonstrated a good agreement with available experimental data in low and high temperatures, and showed a significant improvement of thermodynamic description and predictive capability of the CALPHAD method.

Irina Roslyakova
Ruhr-Universität Bochum
Germany
irina.roslyakova@rub.de

Ingo Steinbach
Ruhr University Bochum
ingo.steinbach@ruhr-uni-bochum.de

MS69

A Homogenization Result in the Gradient Theory of Phase Transitions

A variational model in the context of the gradient theory for fluid-fluid phase transition with small scale heterogeneity is studied. In particular, the case where the scale of the small homogeneities is of the same order of the scale governing the phase transition is considered. In the limit, as the parameter scale tends to zero, there is an interaction between the homogenization and the phase transition process.

Irene Fonseca
Carnegie Mellon University
Center for Nonlinear Analysis
fonseca@andrew.cmu.edu

MS69

Analytic Solution to Nonlocal Equations of Peirtls-Nabarro Models

The Peierls-Nabarro model was first introduced by Peierls Nabarro to describe the continuum model of dislocation in materials. It incorporates the atomic effect into the continuum framework and give us an understanding of dislocation core structure. We focus on the existence of analytic solution to Peierls-Nabarro model including stationary model and dynamic model. Since we incorporate the misfit surface energy into total energy of the system, which leads to a nonlinear boundary condition, the strategy is to first decouple the displacement field and then to uniquely solve a nonlocal equation on boundary.

Yuan Gao
Hong Kong University of science and technology
maygao@ust.hk

Jian-Guo Liu
Duke University
jliu@math.duke.edu

Yang Xiang
Hong Kong University of Science and Technology
maxiang@ust.hk

MS69

Positivity Preserving Scheme for Phase-field Models

Phase-field method is a powerful tool in material science. Flory-Huggins type potential that involves logarithmic function naturally arises through thermal dynamic consideration. These potentials are singular at certain values that correspond to pure states. The positivity of certain physical quantities, which allows the system to avoid the singularities, are essential for the well-posedness. Here we present efficient and unconditionally stable numerical schemes that are able to preserve the positivity of these physical quantities. This is a joint work with Wenbin Chen, Cheng Wang and Steven Wise.

Xiaoming Wang
Florida State University

wxm@mail.math.fsu.edu

MS69

A Generalized Mbo Diffusion Generated Motion for Orthogonal Matrix-Valued Fields

MBO diffusion generated motion is a method introduced by Merriman, Bence, and Osher for evolving the boundary of a set by mean curvature flow. The method consists of two simple steps, which are iterated until convergence. The first is the time evolution of an indicator function of the set by the diffusion equation for a short time. The second is the point-wise thresholding of this function to obtain a new indicator function. Over the last 25 years, this method has been further analyzed, developed, and employed in a variety of interesting applications. In this talk, Ill discuss a generalization of this method to orthogonal matrix valued fields. In particular, following the Ginzburg-Landau approach, we consider a relaxation of the Dirichlet energy for orthogonal matrix valued fields that includes a term that penalizes the matrix not being orthogonal. We introduce a generalization of the MBO diffusion generated motion that effectively finds local minimizers of this relaxed energy. We extend the Lyapunov function of Esedoglu and Otto to show that the method is non-increasing on iterates and hence, unconditionally stable. We also prove that these iterates converge to a local minimum. The algorithm is efficiently implemented using the closest point method and non-uniform FFT. Ill conclude by presenting several numerical experiments to demonstrate the range of behavior for local minimizers of this generalized energy. This is joint work with Braxton Osting.

Dong Wang, Braxton Osting
University of Utah
dwang@math.utah.edu, osting@math.utah.edu

MS70

Density Functional Theory and Many-marginals Optimal Transport with Coulomb and Riesz Costs

We consider two sharp next-order asymptotics problems, namely the asymptotics for the minimum energy for optimal point configurations and the asymptotics for the many-marginals Optimal Transport, in both cases with Coulomb and Riesz costs with inverse power-law long-range interactions. The first problem describes the ground state of a Coulomb or Riesz gas, while the second appears as a semi-classical limit of the Density Functional Theory energy modelling a quantum version of the same system. Recently the second-order term in these expansions was precisely described, and corresponds respectively to a Jellium and to a Uniform Electron Gas model. The present work shows that for inverse-power-law interactions with power d-2¡s¡d, the two second- order constants are equal.

Codina Cotar
University of College at London
codinacotar@ucl.ac.uk

MS70

A Rigorous Formulation of the Kerker Preconditioner for Flapw Methods

In plane-wave methods, the Kerker preconditioner effectively accelerates convergence of electronic structure simulations for a certain class of large metallic systems. The extension of the preconditioner to the FLAPW basis set is non-trivial – it involves adaptation of Weinert's method as well as careful consideration of the charge transfer between muffin-tin region and interstitial. We present this extension and its implementation. Numerical experiments show significantly improved convergence and the typical system-size independence of the SCF convergence.

Miriam Hinzen
Research Center Jülich
m.hinzen@fz-juelich.de

Edoardo A. Di Napoli
Juelich Supercomputing Centre
e.di.napoli@fz-juelich.de

Daniel Wortmann
Institute for Asvanced Simulation
Forschungszentrum Juelich
d.wortmann@fz-juelich.de

Stefan Blügel
Research Center Juelich
s.bluegel@fz-juelich.de

MS70

Globally Constructed Adaptive Local Basis Set for Spectral Projectors of Second Order Differential Operators

Spectral projectors of second order differential operators play an important role in quantum physics and other scientific and engineering applications. In order to resolve local features and to obtain converged results, typically the number of degrees of freedom needed is much larger than the rank of the spectral projector. We develop a method to construct a basis set that is adaptive to the given differential operator. The basis set is systematically improvable, and the local features of the projector are built into the basis set. The spectral projector on the global domain is systematically approximated from such a basis set using the discontinuous Galerkin (DG) method. The global construction procedure is very flexible, and allows a local basis set to be consistently constructed even if the operator contains a nonlocal potential term. We verify the effectiveness of the globally constructed adaptive local basis set using one-, two- and three-dimensional linear problems with local potentials, as well as a one dimensional nonlinear problem with nonlocal potentials resembling the Hartree-Fock problem in quantum physics.

Yingzhou Li
Duke University
yingzhouli0417@gmail.com

Lin Lin
University of California, Berkeley
Lawrence Berkeley National Laboratory
linlin@math.berkeley.edu

MS70

Recent Developments of Fast Algorithms for Hartree-Fock-Like Equations

Hartree-Fock-like equations are very widely used in quantum chemistry and materials science, but the computational cost for solving such these equations is quite high. In a simplified mathematical setting, the solution requires the computation of low-lying eigenpairs of a large matrix in the

form A+B. Here applying A to a vector is easy but A has a large spectral radius, while applying B (the Fock operator) is costly but B has a small spectral radius. It turns out that most eigensolvers are not well equipped to solve such problems efficiently. We will discuss some recently developed strategies to significantly accelerate such calculations, and to enable the solution of Hartree-Fock-like equations for more than 4000 atoms in a planewave basis set. Some of the techniques have been included in community electronic structure software packages such as Quantum ESPRESSO. We also find that the setup of the Hartree-Fock-like equations introduces interesting questions from the perspective of numerical analysis.

Lin Lin
University of California, Berkeley
Lawrence Berkeley National Laboratory
linlin@math.berkeley.edu

MS71

Coherent Virtual Absoprtion in Optical Materials

We discuss the possibility of storing electromagnetic energy and enhancing the interactions of light and matter in nanostructures based on coherent excitation with temporally tailored optical signals. We discuss how metasurfaces and metamaterials may be able to store on demand and release light in plain sight, even in the limit of lossless materials, and the connection of these phenomena with bound states in the continuum. We also shed light on the role that reciprocity plays in these systems, and how these functionalities may play a pivotal role in low-energy nanophotonic opto-electronic and bio-sensing devices.

Andrea Alu
Department of Electrical and Computer Engineering
University of Texas at Austin
aalu@gc.cuny.edu

Alex Krasnok, Younes Radi
University of Texas at Austin
krasnokfiz@mail.ru, younes.radi@utexas.edu

MS71

Deforming Materials with Light

Abstract Not Available At Time Of Publication.

Kaushik Bhattacharya
Howell N. Tyson Sr. Professor of Mechanics
California Institute of Technology
bhatta@caltech.edu

MS71

High-frequency Homogenization of Porous Media Electromagnetic Heat Exchangers

Electromagnetic (EM) heat exchangers are devices which absorb EM radiation converting it into thermal energy to do work, such as run a turbine. Applications involving both solar and microwave energy have garnered increasing attention but have yet to utilize the potential benefits of short-wave interactions when the wavelength is comparable to a materials microstructure. It has been shown for a three-layer laminate the Bragg resonance that occurs at this scale can be used to control steady state temperature and thermal runaway effects. We investigate these effects in a mathematical model approximating a porous medium for use in a heat exchanger. Classical homogenization methods average over the microscale to obtain a macroscopic description of the material, however they are incapable of describing short-wave behavior. High-frequency homogenization methods have been developed but are restricted to cases incompatible with modeling heat exchangers, such as assuming a lossless medium, spatially uniform dielectric constants, and reducing Maxwells equations to the Helmholtz equation. We develop a high-frequency homogenization technique that relax these assumptions, considering a laminate geometry composed of alternating layers of lossy dielectric material and lossless fluid channels in the homogenization limit. This model advances the designing of porous materials for efficient collection of energy in electromagnetic heat exchangers.

Joseph M. Gaone
Worcester Polytechnic Institute
Department of Mathematical Sciences
jmgaone@wpi.edu

Burt S. Tilley
Worcester Polytechnic Institute
Mathematical Sciences Department
tilley@wpi.edu

Vadim Yakovlev
Worcester Polytechnic Institute
vadim@wpi.edu

MS71

Electromagnetic Scattering from Graphene Sheets

In this talk, I will address aspects of the following question: How are surface plasmon-plasmon polaritons (SPPs) excited by electromagnetic waves in the presence of defects or singular geometries of metallic sheets such as graphene? A prototypical case, which will be discussed analytically, is the generation of an SPP by the edge of a large metallic sheet. The time-harmonic Maxwell equations will be the primary focus of attention. Time-dependent implications of this investigation will also be discussed.

Dionisios Margetis
University of Maryland, College Park
dio@math.umd.edu

MS72

Advection Enhanced Diffusion in a Porous Medium

The thermal conductivity of a fluid filled composite changes significantly in the presence of fluid convection. We derive the Stieltjes integral representation for the advection enhanced effective diffusivity and use it to present a series of rigorous bounds on the enhanced diffusivity.

Noa Kraitzman
University of Utah
noa@math.utah.edu

Elena Cherkaev, Kenneth M. Golden
University of Utah
Department of Mathematics
elena@math.utah.edu, golden@math.utah.edu

MS72

Circular Inhomogeneity with Steigmann-Ogden Interface: Local Fields, Neutrality, and Maxwell's

Type Approximation Formula

The boundary conditions for the Steigmann-Ogden (1997, 1999) model are re-derived for a two dimensional surface using general expression for surface energy that include surface tension. The model treats the interface as a shell of vanishing thickness possessing surface tension as well as membrane and bending stiffness. The two-dimensional plane strain problem of an infinite isotropic elastic domain subjected to the uniform far-field load and containing an isotropic elastic circular inhomogeneity whose interface is described by the Steigmann-Ogden model is solved analytically. Closed-form expressions for all elastic fields in the domain are obtained. Dimensionless parameters that govern the problem are identified. The Maxwell type approximation formula is obtained for the effective plane strain properties of the macroscopically isotropic materials containing multiple inhomogeneities with the Steigmann-Ogden interfaces. The neutrality conditions are analyzed. It is demonstrated that while the Steigmann-Ogden model theoretically reduces to the Gurtin-Murdoch (1975, 1978) model when the bending interphase effects are neglected, the two models (for the case of zero surface tension) describe two very different interphase regimes of seven regimes proposed by Benveniste and Miloh (2001).

Sofia Mogilevskaya
University of Minnesota
mogil003@umn.edu

Anna Zemlyanova
Department of Mathematics
Kansas State University
azem@ksu.edu

MS72

An Averaged Mesoscopic Model of Active Particle Systems

Starting from a fine-scale dissipative particle dynamics (DPD) model of self-motile point particles, we derive mesoscale continuum equations by spatial averaging. The resulting stochastic continuum equations are similar to the phenomenological model of Toner and Tu. Unlike that model, our theory provides explicit constitutive equations in terms of the parameters of the DPD model, including a constitutive equation for the averaged stochastic force. Although the self-propulsion force in the DPD model contains no explicit mechanism for aligning the velocities of neighboring particles, the continuum equations include the commonly encountered cubically nonlinear (internal) body force density which is known to promote flocking.

Alexander Panchenko
Washington State University
panchenko@math.wsu.edu

MS72

Numerical and Analytic Study of the Robustness of Checkerboard Dynamic Materials

This work is a numerical and analytical study of wave motion and ¿ energy accumulation in non-perfect checkerboard dynamic materials (DM). Dynamic materials (DM) are materials whose properties vary in space and time. The material property pattern investigated in this work is an extension of the work of Lurie and Weekes in which two materials of matching wave impedance are distributed in the z-t plane in a rectangular checkerboard pattern. For certain values of material parameters, it was shown that there is focusing of characteristics which result in localized energy accumulation in linear waves propagating through the structure. Our work extends the applicability of the checkerboard focusing effect. We show that the focusing effect and energy growth found for the original sharp checkerboard extends to the case of the checkerboard with smooth transitions between materials, and also with impedance mismatch. The robustness of the energy accumulation effects will allow for actual construction of these dynamic materials to meet specific engineering goals.

William C. Sanguinet
Worcester Polytechnic Institute
williamcsanguinet@gmail.com

Suzanne L. Weekes
Worcester Polytechnic Institute (WPI)
sweekes@wpi.edu

MS73

Modeling and Simulation of Moving Contact Lines on Deformable Surfaces

When two immiscible fluids flow on a solid substrate, a contact line would form as the fluid-fluid interface meets the solid surface. Implementing a set of physically meaningful boundary conditions for the moving contact line problem has remained an issue of controversy and debate for many years. In recent models based on the continuum theory, a systematic approach to deriving the boundary conditions has been proposed. In this talk, we will present a continuum model for the elastic-substrate cases where two immiscible fluids flow on a deformable surface. We will focus on the derivation of its boundary conditions from the continuum framework, with its simulations for open-channel flow and droplet wetting as illustrations. We will also compare this model to those for the classical solid-substrate cases.

Hanwen Cui
National University of Singapore
hanwencui@u.nus.edu

Weiqing Ren
National University of Singapore and IHPC, A-Star
matrw@nus.edu.sg

MS73

Numerical Methods for Interfacial Flows with Surfactant

The research of surfactant systems is one of the important areas in soft condensed matter physics. The surfactant behaviors result in various kinds of interface/surface phenomena and also effect greatly on the physical characters of complex fluid systems. Here, we treat these problems in a physical way, and simulate the interface wetting and spreading phenomena of polydimethylsiloxane oil/ surfactant solution systems. We try to understand how the electrostatic/volume effect related to surface change the wetting status.

Yana Di
Institute of Computational Mathematics
Chinese Academy of Sciences
yndi@lsec.cc.ac.cn

Dan Hu
Shanghai Jiao Tong University

hudan80@sjtu.edu.cn

MS73

An Accurate Front Capturing Scheme for Tumor Growth Models with a Free Boundary Limit

In this talk, we are concerned with a class of tumor growth models under the combined effects of density-dependent pressure and cell multiplication, with a free boundary model as its singular limit when the pressure-density relationship becomes highly nonlinear. In particular, the constitutive law connecting pressure p and density ρ is $p(\rho) = \frac{m}{m-1}\rho^{m-1}$, and when $m \gg 1$, the cell density ρ may evolve its support according to a pressure-driven geometric motion with sharp interface along its boundary. The nonlinearity and degeneracy in the diffusion bring great challenges in numerical simulations. Prior to the present paper, there is lack of standard mechanism to numerically capture the front propagation speed as $m \gg 1$. In this paper, we develop a numerical scheme based on a novel prediction-correction reformulation that can accurately approximate the front propagation even when the nonlinearity is extremely strong. We show that the semi-discrete scheme naturally connects to the free boundary limit equation as $m \to \infty$. With proper spatial discretization, the fully discrete scheme has improved stability, preserves positivity, and can be implemented without nonlinear solvers. Finally, extensive numerical examples in both one and two dimensions are provided to verify the claimed properties in various applications.

Zhennan Zhou
Peking University
zhennan@bicmr.pku.edu.cn

MS74

Gradient Plasticity

Abstract Not Available At Time Of Publication.

Elias Aifantis
Aristotle University of Thessaloniki
mom@mom.gen.auth.gr

MS74

Beyond Classical Thermodynamics: Crystal Plasticity

Abstract Not Available At Time Of Publication.

Victor Berdichevsky
Wayne State University
vberd@eng.wayne.edu

MS74

Nonequilibrium Thermodynamic Theory of Dislocation-Mediated Plasticity

Nonequilibrium physics lies at the heart of applied materials research. The most important phenomena, such as deformation and failure, involve flows of energy and entropy through systems that are driven away from mechanical and thermal equilibrium. However, conventional theories of these phenomena have largely been phenomenological and non-predictive. Dislocation theory is an area that seems especially ripe for progress. A basic interpretation of the second law of thermodynamics requires that the dislocations in a deforming crystalline solid be characterized by a thermodynamically well-defined effective disorder temperature that differs greatly from the ambient temperature. Using this idea, plus an analysis of the ordinary thermally activated depinning of entangled dislocation lines, I will show how my colleagues and I are producing quantitative, first-principles explanations of many of the central experimental observations in this field. The list of these observations includes strain hardening, yielding transitions, grain-size effects, and adiabatic shear banding.

James Langer
Physics Department
University of California, Santa Barbara
james.langer@icloud.com

MS74

Thermodynamic Dislocation Theory: Thermal Softening and Shear Band Formation

The statistical-thermodynamic dislocation theory developed in our earlier studies is used here in an analysis of the experimental observations of thermal softening and adiabatic shear banding in steel by Marchand and Duffy (1988). Employing a small set of physics-based parameters, which we expect to be approximately independent of strain rate and temperature, we are able to explain experimental stress-strain curves at six different temperatures and four different strain rates. We make a simple model of a weak notch-like disturbance that, when driven hard enough, triggers shear banding instabilities that are quantitatively comparable with those seen in the experiments. We extend the theory to the case where excess dislocations appear and pile up near the grain boundaries leading to the kinematic hardening.

Khanh Chau Le
Ruhr University Bochum
Ruhr-Universitaet Bochum
chau.le@rub.de

MS75

Adaptive Algorithm for Sampling Large Deviation Functions

Large deviation theory has become a prominent tool in the study of physical systems, with a natural correspondence between mathematical and physical quantities. Indeed, the two main functions of the theory, the cumulant and rate functions, respectively generalize free energy and entropy for non-equilibrium systems. Information on these functions, provide insight on the system at hand, such as the existence of phase transitions. In this talk, we will focus on the numerical estimation of functions associated to fluctuations in time of ergodic averages. Such functions are in general very difficult to compute by direct Monte Carlo Markov Chain simulation, since an efficient sampling requires simulating an exponential number of trajectories with respect to time! This led to designing specific algorithms for this problem. A large family of methods relies on cloning dynamics, which introduce a selection mechanism between replicas to favor a desired behavior. Another range of methods resorts to importance sampling, which involves the estimation of an optimal drift. However, this drift is in general difficult to estimate. For this purpose, we present a strategy based on previous works of Borkar and collaborators, relying on stochastic approximation. The originality of our work is to build on the fly estimators of the cumulant function, its derivative, and the rate function at once. We provide relevant applications on equilibrium

and non-equilibrium toy examples.

Gregoire Ferre
CERMICS, Ecole Nationale des Ponts et Chaussées (ENPC)
gregoire.ferre@enpc.fr

Hugo Touchette
National Institute for Theoretical Physics (NITheP) South Africa
htouchette@sun.ac.za

MS75

Success and Failures of Saddle-Search Algorithms

I will review some recent analytical (and a few computational) results about saddle search algorithms, specifically dimer and GAD type methods. An ongoing struggle for their analysis is the lack of a global merit function, which makes it difficult (impossible?) to construct a globally convergent scheme. I will explain why this is the case, by constructing examples that lead to blow-up and cycling behaviour. Time permitting, I will then show some new attempts (joint work with Letif Mones) that may (or may not?) be able to overcome these limitations.

Christoph Ortner
University of Warwick
c.ortner@warwick.ac.uk

Antoine Levitt
Inria and Ecole des Ponts ParisTech
antoine.levitt@inria.fr

MS75

Accelerated Sampling with Local Entropy

Rough energy landscapes, containing many local minima, appear in a variety of applications, including condensed and soft matter and in uncertainty quantification. This roughness can cripple many sampling techniques. Using a notion of "local" entropy, sampling of rough energy landscapes can be significantly accelerated using an approximation of the smoothed force field. This talk will present the algorithm and examples of the method. Open problems will also be highlighted.

Gideon Simpson
Department of Mathematics
Drexel University
grs53@drexel.edu

MS75

Implementation of Multiscale-Spectral Gfem and Optimal Oversampling

We evaluate a full numerical implementation of the Multiscale-Spectral Generalized Finite Element Method (MS-GFEM) developed in [I. Babuška and R. Lipton, Multiscale Modeling and Simulation 9 (2011), pp. 373-406]. MS-GFEM allows for rough coefficients and therefore does not rely on separation of length scales of material heterogeneity. For particle reinforced composites our simulations demonstrate contrast independent exponential convergence of MS-GFEM solutions. We introduce a method to reduce the computational cost of generating local approximating spaces. This method retains accuracy while reducing the computational work necessary to generate local bases. We go further and introduce new nearly-exponential approximation spaces to further reduce the computational complexity. The nearly exponential convergence is demonstrated and examples are provided.

Ivo Babuska
ICES, The University of Texas at Austin
babuska@ices.utexas.edu

Robert P. Lipton
Department of Mathematics
Louisiana State University
lipton@math.lsu.edu

Paul Sinz
Michigan State University
sinzpaul@msu.edu

Michael Stuebner
University of Dayton Research Institute
michael.stuebner@udri.udayton.edu

MS76

Detection of Capillary-Mediated Interface Energy Fields Using Phase-Field Residuals

Grain boundary grooves are common features observed along polycrystalline solid-liquid and solid-vapor interfaces. Their microstructure profiles may be approximated as variational grain boundary grooves derived from the Euler-Lagrange equation. Such grooves yield Gibbs-Thomson thermo-potential distributions, the vector gradients of which excite capillary-mediated fluxes. These fluxes exhibit divergences that cool the interface slightly, affect its energy budget and speed, and stimulate pattern formation. The existence of active energy fields on grain boundary grooves was uncovered and measured precisely using multiphase-field simulations. Interfacial energy fields introduce small non-linear components into a grooves otherwise linear thermo-potential distribution. Non-linearity was measured here as residuals of the thermo-potential, which are proportional to the interface cooling rate. As will be discussed, phase-field measurements also confirm analytic predictions of persistent bias fields that are derived for grain boundary grooves from sharp-interface thermodynamics, and which cause higher-order self-interactions of groove microstructures with their own capillary fields.

Martin E. Glicksman
Florida Institute of Technology
mglicksman@fit.edu

Kumar Ankit
Arizona State University
kumar.ankit@asu.edu

MS76

Phase-field Modeling of Morphological Evolution During Liquid Metal Dealloying

Liquid metal dealloying (LMD) is a novel technique to produce nanocomposite and open nanoporous metal structures with ultra-high interfacial area for diverse applications. In this talk, we first review the results of a recent combined phase-field simulation and experimental study of dealloying of Ta-Ti alloys by immersion in a Cu melt. The results reveal how diffusion-limited interfacial and bulk transport phenomena interact to form a rich variety of topologically

disconnected and connected structures and allow us to derive scaling laws governing nano/microstructural lengthscales and dealloying kinetics. We then present more recent results that extend this study to the more general case where a bimetallic metal melt contains some fraction of the miscible alloy element by investigating the behavior of Ta-Ti alloys in contact with Cu-Ti melts. Phase-field simulations show that Ti addition in the melt leads to slower dealloying kinetics and increased ligament width. In addition, it yields a transition to a morphologically stable planar dissolution regime when the Ti concentration exceeds a threshold. The existence of this transition is validated experimentally and explained theoretically within the framework of interfacial spinodal decomposition.

Longhai Lai
Northeastern University, USA
lai.lo@husky.neu.edu

Bernard Gaskey
Johns Hopkins University, USA
bgaskey1@jhu.edu

Jonah Erlebacher
Department of Materials Science and Engineering
The Johns Hopkins University
Jonah.Erlebacher@jhu.edu

Alain Karma
Northeastern University
karma@presto.physics.neu.edu

MS76

Phase-Field and CALPHAD: A Successful Liaison

The connection between Phase-Field models and CALPHAD models is discussed against the background of minimization of the total Gibbs energy of a system. Both methods are based on separation of a multiphase system into individual contributions of the bulk phases, which are described by appropriate models in composition, temperature, and pressure. While the CALPHAD method uses a global minimization of the total Gibbs energy, the Phase-Field method introduces local interactions, interfaces, and diffusion and allows for non-equilibrium situations. Thus, the Phase-Field method is much more general by its concept, however, it can profit a lot if realistic thermodynamic descriptions, as provided by the CALPHAD method, are incorporated. The talk discusses details of a direct coupling between the Multiphase-Field method and the CALPHAD method. Special emphasis is given to the case of sub-lattice ordering in the CALPHAD framework, but with extension to external constraint coming from the local constitutive fields.

Ingo Steinbach
Ruhr University Bochum
ingo.steinbach@ruhr-uni-bochum.de

MS76

Phase Field Modeling with Strong Interfacial Energy Anisotropy and Bulk Diffusivity

Phase field methods are well suited to modeling microstructure evolution in materials science. However, incorporation of realistic physical effects can introduce technical challenges as well as increased computational cost. This is particularly true in the case of strong interfacial energy anisotropy, where sharp corners (edges) form in the equilibrium shape of a second-phase particle. Interfaces with unstable orientations undergo thermal faceting, in which interfaces with thermodynamically unstable orientations decompose into stable ones. Here, we present new analysis of an existing model, which uses a higher-order regularization term to round sharp corners and ensure well-posedness of the thermal faceting process. We show via asymptotic analysis how a linear regularization term leads to a modification of the anisotropic interfacial energy, which explains regularization-dependent changes to the equilibrium shape observed in simulations. Exploring the relationship between model inputs (anisotropy and regularization parameters) and the modified interfacial energy, we show that this model can be parametrized to effectively provide the desired interfacial energy and the resulting equilibrium shape. Finally, we discuss the differences between this model and others currently in use, notably those that convexify the interfacial energy anisotropy, as well as another existing formulation that results in a constant interfacial width with respect to orientation.

W. Beck Andrews, Katsuyo Thornton
Department of Materials Science and Engineering
University of Michigan
wband@umich.edu, kthorn@umich.edu

MS77

Generalized Disclinations in Defect Mechanics

The geometrical aspects of the work of Weingarten and Volterra related to defects in solids consider the question of characterizing the possible jumps in the displacement and rotation fields corresponding to a *locally* compatible C^2 strain field in a non-simply connected domain. The question has a natural 'dual' in compact simply connected domains leading to singularities concentrated on curves called *dislocations* and *disclinations*. A close examination of this idea motivated by possible extensions for dealing with strain fields that are not smooth as well (as arises in dealing with solid-solid to phase transformations) naturally leads to the definition of the concept of *generalized disclinations* (g.disclinations). We discuss this construction and its physical realizations in grain and phase-boundary mechanics like disconnections and penta-twins, provide the Burgers vector of a g.disclination dipole, and show that even though a g.disclination dipole and a dislocation can be topologically indistinguishable, the dipole can be energetically favored in many circumstances.

Amit Acharya
Civil and Environmental Engineering
Carnegie Mellon University
acharyaamit@cmu.edu

Chiqun Zhang
Carnegie Mellon University
Civil and Environmental Engineering
chiqun0524@gmail.com

MS77

Purely Metric Characterizations of Dislocations

The rigorous analysis of dislocations and their homogenization has seen significant advances in recent years, notably using Gamma-convergence techniques. The standard approach is to model dislocations using a strain field, which is not the gradient of a displacement field. Another approach, which is more geometric in nature, is to model the defect through the intrinsic geometry (a Riemannian metric) of

the body manifold. In this lecture, I will demonstrate how many of the recent results are naturally obtained within this framework. This is a joint work with Cy Maor.

Raz Kupferman
Hebrew University
Israel
raz@math.huji.ac.il

MS77

Elastic Energies of Continuous Distributions of Dislocations

Continuous distributions of dislocations are often modeled by manifolds endowed with flat, non-symmetric connections; these models are typically not associated with any specific constitutive relations. In this talk I will show how recent notions of homogenization of dislocations can be applied to obtain elastic energies for bodies with distributed dislocations, and how this sheds light on the relation between the above-mentioned connection and the Noll-Wang notion of "material connection" associated with a constitutive relation.

Cy Maor
Department of Mathematics
University of Toronto
cmaor@math.toronto.edu

Raz Kupferman
Institute of Mathematics,
The Hebrew University
raz@math.huji.ac.il

Marcelo Epstein
University of Calgary
Calgary, AB, Canada.
mepstein@ucalgary.ca

MS77

Discrete Structures in Continuum Descriptions of Defective Crystals

I discuss various mathematical constructions that combine together to provide a natural setting for discrete and continuum geometric models of defective crystals. In particular I provide a quite general list of 'plastic strain variables', which quantifies inelastic behaviour, and exhibit rigorous connections between discrete and continuous mathematical structures associated with crystalline materials that have a correspondingly general constitutive specification.

Gareth Parry
University of Nottingham
gareth.parry@nottingham.ac.uk

MS78

A Local Morphological Descriptor of Particulates, Cells and Porous Media, and Its Uses

I present a method to characterize quantitatively the local morphology of particulate, cellular, and porous media in two and three dimensions. The method is based on a special tessellation by quadrons, each of which is assigned a structure tensor. The advantages of the method are described. I then describe the usefulness of the method for a number of applications:
1. It forms the basis for a statistical mechanical formalism of a-thermal particulate systems [Blumenfeld and Edwards, Phys. Rev. Lett. 90, 114303 (2003)] [Blumenfeld and Edwards, Eur. Phys. J. E 19, 23 (2006)] [Blumenfeld et al., Phys. Rev. Lett. 109, 238001 (2012)] [Blumenfeld et al., Phys. Rev. Lett. 116, 148001 (2016)].
2. The structure tensor is useful for closing the stress equations in isostatic systems [Ball and Blumenfeld, Phys. Rev. Lett. 88, 115508 (2002)] [Blumenfeld, Phys. Rev. Lett. 93, 108301 (2004)] [Gerritsen et al., Phys. Rev. Lett. 101, 098001 (2008)].
3. It makes possible to detect subtle characteristics that distinguish different structures from one another [Matsushima and Blumenfeld, Phys. Rev. Lett. 112, 098003 (2014)] [Hihinashvili and Blumenfeld, Granular Matter 14, 277 (2012)].
4. It makes possible systematic derivations of the dependence of macroscopic physical properties, such as permeability to flow, catalysis and heat exchange, on the statistical characteristics of the microstructure. Time permitting, the derivation procedure will be outlined.

Rafi Blumenfeld
Pekign U., Imperial College, & Cambridge U.
rbb11@cam.ac.uk

MS78

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Sharon C. Glotzer
Chemical Engineering
University of Michigan
sglotzer@umich.edu

MS78

Machine Learning of Complex Crystal Structures *via* Local Bond Orientational Order Diagram Fingerprints

Bond orientational order diagrams, or BOODs, have been used for many years as fingerprints to identify crystals in simulations. While they often work well to identify single-crystalline regions, BOODs can be difficult to use when examining polycrystalline samples or analyzing systems *via* machine learning. In this talk we discuss an alternative characterization of near-neighbor bonds using rotationally-invariant local environment descriptors and show the application of these local BOODs for crystal identification. Armed with these descriptors, we can generate machine learning models for enhanced sampling, high-throughput analysis, and automatic experiment design.

Matthew Spellings, Julia Dshemuchadse, Sharon Glotzer
University of Michigan
mspells@umich.edu, djulia@umich.edu, sglotzerkjc@umich.edu

MS78

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Juan de Pablo
University of Chicago

depablo@uchicago.edu

MS79

On the Universal Korn Interpolation and Korn's Second Inequalities for Shells with Nonconstant Thickness

We consider shells of non-constant thickness in three dimensional Euclidean space around compact regular surfaces which have bounded principal curvatures. We derive Korns interpolation and second inequalities on that kind of domains for H^1 vector fields, imposing no boundary or normalization conditions on u. This is the first work that determines the asymptotics of the optimal constant in the classical Korn second inequality for shells in terms of the domain thickness in almost full generality, the inequality being fulfilled for practically all thin domains $\Omega \subset R^3$ and all vector fields $u \in H^1(\Omega)$. Moreover, the Korn interpolation inequality is stronger than Korns second inequality, and it remains sharp for all the main shell-curvature situations (positive, negative and zero Gaussian curvatures).

Davit Harutyunyan
University of Utah
harutyunyan@ucsb.edu

MS79

On Thin Rods with Misfit

There are many examples in nature of thin rods with misfit (or prestrain), including the metallic bilayer and the tendrils of a plant. We explain the shape that these rods take. In particular, we show that the thin-rod Gamma-limit of a three-dimensional elastic energy functional with misfit yields a rod theory with intrinsic bend or twist. In the examples mentioned above we show that our rod theory agrees with the literature, and explain the connection between the classical calculations and the present result. Finally, we ask what additional information we can gain if we do not know the exact form of the misfit, but only that it has certain symmetries.

Ethan O'Brien
Courant Institute of Mathematical Sciences
New York University, USA
obrien@cims.nyu.edu

MS79

An Asymptotic Variational Problem Modeling An Elastic Sheet on Water, Lifted at One End

We discuss a $1D$ variational problem modeling an elastic sheet on water, lifted at one end. Its terms include the membrane and bending energy of the sheet as well as terms due to gravity and surface tension. By studying a suitable *Gamma*-limit, we identify a parameter regime in which the sheet is inextensible, and the bending energy and weight of the sheet are negligible. In this regime, the problem simplifies to one with a simple and explicit solution. This project was motivated by discussions with Benjamin Davidovitch (who is currently analyzing the same problem using different methods).

David Padilla-Garza
Courant Institute of Mathematical Sciences
New York University
dpg310@nyu.edu

MS79

Non-Euclidean Elasticity and Asymptotic Rigidity of Manifolds

The fundamental problem of non-Euclidean elasticity is finding an immersion of a body in the ambient space which minimizes the elastic energy (distortion). Let $(M, g), (N, h)$ be Riemannian manifolds. Every mapping $f : (M, g) \to (N, h)$ has an associated measure of distortion - an average distance of df from being an isometry. Reshetnyak's rigidity theorem states that a sequence of mappings between Euclidean domains whose mean distortion tends to zero has a subsequence converging to an isometry. I will present a generalization of Reshetnyaks theorem to the general Riemannian setting, and discuss some applications to elasticity theory.

Asaf Shachar
Hebrew University
asaf.shachar@mail.huji.ac.il

Raz Kupferman
Institute of Mathematics,
The Hebrew University
raz@math.huji.ac.il

Cy Maor
Department of Mathematics
University of Toronto
cmaor@math.toronto.edu

MS80

CALPHAD: Past, Current and Future

The CALPHAD (CALculation of PHAse Diagram) method is the key component in materials design. In this presentation, its history of is briefed, its current status is reviewed, and future directions are discussed. The CALPHAD computational tools and algorithms developed over the years are represented by three commercial software packages. More recent development includes the new algorithms and open-source programs for equilibrium calculations and open-source program for high-throughput thermodynamic modeling and uncertainty quantification. Remaining challenges will also be examined.

Zi-Kui Liu
Department of Materials Science and Engineering
Penn State University
prof.zikui.liu@psu.edu

MS80

Energy Minimization Challenges: Metastability, Vacancies and Uncertainty

This talk will discuss several mathematical challenges associated with traditional CALPHAD formalism, including uncertainty quantification (UQ) and the pitfalls of global Gibbs energy minimization. There is an obvious lack of UQ tools capable of assessing the uncertainty in thermodynamic calculations. This work focuses on developing quantitative measures of uncertainty associated with constructing the phase diagram from a given Gibbs energy, which complements efforts in assessing the errors associated with the choice of the Gibbs functionals and experimental measurements. Depending on the numerical solver

used, the choice of the initial condition and formulation of the optimization problem, the user might arrive at the stable solution or get stuck in a metastable equilibrium. We will introduce the concept of uncertainty diagram which helps quantify the energy gap between nearby equilibria and discuss how different analytically equivalent Gibbs energy minimization formulations may lead to drastically different solutions. Some practical recommendations will be made to help avoid some of these complications.

Jeff Snider, Maria Emelianenko, Igor Griva
George Mason University
jeff@snider.com, memelian@gmu.edu, igriva@gmu.edu

MS80

Bayesian Analysis of Thermodynamic Data

Modeling thermodynamic properties of multi-component materials is important for both basic science and engineering applications. Unfortunately, many journal articles report thermodynamic data especially phase equilibrium diagrams without uncertainty/confidence intervals. In addition, the complexity of the physics and chemistry of the multi-component materials makes evaluating the quality of the data and models quite difficult. In this work, we discuss the theoretical, mathematical and computational challenges associated with quantifying uncertainty in a multi-dimensional parametric space with application to thermodynamic data sets and equilibrium phase diagrams. The scientific approach involves a Bayesian method that simultaneously accounts for different types of data and its provenance to deliver uncertainty intervals. Data analysis is enhanced by machine learning methods. The presentation ends with a discussion of the changing role of computation in materials design.

Marius Stan, Noah Paulson, Elise Jennings
Argonne National Laboratory
mstan@anl.gov, npaulson@anl.gov, ejennings@anl.gov

MS80

Integration of Thermodynamic Potentials into Phase-Field Models and Transport Phenomena

There has been recent interest in the incorporation of CALPHAD-type thermodynamic potentials as driving forces for transport phenomena and phase evolution, an approach which can ensure thermodynamically self-consistency and increase the accuracy and robustness of modelling techniques. This work describes a method of combining single phase thermodynamic potentials into a multiphase composite potential suitable for integration in temperature dependent, multicomponent phase-field models. Implicit interfacial energy contributions are avoided by starting from a grand potential formulation and approximating the Legendre transform between grand and Helmholtz potentials about a known equilibrium state. The resulting composite function is explicit, reproduces the equilibrium states exactly, approximates the non-equilibrium energy surface well, and is smooth such that it can be differentiated to provide the driving forces for coupled heat and mass transport and phase change in a thermodynamically self-consistent manner. Examples include simulation of a sequence of phase transformations for intermetallic growth in Al-Mg, interdiffusion for advanced nuclear research reactor fuel, and in transient heating experiments with phase change.

Michael Welland
Canadian Nuclear Laboratories
Canada
michael.welland@cnl.ca

Eric Tenuta, Markus Piro
Univ. Ontario Inst. Tech.
eric.tenuta@uoit.net, markus.piro@uoit.ca

Stephen Hibbins, Ning Wang
Canadian Nuclear Laboratories
stephen.hibbins@cnl.ca, ning.wang@cnl.ca

MS81

Fundamental Limits to the Optical Response of Materials, Over Any Bandwidth

Near-field nanophotonics offers the promise of orders-of-magnitude enhancements for phenomena ranging from spontaneous-emission engineering to Casimir forces via zero-point quantum fluctuations. An increasing variety of approaches–photonic crystals, metamaterials, metasurfaces, antennas, and more–has underscored our lack of understanding as to how large these effects can be. We provide a general answer to this question, deriving the first sum rule for near-field optical response as well as general upper bounds for *any* bandwidth, i.e. power–bandwidth limits. Our framework relies on a unification of the analytic properties of causal functions with energy-conservation constraints that emerge in any scattering system. We computationally verify the sum rule, and demonstrate the capability of the power-bandwidth limits to identify optimal nanophotonic materials for any combination of frequency and bandwidth

Owen D. Miller
Yale Applied Physics
owen.miller@yale.edu

MS81

Modeling Photo-Actuation in Ribbons

Abstract Not Available At Time Of Publication.

Paul Plucinsky
University of Minnesota
plucinsp@gmail.com

MS82

A Novel Coarse-Grained Formulation of Density Functional Theory for Studying Defects in Crystalline Materials

Density Functional Theory (DFT) has the highest accuracy to cost ratio among all electronic structure methods and provides valuable insight in understanding and predicting a wide range of materials properties. Defects in crystalline solids, play crucial role in determining macroscopic properties of materials. The profound significance of defects underlies from the coupling between the discrete effects of the lattice, chemical effects of the core and the long-range effects of the elastic field. While DFT is capable of accurately describing the chemistry of the defect core, but are too complicated and expensive for defects with long range fields, methods capable for describing long-range fields rely on empiricism and lack fidelity. This poses an outstanding dual challenge to simulate defects from first principles. To overcome this, we develop a novel coarse-grained formulation of DFT. We employ Linear Scaling Spectral Quadra-

ture method to solve for the electronic fields and develop a coarse-graining strategy based on updated Lagrangian method to describe the long-range fields. We discuss a real space formulation based on high-order finite differences, local reformulation of electrostatics, reformulation of the atomic forces and a parallelization strategy based on domain decomposition method. The developed formulation is sublinear scaling with respect to the system size and has to potential to efficiently simulate defects in crystalline materials from first principles.

Swarnava Ghosh
CalTech
swarnava@caltech.edu

Kaushik Bhattacharya
Howell N. Tyson Sr. Professor of Mechanics
California Institute of Technology
bhatta@caltech.edu

Michael Ortiz
California Institute of Technology
ortiz@aero.caltech.edu

MS82

Continuous and Discontinuous Methods for Accurate, Large-Scale Electronic Structure Calculations

In this talk, we discuss recent developments in finite element (FE) based methods for the solution of the Kohn-Sham equations that have made possible larger, more realistic calculations than possible before, of metals and insulators alike. In particular, we discuss recent partition of unity enriched finite element (PUFE) methods, which build known atomic physics into the basis while retaining strict locality and systematic improvability. By incorporating known physics, these methods can achieve the required accuracies with an order of magnitude fewer degrees of freedom (DOF) than required by traditional planewave based methods as implemented in widely used VASP and ABINIT codes, among many others. However, with such enrichment comes more costly quadrature, nonorthogonality, and some degree of ill-conditioning. We discuss two directions we are currently pursuing to address these issues while retaining strict locality and systematic improvability: Discontinuous Galerkin (DG) and Flat-Top Partition of Unity (FT-PU) methods. Both approaches yield compact, well conditioned, standard discrete eigenvalue problems amenable to efficient parallel solution via Chebyshev-polynomial filtered subspace iteration. We conclude with recent results for quantum molecular dynamics of general metallic and solid-liquid interface systems of 4,000 atoms and more, with application to lithium-ion batteries, and discuss current progress taking us to 10,000 atoms and more.

John Pask
Lawrence Livemore National Lab
pask1@llnl.gov

MS82

Electronic and Thermal Transport for Thermoelectric Materials

Thermoelectrics are used for the conversion of thermal and electrical energy. They offer a number of advantages over competing technologies including scalability to small sizes and temperature differences, simple reliable designs and often low cost. However, these devices have not seen wide application in energy applications due to their limited conversion efficiency. This is a consequence of the limited performance of current thermoelectric materials, which can be characterized by a dimensionless figure of merit, ZT, which is proportional to square Seebeck coefficient, conductivity and temperature and inversely proportional to thermal conductivity. There is no known fundamental limit on ZyT. However, the combination of transport parameters entering ZT is a contradictory combination that does not occur in ordinary materials. Boltzmann transport calculations show that electronic structure plays a remarkably subtle role in thermoelectric performance. A long sought connection is drawn between topological insulators and high ZT thermoelectrics, explaining the overlap between these two interesting materials classes. Characteristics that can be used to identify new thermoelectric compositions are discussed and an efficient computational screening method based on an electronic fitness function is presented.

David Singh
University of Missouri
singhdj@missouri.edu

MS82

A Numerical Linear Algebra Perspective of Projection Based Embedding Theory

Embedding methods play an important role in reducing the computational cost of electronic structure calculations, both in mean field and many body quantum theories. Its main application arises in the modeling of perturbations (or defects) in materials, in which the perturbation is embedded in an underlying environment whose effect is incorporated via boundary conditions. The choice of the boundary conditions is, in general, discretization-dependent and can greatly affect the accuracy of the model. In this talk we study the recently developed Projection based Embedding Theory (PET) from a linear algebra perspective. We show how it seamlessly provides versatile boundary conditions independently of the discretization. In addition, we present a perturbation based extension to the method, which improves the accuracy by solving a small set of linear problems. We will also demonstrate the performance of PET for electronic structure calculations of real chemical systems using the KSSOLV software package.

Leonardo Zepeda
Lawrence Berkeley National Laboratory
lzepeda@lbl.gov

MS83

Rigidity Percolation in Composite Materials

Mechanical or rheological percolation is a phenomenon in materials processing wherein ‘filler rod-like particles are incorporated into polymeric materials to enhance the composites mechanical properties. Experiments have well characterized a nonlinear phase transition from floppy to rigid behavior at a threshold filler concentration that is beyond the electrical percolation threshold. However, the underlying mechanism is not well understood. It is our hypothesis thatin appropriate experimental systemsthis phenomenon coincides with the formation of a spatially extended component of rods that is not only connected, but furthermore the topology of inherent contacts restricts any nontrivial degrees of freedom within the component (rigidity percolation). In order to validate this hypothesis, we develop an iterative graph compression algorithm to characterize rigidity in Monte Carlo samples of rod dispersions. In a

previous presentation of SIAM-MS, we demonstrated the efficacy of this approach by estimating the rigidity percolation threshold in random 2D fiber dispersions, wherein rigidity percolation has already been characterized. Here, we extend this method to estimate the rigidity percolation threshold and associated correlation length parameter in systems of randomly dispersed 3D fibers, wherein rigidity percolation has not been previously investigated. Furthermore, we vary the anisotropy of the rod dispersions in order to mimic realistic processing conditions.

Samuel Heroy, Feng Shi
UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL
SAM.HEROY@GMAIL.COM, bill10@email.unc.edu

Dane Taylor
Department of Mathematics
University of North Carolina at Chapel Hill
danet@buffalo.edu

Greg Forest
UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL
forest@unc.edu

Peter J. Mucha
University of North Carolina
mucha@unc.edu

MS83

Numerical Methods for Singular Integro-Differential Equations with Applications to Surface Elasticity

The mechanical problems with boundary surface energies of the GurtinMurdoch or Steigmann-Ogden type can often be reduced to systems of singular integro-differential equations. These systems include derivatives of the unknowns of the first and third orders, correspondingly. Several methods exist in scientific literature to obtain numerical solutions to systems appearing in problems with Gurtin-Murdoch surface energy. Those include approximations by Chebyshev polynomials and approximations by splines. At the same time, due to the higher order terms, not much is known about numerical solution of systems of singular integro-differential equations with Steigmann-Ogden energy. In this talk, we will review the main methods used for the Gurtin-Murdoch type of problems and derive the numerical method for tackling the singular integro-differential equations appearing in the Steigmann-Ogden theory.

Alexia J. Machina
Kansas State University
ajmachina@ksu.edu

MS83

Multiscale Modeling of Weakly Interacting Incommensurate 2Dimensional Lattices

I derive a continuum variational model for a two-dimensional deformable lattice of atoms interacting with a two-dimensional rigid lattice. The starting point is a discrete atomistic model for the two lattices, which are assumed to have slightly different lattice parameters and, possibly, a small relative rotation. This is a prototypical example of a three-dimensional system consisting of a graphene sheet suspended over a substrate. A discrete-to-continuum procedure is used to obtain a continuum model that recovers both qualitatively and quantitatively the behavior observed in the corresponding discrete model. The continuum model predicts that the deformable lattice develops a network of domain walls characterized by large shearing, stretching, and bending deformation that accommodates the misalignment and/or mismatch between the deformable and rigid lattices. Two integer-valued parameters, which can be identified with the components of a Burgers vector, describe the mismatch between the lattices and determine the geometry and the details of the deformation associated with the domain walls.

Patrick Wilber
University of Akron
jw50@uakron.edu

MS83

Size-Dependency in Fracture Modeling with Steigmann-Ogden Surface Energy

A problem of a straight mixed mode non-interface fracture in an infinite plane is treated analytically with the help of complex analysis techniques. The surfaces of the fracture are subjected to surface elasticity in the form proposed by Steigmann and Ogden. The boundary conditions on the banks of the fracture connect the stresses and the derivatives of the displacements. The mechanical problem is reduced to two systems of singular integro-differential equations which are further reduced to the systems of equations with logarithmic singularities. It is shown that modeling of the fracture with the Steigmann-Ogden elasticity produces the stress and strain fields which are bounded at the crack tips. The existence and uniqueness of the solution for almost all the values of the parameters is proved. Additionally, it is shown that introduction of the surface mechanics into the modeling of fracture leads to the size-dependent equations. A numerical scheme of the solution of the systems of singular integro-differential equations is suggested, and the numerical results are presented for different values of the mechanical and the geometric parameters.

Anna Zemlyanova
Department of Mathematics
Kansas State University
azem@ksu.edu

MS84

Dislocation Dynamics Simulations of Materials with Complex Physics

Discrete dislocation dynamics (DDD) simulations provide a technique for examining the effects of fundamental dislocation physics on the plastic response of crystalline solids. Many DDD simulations focus on relatively simple materials and loading conditions, such as glide-motion-dominated plasticity of pure face-centered and body-centered cubic crystals. In this presentation, we provide an overview of the more complex physical aspects of dislocation-mediated plasticity in the context of DDD. We consider both physics that are intrinsic to the crystal lattice (elastic anisotropy, nonlinear drag, and low crystallographic symmetry) and extrinsic physics that are due to defects other than dislocations (solutes, vacancies, precipitates, and grain boundaries). For each of these classes of physics, we first discuss the conditions under which they are relevant, followed by an examination of the fundamental ways in which the behaviors of dislocations are affected by the physics, and finally a presentation of the methods that have been de-

veloped for incorporating the physics in DDD. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Sylvie Aubry
Lawrence Livermore National Laboratory
sylvie.aubry@llnl.gov

MS84

The Role of Complexity in Dislocation Mechanics

Abstract Not Available At Time Of Publication.

Mick Brown
Cavendish Laboratory, Cambridge
lmb12@cam.ac.uk

MS84

The Mathematical Development of Continuum Dislocation Dynamics Equations at Finite Deformation

We present a finite deformation, density based dislocation dynamics approach for mesoscale deformation of single crystals. A derivation of the dislocation transport equations at finite strain and lattice rotation in Lagrangian and Eulerian forms is outlined, with a special focus on the kinematic coupling of dislocation density evolution on individual slip systems and to the coupling via cross slip and dislocation reactions. The relevant crystal mechanics, thermodynamics, and constitutive closure questions will be discussed.

Anter El-Azab
Purdue University
aelazab@purdue.edu

Kyle Starkey
purdue
starkeyk@purdue.edu

MS84

Mesoscale Modeling of Dislocations in Face-Centered Cubic Metals

Dislocations are prevalent in metals and play an important role in plastic deformation. While atomistic simulations are desirable in studying dislocations, they are limited to nano/submicron length scale. On the other hand, classical continuum models do not naturally incorporate the discrete atomic-scale degrees of freedom needed to define the dislocation core structure. In this work, we explore the core structure/energy/stress of dislocations in Al using a variety of meso-scale dislocation models, i.e., concurrent atomistic-continuum modeling [Xu et al., Int. J. Plast. 72 (2015) 91], phase-field dislocation dynamics [Beyerlein and Hunter, Philos. Trans. R. Soc. A 374 (2016) 20150166], and atomistic phase-field microelasticity [Mianroodi and Svendsen, J. Mech. Phys. Solids 77 (2015) 109]. In particular, special attention is paid to mixed-type dislocations, whose characteristics cannot be extrapolated from those of pure characters and which have received less attention in the literature up to this point. For phase-field-based modeling of these, the generalized stacking fault energy surface of Al is calculated using density functional theory. Results are benchmarked against molecular statics and possible sources of errors in these mesoscale calculations are discussed. A dislocation loop is then modelled using these approaches to shed light on their abilities to describe more realistic mixed-type configurations, potentially assisting in designing stronger metallic materials.

Shuozhi Xu
University of California, Santa Barbara
shuozhixu@ucsb.edu

Jaber Mianroodi
RWTH Aachen
Max-Planck-Institut fur Eisenforschung GmbH
jaber.rezaeimianroodi@cmm.rwth-aachen.de

Abigail Hunter
Los Alamos National Laboratory
ahunter@lanl.gov

Irene Beyerlein
UCSB
beyerlein@ucsb.edu

Bob Svendsen
Aachen University
b.svendsen@mpie.de

MS85

Numerical Methods for Deterministic and Stochastic Total Variation (tv) Flow

The total variation (TV) flow is a gradient flow for the TV energy functional, it arrives from various applications in image processing and materials science and has been intensively studied analytically and numerically. In order to incorporate uncertainties/noises from materials and images, it is necessary to consider stochastic version(s) of the TV flow. In this talk, we shall first review some known analytical and numerical works for the deterministic TV flow. We then introduce a stochastic TV flow (sTV) driven by additive or multiplicative noises and present some newly obtained well-posedness results for the sTV flow based on two different variational inequality weak formulations. We also present a complete finite element numerical analysis for the sTV flow based on one variational formulation. Finally, Computation experiment results will also be given for the proposed finite element methods. This is a joint work with Andreas Prohl of University of Tubingen, Germany, and Shu Ma of Northwest Polytechnical University, China.

Xiaobing H. Feng
The University of Tennessee
xfeng@math.utk.edu

MS85

Singularity Formation in Solid Thin Films Using Lubrication-Type Equations

Following recent studies by Liu and Xu (2016) we investigate a fourth order partial differential equation with exponential nonlinearity. This is a solid thin film model that describes the evolution of crystal surfaces, and is also related to a family of modified lubrication equations. Due to the singular nature of the PDE, we show that for proper initial conditions the solution can blow up in finite time in a non-self-similar manner.

Hangjie Ji
Duke University, Department of Mathematics

hangjie@math.ucla.edu

MS85

The Threshold Dynamics Method and Applications

In this talk, I will review some recent work on the threshold dynamics method for diffusion generated motion of the interface on solid surface. We also analyze the contact line behavior of the method from asymptotic expansion and the contact line dynamics is also derived. Applications to wetting on solid surface, image segmentation are presented.

Xiaoping Wang
Hong Kong University of Science and Technology
mawang@ust.hk

MS85

Bound States of 'Multiple Domain Wall' Dirac Operators and 'Multiple-edge States' in Honeycomb Structures

We study bound states of a one-dimensional Dirac operator with spatially varying 'mass' term which controls the existence of states localized along appropriate 'edge' defects in honeycomb structures. It is well known that when the mass function has the form of a 'kink', or *domain wall*, the Dirac operator has a unique *zero mode*: an eigenfunction with eigenvalue zero. By a Liapunov-Schmidt reduction to an effective matrix problem, we prove that when the mass function has the form of *two* domain walls separated by a sufficiently large distance, the Dirac operator has two near-zero eigenvalues, whose associated eigenfunctions are linear combinations of shifted copies of the single domain wall zero mode. Our methods extend easily to the case of n domain walls equally spaced from each other, and to more general spatial separations of the domain walls. Our results suggest that appropriate 'n edge' defects in honeycomb structures will spawn precisely n states localized to the defects.

Alexander Watson
Duke University
Department of Mathematics
abwatson@math.duke.edu

Jianfeng Lu
Mathematics Department
Duke University
jianfeng@math.duke.edu

Michael I. Weinstein
Columbia University
miw2103@columbia.edu

MS86

A Hierarchy of Boundary Conditions for Crystal Defect Calculations

I will present a sequential multi-scale approach for defect calculations in atomic crystals. These defects include point defects as well as dislocations. At the heart of the approach is a new hierarchy of boundary conditions used for the atomistic relaxation that is derived from a precise understanding of the elastic far-field generated by the defect. This is joint work with Christoph Ortner and Thomas Hudson.

Julian Braun
University of Warwick
j.braun@warwick.ac.uk

MS86

Numerical Methods for Large-scale Real-space Kohn-Sham DFT Calculations

We present recent developments in large-scale real-space Kohn-Sham DFT calculations using finite element discretization, which include the efficacy of higher-order and enriched finite-element discretizations in DFT calculations, and the demonstration of the efficiency and scalability of Chebyshev filtering algorithm for pseudopotential and all-electron calculations. Further, the development of a subquadratic-scaling approach based on a subspace projection and Fermi-operator expansion will be discussed, which will be the basis for the future development of coarse-graining techniques for Kohn-Sham DFT. The developed techniques have enabled, to date, pseudopotential calculations on $\sim$ 10,000 atoms, as well as all-electron calculations on systems containing $\sim$ 10,000 electrons.

Vikram Gavini
Mechanical Engineering, University of Michigan
vikramg@umich.edu

Phani S. Motamarri, Bikash Kanungo
University of Michigan
phanim@umich.edu, bikash@umich.edu

MS86

Coarse-Grained Modeling of Defects at Grain Boundaries by the Amplitude Expansion of the Phase-Field Crystal Model

The Phase-Field Crystal (PFC) approach describes the dynamics of the local atomic probability density, n, on diffusive time scales. It generally requires a fine spatial discretization, which limits its applications to small systems. The amplitude expansion of the PFC model (APFC) consists in a coarse-grained method accounting for the evolution of the slowly varying periodic amplitudes of n. However, the limited number of parameters of the model pose some restrictions in the quantitative description of material properties. Moreover, the method has not been exploited to describe three-dimensional systems. We present a detailed modeling of grain boundaries between tilted/twisted crystals by means of the APFC model. This is achieved thanks to the implementation within a Finite Element Method framework with advanced computational features. The method allows for the study of planar grain boundaries according to specific rotations and symmetry, namely triangular/honeycomb in 2D as well as body-centered cubic and face-centered cubic in 3D. Moreover, spherical grain boundaries and their shrinkage are addressed. In order to apply this framework to the study of real systems, the standard approach has been also extended by including an additional energy term allowing for the control of the energy of solid-liquid interfaces and of defects.

Marco Salvalaglio
Institute of Scientific Computing, TU Dresden, Germany
marco.salvalaglio@tu-dresden.de

Rainer Backofen
TU Dresden
rainer.backofen@tu-dresden.de

Ken Elder

Dept Physics
Oakland U.
elder@oakland.edu

Axel Voigt
TU Dresden
axel.voigt@tu-dresden.de

MS86

Coupling Methods of Nonlocal and Local Models

Multiscale models for materials with fractures or defects involve local interaction where classical models work well and nonlocal interaction where defects display. In this talk, we present two types of energy-based coupling methods that combines nonlocal models and local models. The first idea comes from peridynamics model with a heterogeneous nonlocal horizon(interaction length). By allowing a smooth change of horizon from nonzero to zero, we effectively have a seamless coupling of nonlocal and local models. Another idea is borrowed from the quasicontiumm method in the atomistic-to-continuum coupling which leads to a way to get a well-posed model that passes the patch test.

Xiaochuan Tian
University of Texas at Austin
xtian@math.utexas.edu

MS87

On the importance of accounting for Nuclear Quantum Effects in Ab Initio Calibrated Force Fields

In many important processes in chemistry, physics, and biology, the nuclear degrees of freedom cannot be described using the laws of classical mechanics. At the same time, the vast majority of molecular simulations, which employ wide-coverage Force Fields, treat atomic motion classically. In light of the increasing desire for, and accelerated development of QM-parameterized interaction models, we re-examine whether the classical treatment is sufficient for a simple but crucial chemical species alkanes. We show that when using an interaction model or Force Field, which is in excellent agreement with the gold standard QM data, even very basic simulated properties of liquid alkanes, such as densities and heats of vaporization, deviate significantly from experimental values. Inclusion of Nuclear Quantum Effects (NQE) via techniques that treat nuclear degrees of freedom using the laws of classical mechanics serves to bring the simulated properties much closer to reality

Ganesh Kamath
Interyx Inc
gkamath9173@gmail.com

MS87

Machine Learning Coarse Grained Models from Atomistic Trajectories

The ability to perform accurate calculations efficiently is crucial for computational materials design. Molecular dynamics (MD) is one such popular technique for materials design and provides information on structure, dynamical evolution and transport properties of ion conducting materials. The accuracy and efficiency of MD, however, hinges strongly on the quality of the force fields that describe the various inter/intramolecular interactions. Historically, force field (FF) development for MD, especially for ion conducting materials such as oxide interfaces, can take months to several years while being limited to specific material systems. In this talk, we will discuss how our streamlined approach to FF development using first principles training data and machine learning algorithms is dramatically bringing down this timeframe to weeks to days [1-3]. Our procedure involves several steps including (a) generation and manipulation of extensive fitting data sets through electronic structure calculations and/or experiments, (b) defining functional forms, (c) formulating novel highly optimized training procedures, (d) coarse-graining to improve efficiency while retaining accuracy, and (e) subsequently coding and implementing these algorithms on high performance computers (HPCs). We will specifically discuss the validation of this approach on a diverse class of materials from oxides, nitrides, 2D material to even water.

Subramanian Sankaranarayanan
University of Chicago
Argonne National Lab
skrssank@anl.gov

MS87

Automated Generation of High-Accuracy Interatomic Potentials Using Quantum Data

Molecular dynamics (MD) simulation is a powerful materials simulation method for bridging between macroscopic continuum models and quantum-mechanical methods that are limited to a few hundred atoms. However, MD itself is limited by the accuracy of the interatomic potential. The growing availability of large data sets has made it possible to use automated machine-learning approaches for interatomic potential development. The SNAP approach strikes a balance between flexibility and computational cost. The energy is expressed as a closed form expression in the bispectrum components, which are a very general set of geometric invariants that characterize the local neighborhood of each atom. The SNAP approach has been used to develop potentials for studying plasticity in tantalum, site defects in indium phosphide, and plasma surface interactions in tungsten. In each case, large quantum-mechanical data sets of energy, force, and stress are accurately reproduced and cross-validation on additional test data is performed. The resultant potentials enable high-fidelity MD simulations with thousands to millions of atoms. The relatively large computational cost of the SNAP implementation in LAMMPS is offset by the excellent parallel and size scalability.

Aidan Thompson
Sandia National Lab
athomps@sandia.gov

MS88

Quantitative Phase Field Approach for Void Evolution in Irradiated Solids: Diffuse and Sharp-Interface Theory and Asymptotic Matching

We discuss the theoretical and computational development of a phase field approach for void dynamics in irradiated solids. This development includes three parts: 1) a thermodynamically-based phase field model for void nucleation and growth under irradiation, 2) a thermodynamically-based sharp interface model of the same, and 3) asymptotic matching of the two models. Quantitative results for void evolution are demonstrated.

Anter El-Azab

Purdue University
aelazab@purdue.edu

Karim Ahmed
Texas A&M
karim.elsayeed@gmail.com

MS88

Structural Phase Transitions in Transition Metal Dichalcogenide Monolayers

Two-dimensional (2D) materials, such as graphene and monolayers of transition metal-based compounds, exhibit a rich variety of electronic properties and novel 2D physics. In certain classes of layered transition metal-based compounds, recent work has indicated that it may be possible to exploit strain-induced structural transformations to rapidly switch between semiconducting and metallic in-plane crystal structures. To this end, we have developed an ab-initio informed, mesoscale continuum model to investigate such transformations. The model incorporates the effects of transformation strains, domain boundaries and interfacial energies between the symmetry-related orientational variants of the transformed phase, long-range elastic interactions between domains, out-of-plane deformations, and coupling to applied strain. Simulation results for both substrate-supported quasi-2D monolayers and suspended monolayers that can deform out of the 2D plane will be discussed, and issues of transformation reversibility and recoverability will be explored. This work has been supported as part of the Center for Computational Design of Functional Layered Materials (CCDM), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science under Award #DE-SC0012575.

Mikko Haataja
MAE Department
Princeton University
mhaataja@princeton.edu

MS88

Realistic Phase-Field Modeling: A Path Towards Microstructure Tailoring?

The coupling of phase-field modeling (PFM) to thermodynamic and kinetic databases (CALPHAD methodology) is important for realistic parameterization of PFM [Fattebert at al., Phase-field modeling of coring during solidification of Au-Ni alloy using quaternions and CALPHAD input, Acta Mater. 62 89-104 (2014)]. The present work aims at studying solidification in metallic alloys from equilibrium to far-from-equilibrium conditions to address the challenge of rapid-solidification processes encountered during laser-based additive manufacturing (AM). Experiments consist of laser surface melting and re-solidification in bulk alloys (Ti-Nb) [Roehling et al., Rapid solidification in bulk Ti-Nb alloys by single-track laser melting, JOM (submitted)], and in situ laser melting and rapid solidification in thin-film alloys (Cu-Ni) [Perron et al., Matching time and spatial scales of rapid solidification: dynamic TEM experiments coupled to CALPHAD-informed phase-field simulations, Modelling Simul. Mater. Sci. Eng. 26 014002 (2018)]. Modeling successes and challenges will be discussed and compared with experimental data. Finally, a discussion about microstructure control during AM process using PFM will be initiated. This work was performed under the auspices of the U.S Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Work at LLNL was funded by the Laboratory Directed Research and Development Program under project tracking code 18-SI-003.

Aurelien Perron
Lawrence Livermore National Laboratory
perron1@llnl.gov

Jean-Luc Fattebert
Lawrence Livermore National Lab.
fattebertj@ornl.gov

Patrice E. A. Turchi
Lawrence Livermore Nat. Lab.
turchi1@llnl.gov

Tomorr Haxhimali, John Roehling, Manyalibo Matthews, Joseph McKeown
Lawrence Livermore National Laboratory
haxhimali1@llnl.gov, roehling1@llnl.gov, matthews11@llnl.gov, mckeown3@llnl.gov

MS89

The Canonical Connection on a Homogeneous Space As a Measure of Lattice Defectiveness

The kinematic model of continuous defective crystals of Davini (ARMA 96, (1986) 295-317) in which a state of a smooth solid crystalline structure is defined by prescribing on a body manifold three linearly independent lattice vector fields (a frame), focuses mainly on objects which are invariant under elastic deformations. Such objects, in particular, the dislocation density tensor S, and its derivatives, are viewed as providing a measure of crystals defectiveness. When the dislocation density tensor is material point independent, the underlining continuum can be viewed as a Lie group acting on itself. The non-uniformity of the distribution of defects implies, on the other hand, that the underlying continuum can be viewed as a non-trivial homogeneous space of the ambient Lie group G the algebra of which is isomorphic to the Lie algebra of vector fields generated by the given frame. In our presentation, we shall focus on the non-uniform case discussing the relation between the form of the lattice algebra (Lie algebra of the group G) and the geometry of the said homogeneous space as characterized by the canonical principal connection. As the canonical connection on a homogeneous space may have not only a non-vanishing torsion but also a non-vanishing curvature, one hopes to be able to account within this model for distributions of dislocations as well as disclinations.

Marek Elzanowski
Portland State Univesity
hmmz@pdx.edu

MS89

The Role of Weak Forces in the Self-Similar Buckling of Non-Euclidean Elastic Sheets

The mechanics of thin elastic sheets can exhibit extreme properties, from crumpled paper to lettuce leaves. The former are quite rigid; whereas the latter are floppy. We argue that the inherent floppiness of non-Euclidean elastic sheets (like lettuce) is governed by and may, in turn, be quantified by novel geometric defects. These localized defects characterize topological properties of the sheet and are easily manipulated by weak forces, which play a role in generating intricate wrinkling shapes, e.g, along edges of torn plastic sheets and growing leaves. Our investigations suggest that complex morphologies result from the selec-

tion of potentially non-smooth configurations with vanishing in-plane strain (i.e., no stretching) that contain such geometric defects influenced by weak forces, i.e., effects other than stretching or bending.

Kenneth K. Yamamoto
Program in Applied Mathematics, University of Arizona
kyamamoto@math.arizona.edu

Shankar C. Venkataramani
University of Arizona
Department of Mathematics
shankar@math.arizona.edu

Toby Shearman
Program in Applied Mathematics, University of Arizona
toby.shearman@gmail.com

MS89

Line and Point Defects in Nonlinear Anisotropic Solids

In this talk, we present some analytical solutions for the stress fields of nonlinear anisotropic solids with distributed line and point defects. In particular, we determine the induced stress fields of a parallel cylindrically-symmetric distribution of screw dislocations in infinite orthotropic and monoclinic media as well as a cylindrically-symmetric distribution of parallel wedge disclinations in an infinite orthotropic medium. For a given distribution of edge dislocations, the material manifold is constructed using Cartan's moving frames and the stress field is obtained assuming that the medium is orthotropic. Also, we consider a spherically-symmetric distribution of point defects in a transversely isotropic spherical ball. We show that for an arbitrary incompressible transversely isotropic ball with the radial material preferred direction, a uniform point defect distribution results in a uniform hydrostatic stress field inside the spherical region the distribution is supported in.

Ashkan Golgoon, Arash Yavari
Georgia Institute of Technology
agolgoon3@gatech.edu, arash.yavari@ce.gatech.edu

MS89

Two-Dimensional Defective Crystals, with 3-Dimensional Algebras of Lattice Vector Fields

I will talk about continuum mechanics of 2 dimensional defective crystals with lattice vector and dislocation density tensor governed by 3 dimensional Lie algebras of lattice vector fields. There are several cases corresponding to nilpotent, solvable, or simple Lie algebras. I will also describe some examples of discrete defective crystal structures which emerge in this framework. Those structures correspond to discrete symmetry groups, but may be different from crystal structures of perfect crystals.

Maxim Zyskin
School of Mathematical Sciences, University of Nottingham
maxim.zyskin@nottingham.ac.uk

MS90

Stochastic Multi-Scale Design Optimization of Microstructures Using a Linear Solver

Microstructure design has been traditionally addressed as a deterministic optimization problem. However, the microstructures are inherently stochastic, and their stochastic nature can lead to deviations in material properties. The current state of the art focuses on the direct uncertainty quantification (UQ) problem such that the effect of microstructural uncertainties on properties is predicted. The inverse stochastic problem, which aims to predict the microstructural uncertainty given prescribed probability distributions of the material properties, has not been addressed. In this work, we present an analytical UQ formulation based on the multivariate Gaussian representation of the microstructural texture to solve the inverse problem. The analytical algorithm implements a linear programming (LP) solution to obtain the optimum microstructural probability distributions given the distributions of the material properties. The solution is exercised on problems, set separately for maximization of the magnetostriction and yield stress of Galfenol. The stochastic optimum designs are found to provide material properties that are comparable to the values in the deterministic designs. A linear scheme is implemented to identify the multiple optimum microstructure designs of the deterministic and stochastic problems. The solutions are compared to each other, and similar features are observed.

Pinar Acar
Virginia Tech
pacar@vt.edu

MS90

Materials Forensics for Inverse Microstructure and Processing Path Design

Materials forensics uses materials and microstructure correlations as signatures that can be linked to the original processing conditions and parameters. The linkage to synthesis and processing requires multi-scale modeling approaches and mechanism based modeling efforts. Inverse computational design of materials is a formidable task requiring solutions to strongly coupled properties and constraints and direct linkage to microstructures. The resulting coupled field equations for these problems can be solved using a variety of direct and indirect methods. However, a rigorous link between statistical continuum mechanics relations and properties requires a complete representation of microstructure. Microstructure and material representation in the form of correlation functions or a series expansion of a set of orthogonal functions is at the core of such methodologies. Such a representation can be achieved using direct tessellation techniques or indirect statistical methodologies. Such a linkage is also an important tool for inverse computational materials design. Not only can it provide the set of microstructures possible from a specific process path or a class of synthesis methods but it can also provide a direct link to the final or the original microstructure based on similar processing methodologies. These methodologies have been applied to several manufacturing and forming processes and will be examined during the talk.

Hamid Garmestani
Georgia Institute of Technology

hamid.garmestani@mse.gatech.edu

MS90

Roundness of Cells in Cellular Microstructures

Cellular microstructures, such as foams or polycrystalline materials, are composed of cells of varying size and shape. Typically, the cells have the combinatorial types of 3-dimensional simple polytopes, and together they tile 3-dimensional space. Now, some of the occurring cell types in the microstructures are substantially more frequent than others - and we will see that the frequent types are "combinatorially round". This property of cell types then gives us a starting point for a topological analysis of cellular microstructures.

Frank H. Lutz
TU Berlin
lutz@math.tu-berlin.de

MS90

The Effect of Microstructure Topological and Geometrical Disorder on Mechanical Properties of 2D Materials

We describe measure(s) of the topological and geometrical information of 2D polycrystalline microstructures using Rényi entropy-based mesoscale approaches. We carry out sensitivity analysis to investigate dependence between materials mechanical response and mesoscale representations of microstructure networks by performing simulations of quasi- static uniaxial compression loading tests on an idealized material using grain-level micro-mechanical discrete element model (DEM). The results allow us to make observations about the sensitivity of mechanical parameters such as Young's modulus, proportional limit, first yield stress, toughness and amount of microstructure damage to different entropy measures.

Katerine I. Saleme Ruiz
Department of Mathematical Sciences
George Mason University
katerinesaleme@gmail.com

MS91

Neo-Hookean Laminated Composites: Instabilities and Post-Bifurcation Response

In this work, the relaxation of the homogenized energy potential for a certain class of two-dimensional Neo-Hookean laminates is obtained. It is known that the macroscopic response of such hyperelastic composites can lose strong ellipticity [Geymonat, G. and Müller, S. and Triantafyllidis, N. [1993], "Homogenization of nonlinearly elastic materials, microscopic bifurcation and macroscopic loss of rank-one convexity,' Archive for Rational Mechanics and Mathematics 122, 231–290], but the post-bifurcation response is not known. Here it will be shown that the laminates can lose (global) rank-one convexity before losing (local) strong ellipticity. The post-bifurcation solution is then shown to correspond to the formation of lamellar domains.

Joshua Furer
Department of Applied Mathematics and Computational Science
University of Pennsylvania
jfurer@sas.upenn.edu

Pedro Ponte-Castañeda
Department of Mechanical Engineering and Applied Mechanics
University of Pennsylvania
ponte@seas.upenn.edu

MS91

Comparison of Numerical and Experimental Deformation Values in Beams Using Different Concrete Additives

Nowadays, there is an increasing tendency to choose high resistivity materials, in an attempt to reduce cost and maintenance frequency in construction. Concrete is one of the most used materials due to its ease of use and molding; one of its main applications is the elaboration of rigid pavements. The performance of a structure depends on several factors. One of most important features is the capacity to respond to flexion stress. In this paper, we tested the performance of three different concrete mixtures: the first one is a conventional concrete mixture with a water-cement ratio of 0.43, the second one includes a fluidizing additive with a ratio of 0.35, and the third one, with the same ratio, uses an organic polymer as a fluidizing additive. According to the age of the samples, several prismatic specimens were manufactured and subject to the bending tests. For benchmarking, a Galerkin finite element solution of Euler-Bernoulli beam equation was calculated to compare against the experimental results. The numerical and experimental results show a strong coincidence, and led to conclude that the use of the organic polymer increases notably the flexibility of the mixture. This is an encouraging result since it could be reflected in a low maintenance cost in actual buildings.

José A. Guzmán-Torres
Facultad de Ciencias Físico Matemáticas
Universidad Michoacana de San Nicolás de Hidalgo
albertoguzman1506@gmail.com

Francisco J Domínguez-Mota, Elia M Alonso-Guzmán, Wilfrido Martinez Molina, Gerardo Tinoco-Ruíz, Hugo L Chávez Garcia
Universidad Michoacana de San Nicolás de Hidalgo
dmota@umich.mx, eliamercedesalonso@gmail.com, wilfridomartinezmolina@gmail.com, jtinoco@umich.mx, hchavezenator@gmail.com

MS91

Characterization of Rock Strength in Irregular Rock Lumps Using the Point Load Method As An Inverse Problem

Rocks are hard and compact natural aggregates of mineral particles with strong permanent cohesive bonds. Due to this fact, they are currently used in almost all building processes in civil engineering, and different physical and mechanical tests are constantly carried out to improve processes of construction. These results help to understand their behavior, however, we must bear in mind that the analysis and treatment of the information obtained raise inverse problems. An example of the latter is the point load test regulated by American norm ASTM D 5731, which describes the use of Point Load equipment to determine the mechanical strength in untreated rocks with an approximate size of 4 inches in diameter. The number of tests that were performed on the rocks allows multivariate regression analysis in order to obtain a mathematical model. Among the tests performed on the rocks are ultrasonic ve-

locity, density, point load index, absorption and capillary suction tests. The analyzed data came from samples obtained from stone material banks in the Morelia, Michoacn region. The mathematical model obtained allows correlating the rock parameters to the effect of the aggregates in the elaboration of mixtures of concrete and asphalt.

Marco A. Navarrete-Seras
Facultad de Ingeniería Civil
Universidad Michoacana de San Nicolas de Hidalgo
marcoantonionavarreteseras@gmail.com

Francisco Domínguez-Mota
Facultad de Ciencias Físico Matemáticas
Universidad Michoacana de San Nicolás de Hidalgo
dmota@umich.mx

Elia Mercedes Alonso-Guzmán
Facultad de Inganiería Civil
Universidad Michoacana de San Nicolás de Hidalgo
eliamercedesalonso@gmail.com

Jose Tinoco-Ruiz
Facultad de Ciencias Físico Matemáticas
Universidad Michoacana de San Nicolás de Hidalgo
jgtinoco@gmail.com

Wilfrido Martínez-Molina, Hugo Luis Chávez-García
Facultad de Inganiería Civil
Universidad Michoacana de San Nicolás de Hidalgo
wilfridomartinezmolina@gmail.com, hchavezenator@gmail.com

MS92

Computational Approximation of Mesoscale Field Dislocation Mechanics at Finite Deformation

Dislocations play a pivotal role in determining the strength and mechanical properties of engineering materials. Understanding complex dislocation interactions using first principles limits the system sizes and simulation times due to steep computational cost associated with them. Hence, a continuum scale 'fundamentally accurate model that enables a predictive understanding of dislocation-mediated deformation serves a complementary purpose. We describe finite deformation results of a PDE based model (Mesoscale Field Dislocation Mechanics) to understand meso-macroscale plasticity in solids. We demonstrate the stress-field path followed in a body corresponding to a sequence of dislocations starting from a single dislocation to a stress-free dislocation wall constituting a grain boundary. Results quantifying the change in volume of the body upon introduction of dislocations will also be presented. Size effect and development of strong in-homogeneity in the simple-shearing of physically constrained and unconstrained grains will also be demonstrated. When the dislocation density field is localized, dislocation velocity obtained from thermodynamical constraints has the property that the dislocation curve moves perpendicular to itself in space. Adopting this as a kinematical implication, we present a simple example demonstrating longitudinal shear band propagation through essentially the motion of its tip wherein the driving force is uncoupled to the stresses.

Rajat Arora
Carnegie Mellon University
rarora1@andrew.cmu.edu

Amit Acharya
Civil and Environmental Engineering
Carnegie Mellon University
acharyaamit@cmu.edu

MS92

Understanding Dislocation Mechanics at the Mesoscale Using Phase Field Dislocation Dynamics

Abstract Not Available At Time Of Publication.

Irene Beyerlein
UCSB
beyerlein@ucsb.edu

MS92

Computing Singularly Perturbed Differential Equations and Plasticity without Constitutive Assumptions

Obtaining coarse response of systems of ordinary differential equations (ODE) containing rapidly oscillatory response as well as fast monotonic decay without detailed information on the evolution of the original (fine) variables is an interesting, but challenging task. For a given autonomous system of ODE, we consider developing practical models for determining the slow/coarse behavior of the ODE system which reflect a measurement of the underlying dynamics. We define coarse variables using modern mathematical tools like Young Measure and Practical Time Averaging (PTA) which incorporates many rigorous ideas. Finally, we apply this method to develop a macroscopic model to compute the plastic strength and study the microstructure of crystalline materials at the meso-macro scale from the underlying motion of crystal defects. We couple an exact, non-closed partial differential equation based theory (Mesoscale Field Dislocation Mechanics) representing the evolution of space-time averaged dislocation dynamics, that contains well-defined place-holders for microscopic dislocation dynamics based input. The rationale behind adopting such a coupled PDE-ODE approach instead of a completely DD based approach is primarily the vast separation in time-scales between plasticity applications that operate at quasi-static loading rates and the fundamental time scale of dislocation motion as embodied in DD which makes it impractical to reach appreciable applied strain using DD alone.

Sabyasachi Chatterjee
Carnegie Mellon University
sabyasac@andrew.cmu.edu

Amit Acharya
Civil and Environmental Engineering
Carnegie Mellon University
acharyaamit@cmu.edu

MS92

Statistical Characteristics of Dislocation Ensembles

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Vlad Soutyrine
VP, Algorithm and Software Dev.
vlad.soutyrine@gmail.com

MS93

Herglotz Functions in the Free Noncommutative

Setting: Results and Open Problems

Herglotz functions (variously otherwise known as Pick functions or R-functions) classically are holomorphic functions mapping the upper half plane to itself. Such functions come up in the discussion of the spectral theory for selfadjoint operators (including the unbounded case), as well as in Loewner's characterization of operator monotone functions, i.e., functions f defined on a real interval (a, b) such that: whenever A, B are selfadjoint operators with spectra contained in (a, b) such that $A \preceq B$ (in the sense that $B - A$ has spectrum in the positive real line), then $f(A) \preceq f(B)$. A fundamental result is that such functions f can be characterized via an integral representation, the precise form of which depends on the asymptotics of f along the positive imaginary line. There has now been some progress on multivariable extensions of these results (see work of Agler, McCarthy, Young, Tully-Doyle, Ball, Kaluzhnyi-Verbovetskyi for the case of commuting matrix variables, and of Pascoe, Tully-Doyle, and Palfia for the case of freely noncommuting variables). The inspiration for much of this work has been from multidimensional linear system theory and free probability/random matrix theory; possible connections with composite materials and multivariable versions of the Dirichlet-to-Neumann map remains to be worked out. The talk will survey and highlight these recent developments.

Joseph A. Ball
Virginia Tech
Department of Mathematics
ball@math.vt.edu

MS93

Herglotz Functions and Anderson Transitions in Composite Media

Anderson transitions, such as the metal-insulator transition where electronic wave functions become localized with sufficient disorder in the system, have been observed throughout the physics of waves in solids, optics, acoustics, and fluids. We recently uncovered the hallmarks of the Anderson transition for classical homogenized transport coefficients in two phase composite materials, such as the effective thermal conductivity or complex permittivity - without wave interference or scattering effects. We analyze the eigenvalues of a key random matrix governing transport in the analytic continuation method for obtaining Stieltjes integrals for the homogenized parameter. As one of the phases becomes connected and develops long range order, such as brine in sea ice forming channels through which fluid can flow, we observe striking transitional behavior. The eigenvalues transition from obeying uncorrelated Poisson-like statistics to repulsive, universal Wigner-Dyson statistics, and the field eigenvectors become delocalized. Our results are related to surface plasmon resonances in metal-insulator composites, such as gold nanoparticles suspended in a liquid, interacting with light in the quasistatic regime. Finally, we also report on recent results in extending the analytic continuation method to other homogenization problems, such as advection enhanced diffusion and quasistatic ocean wave propagation in the marginal ice zone of the Arctic and Antarctic sea ice packs.

Kenneth M. Golden
University of Utah
Department of Mathematics
golden@math.utah.edu

MS93

Extraction of the Size of An Inclusion from Boundary Measurements in Time

In this talk we will show an application of the so-called analytic method (Bergman, Milton, and Golden and Papanicolaou), a method based on the analyticity of the effective tensor of a composite with respect to the moduli of the components. Specifically, due to the analogy, established by Milton, between the problem of finding the effective tensor in the abstract theory of composites, and the problem of finding the Dirichlet-to-Neumann (DtN) map for an inhomogeneous body, one can apply the analytic method to determine bounds on the DtN map. In particular, the bounds are determined in the time domain and those involving the volume fraction of the inclusion turn out to be very tight at specific moments of time. Therefore, these bounds can be used in an inverse fashion to determine the size of the inclusion by probing the body with time-dependent fields and then performing boundary measurements at those specific times.

Ornella Mattei
University of Utah
mattei@math.utah.edu

Graeme W. Milton
University of Utah
Department of Mathematics
milton@math.utah.edu

MS93

Sum Rules and Power-Bandwidth Limits to Near-Field Optical Response

Near-field nanophotonics offers the promise of orders-of-magnitude enhancements for phenomena ranging from spontaneous-emission engineering to Casimir forces via zero-point quantum fluctuations. An increasing variety of approaches–photonic crystals, metamaterials, metasurfaces, antennas, and more–has underscored our lack of understanding as to how large these effects can be. We provide a general answer to this question, deriving the first sum rule for near-field optical response as well as general upper bounds for any bandwidth, i.e. power–bandwidth limits. Our framework relies on a unification of the analytic properties of causal functions with energy-conservation constraints that emerge in any scattering system. We computationally verify the sum rule, and demonstrate the capability of the power-bandwidth limits to identify optimal nanophotonic materials for any combination of frequency and bandwidth.

Hyungki Shim
Yale Applied Physics
Yale Physics
hyungki.shim@yale.edu

Owen D. Miller
Yale Applied Physics
owen.miller@yale.edu

MS94

Machine Learning Interatomic Potentials for Reac-

tive Simulations from First Principles Data

The growth of stanene on a Bi2Te3 substrate and of germanene on multiple substrates has engendered a great deal of interest. However, atomistic investigations of growth mechanisms (needed to guide synthesis), of phonon transport (crucial for designing thermoelectrics), and of thermomechanical behavior are scarce. This paucity is primarily due to the lack of inter-atomic potentials that can accurately capture atomic interactions in these materials. To address this, we have developed machine learnt potentials for these materials based on the Tersoff and Stillinger-Weber formalisms that were trained to reproduce the (a)structure, (b)equation of state, (c)elastic constants, and (d)phonon dispersions obtained from our density functional theory calculations. To optimize these potentials, we employed a hybrid global optimization scheme based on genetic algorithms and Nelder-Mead simplex. Finally, we employed our newly developed potentials to study the anisotropy in thermal conductivity of stanene sheets and nanotubes, as well as the growth mechanism of germanene.

Mathew Cherukara
Argonne National Lab
mcherukara@anl.gov

MS94

Creative AI for Molecule Discovery

Designing new molecules and materials with optimized attributes is one the ultimate needs in areas such as drug discovery, agriculture, energy generation and storage, structural and advanced polymers, etc. The chemical space is discrete, unstructured and unimaginably large, with an estimated size ranging 10^30 to 10^100. Optimizing over such a space is very challenging, as well as time and resource-intensive. Deep generative models have attained inspiring success in image and text generation in recent years. Advances in deep generative models are at the forefront of deep learning research because of their potential in data-efficient learning, and model-based reinforcement learning. In this talk, I will discuss the development and application of deep generative models for new molecule design, which require training on multi-dimensional data in an optimal manner.

Payal Das
IBM
daspa@us.ibm.com

MS94

Accelerated exploration and rational engineering of biomolecular folding and colloidal assembly using neural networks and manifold learning

Data-driven modeling and machine learning have opened new paradigms and opportunities in the understanding and design of soft and biological materials. Rational engineering of structural and functional polymers and colloids requires an understanding of the underlying free energy landscapes dictating thermodynamic stability and kinetically accessibility. In the first part of this talk, I will discuss our use of auto-encoding deep networks to perform on-the-fly collective variable discovery and accelerated sampling of free energy landscapes in molecular dynamics simulation of proteins. In the second part of this talk, I will describe our use of nonlinear manifold learning to determine low-dimensional assembly landscapes for self-assembling patchy colloids and rational sculpting of these landscapes to engineer the stability and accessibility of desired aggregates.

Andrew L. Ferguson
Univ Illinois Champaign Urbana
alf@illinois.edu

MS94

From Data to Materials Discovery: Challenges in Learning and Design

Abstract Not Available At Time Of Publication.

Turab Lookman
Los Alamos National Laboratory
txl@lanl.gov

MS95

Lie Groupoids Theory for FGM Materials

In this paper we will present an application of the theory of Lie groupoids to a large class of materials known as Functionally Graded Materials (FGM). For a FGM we can compare the material symmetry groups at two different points even if the material does not enjoy uniformity. A kind of homogeneity adapted to this situation will be discussed.

Manuel De León
ICMAT-CSIC
mdeleon@icmat.es

MS95

Material Groupoids, Algebroids and Distributions

Any local constitutive law over a material body (or over a body-time manifold) and a criterion for comparing responses at different points (and instants) give rise to a uniquely defined material groupoid. In the case of a transitive Lie groupoid (corresponding to concepts such as smooth uniformity and anelastic evolution) the associated Lie algebroid plays a role in the description of material defects. For the more general case, the concept of material distribution can be introduced. Its associated singular foliation provides a unique subdivision of the material groupoid into strictly transitive components of various dimensions.

Marcelo Epstein
University of Calgary
Calgary, AB, Canada.
mepstein@ucalgary.ca

MS95

On the Kinematics of Defects

In a general geometric theory, the distribution of the crystalline structure of a solid body is specified by a de Rham r-current T on an n- manifold. Defects are described by the boundary ∂T. For a motion of defects associated with a family of diffeomorphisms of the body, we show that the rate of change of the distribution of defects is given by the dual of the Lie derivative operator.

Reuven Segev
Ben-Gurion University
Israel

rsegev@post.bgu.ac.il

Marcelo Epstein
University of Calgary
Calgary, AB, Canada.
mepstein@ucalgary.ca

MS96

Consistent Hydrodynamics for Phase Field Crystals

Phase field crystal (PFC) models were originally introduced in order to couple diffusive time scales with atomistic spatial resolution and are a suitable candidate for a phase transitions over a wide range of temporal scales. One of the important advantages of the PFC models is the intrinsic incorporation of elastic energy associated with a fixed interatomic length scale. However, this poses a great challenge for the dynamics of the system: elastic excitations emit phonons which cannot be described using over-damped, purely dissipative dynamics. In this work, we investigate the fast time scales in the dynamics by coupling a coarse-grained version of the PFC with hydrodynamics. In particular, we coarse-grain the mass density and velocity fields by using the amplitude expansion framework where the structure is described by the amplitudes of the atomistic density oscillations instead of the PFC mass density field itself. This framework allows for a description of the material by smooth fields and it can be shown to reduce to well-known macroscopic theories. The displacement field is naturally coupled to the amplitudes of the density oscillations and to the velocity field, with no need for additional assumptions. We show that the dynamics allows for long wavelength phonon modes and demonstrate the theory numerically showing that the elastic excitations in the system are relaxed through phonon emission.

Vili Heinonen
Massachusetts Institute of Technology
vili@mit.edu

C.V. Achim
Universidad de Concepción
cristian.v.achim@gmail.com

J.M. Kosterlitz, See-Chen Ying
Brown University
j_kosterlitz@brown.edu, see-chen_ying@brown.edu

John Lowengrub
University of California, Irvine
lowengrb@math.uci.edu

John Lowengrub
Department of Mathematics
University of California at Irvine
lowengrb@math.uci.edu

T. Ala Nissila
Loughborough University, UK
Aalton University, Finland
t.ala-nissila@lboro.ac.uk

MS96

Dynamic Failure of High Energy Materials

Polymer bonded explosives consist of high energy particles in a polymeric binder. When these composites are subjected to heat, impact, or other stimulus they undergo a rapid chemical change. The sensitivity to initiation depends on the amount of energy available in the system and on the rate at which it is released. This process is controlled by the formation of high temperature localized regions known as hot spots. The mechanisms of hot spot nucleation are controlled by the microstructure, for example in the same sample some particles ignite while others do not. Finite element simulations that explicitly describe particles, are performed to study the sensitivity of the microstructure to initiation and to identify the mechanisms of hot spot formation under a range of mechanical stimulus. The finite element model incorporates plasticity, fracture and heat transport using a phase field approach. Different microstructures with initial defects, including cracks, debonding and voids are analyzed. Our work suggests that heat generated by friction at preexisting microcracks and at particle binder interfaces are of key importance for hot-spot formation.

Marisol Koslowski, Nicolo Grilli, Camilo Duarte
Purdue University
marisol@purdue.edu, ngrilli@purdue.edu, cduartec@purdue.edu

MS96

Development of a Quantitative Phase Field Model to Predict the Impact of Microstructure on Brittle Fracture Implemented Using an Implicit Finite Element Method

Fracture in brittle materials is dictated by crack initiation and growth within the material. Microstructural features, such as grain boundaries, precipitates, impurities, dislocations, and pores, are typical sites for crack initiation. Thus, in order to accurately determine the fracture properties, we must consider the impact of microstructure. In this work, we present a quantitative phase field fracture model that considers the impact of grain boundaries, pores, and other heterogeneities on the fracture behavior. The fracture toughness of the various microstructural features in the model can be obtained from atomistic simulations or from experimental data. The model also considers anisotropic elastic properties of the microstructural features, though preferred cleavage planes are not currently considered. The model is implemented using the open source MOOSE finite element framework with implicit time integration.

Shuaifang Zhang, Michael Tonks
University of Florida
zhang.s@ufl.edu, michael.tonks@ufl.edu

Wen Jian
Idaho National Laboratory
wen.jiang@inl.gov

Pritam Chakraborty
India Institute of Technology, Kanpoor
cpritam@iitk.ac.in

MS96

Integrating Phase Field with Finite Deformation Plasticity in a Spectral Solver for 3D Simulation of Thermo-Mechanical Processing

We present an integrated full-field modeling scheme that couples the mechanical response with the underlying microstructure evolution. Here we integrate a fast Fourier transform-based elasto-viscoplastic (FFT-EVP)

model with a phase-field (PF) recrystallization model, and carry out three-dimensional simulations of dynamic recrystallization (DRX) in polycrystalline copper and rafting during creep in γ/γ' superalloys. A physics-based coupling between FFT-EVP and PF is achieved by (1) adopting a dislocation-based constitutive model in FFT-EVP, which allows the predicted dislocation density distribution to be converted to a stored energy distribution and passed to PF, and (2) implementing a stochastic nucleation model within the phase field. For both cases the coupling illuminates features of the microstructure evolution that would not be apparent from either the micro-mechanical or phase field simulation alone. For DRX it is observed that the resulting stress redistribution due to strain compatibility is found to have a profound influence on the subsequent dislocation evolution and softening, and for rafting the relaxation of strain energy due to plastic dissipation is shown to affect local diffusion potential and alter the kinetics of rafting.

Stephen Niezgoda
Ohio State University
niezgoda.6@osu.edu

Pengyang Zhao
The Ohio State University
zhao.247@osu.edu

Yunzhi Wang
Ohio State University
wang.363@osu.edu

MS97

Broadband Non-Reciprocity in Spatio-Temporally Modulated Metamaterials

In this talk, we will review our recent progress towards the concept, design and realization of magnet-free non-reciprocal electromagnetic devices and arrays of them with strong non-reciprocal response to realize broadband isolators and circulators. We will discuss in particular our approaches to achieve the ultimate limits on the bandwidth of spatio-temporally modulated devices with strong non-reciprocal responses, the relation with bounds on the bandwidth of passive devices, even in the limit in which spatio-temporal modulation is hidden within the device, and for an external observer its response is pseudo-linear-time-invariant.

Andrea Alu
Department of Electrical and Computer Engineering
University of Texas at Austin
aalu@gc.cuny.edu

Ahmed Kord, Dimitrios Sounas
University of Texas at Austin
ahmedkord@gmail.com, dimitrios.sounas@utexas.edu

MS97

Matrix Valued Herglotz Functions and Internal Memory Variables for Composites

The resolvent representation of the effective properties of anisotropic heterogeneous material results in a matrix valued Herglotz function representation. We show that the spectral measure in this integral representation provides an efficient way to introduce the internal memory variables in composites. We discuss applications to inverse homogenization and to numerical simulation of wave propagation in composite materials.

Elena Cherkaev
University of Utah
Department of Mathematics
elena@math.utah.edu

MS97

Physical Bounds on Metamaterial Structures, and Extreme Electromagnetic Effects

In this talk, we will review some of our recent efforts on deriving physical bounds and limits for metamaterial structures and devices, and our investigations of some extreme electromagnetic effects that are seemingly at odds with physical intuition. In the first half of our presentation, we will discuss the limitations – stemming from linearity, causality, energy conservation, and stability – on anomalous effects enabled by metamaterial concepts, especially in the context of scattering suppression with passive and active cloaking devices. The second half of this talk will instead be devoted to our investigations of some extreme – seemingly unbounded – electromagnetic effects, most notably embedded eigenstates and exceptional points, as well as their relation to passivity, reciprocity, and topological concepts.

Francesco Monticone
Cornell University
Electrical and Computer Engineering
francesco.monticone@cornell.edu

MS97

Bounds on the Dirichlet-to-Neumann Map in Approximate Cloaking Problems

Abstract Not Available At Time Of Publication.

Aaron Welters
Florida Institute of Technology
awelters@fit.edu

PP1

Analysis of Earthquake Time Series by Using Stochastic Volatility Model

This work is devoted to the study of modeling geophysical time series. We collected the seismograms containing the seismic waves generated by the earthquakes recorded by two nearby seismic stations (IU.TUC and US.ANMO) and observe that they generate different frequency spectra. A stochastic technique with time-varying parameters is used to forecast the volatility of time series in a stationary environment. The modeling of stationary time series with consistent properties facilitates prediction with much certainty. In this study, the volatility is defined as a logarithmic first-order autoregressive process. We observe that the inclusion of log-volatility into the time-varying parameter estimation significantly improves forecasting which is facilitated via maximum likelihood estimation. The estimation algorithm for the corresponding one-step-ahead predicted volatility (with ± 2 standard prediction errors) is very feasible since it possesses good convergence properties with large data sets. Our results suggest that the stochastic process to forecast the earthquake time series is more effective in enforcing the characteristic of time-varying parameters than the commonly used deterministic process.

Md Al Masum Bhuiyan

Ph.D. candidate
The University of Texas at El Paso
mbhuiyan@miners.utep.edu

Maria C. Mariani
Department of Mathematical Sciences
The University of Texas at El Paso
mcmariani@utep.edu

PP1

Pde Analysis of a Class of Thermodynamically Compatible Viscoelastic Rate-Type Fluids with Stress-Diffusion

We provide a uniform approach how to rigorously derive thermodynamically consistent viscoelastic rate-type model with a stress-diffusion term for incompressible heat conducting fluids with material parameters depending on temperature. Furthermore, we show how the approach can be used to obtain new a priori estimates arising from the entropy inequality. Finally, we establish the long-time existence of large-data weak solutions to the system of interest, which governs the motion of non-Newtonian fluids described by a simplified viscoelastic rate-type model with a stress-diffusion term. The simplified model shares many qualitative features with more complex viscoelastic rate-type models that are frequently used in the modeling of fluids with complicated microstructure. As such, the simplified model provides important preliminary insight into the mathematical properties of these more complex and practically relevant models of non-Newtonian fluids. The simplified model that is analyzed from the mathematical perspective is shown to be thermodynamically consistent, and we extensively comment on the interplay between the thermodynamical background of the model and the mathematical analysis of the corresponding initial-boundary-value problem.

Miroslav Bulicek
Charles University in Prague
Faculty of Mathematics and Physics
mbul8060@karlin.mff.cuni.cz

PP1

Verification and Validation of the Flag Hydrocode for Impact Cratering Simulations

Impact cratering is the dominant geologic process in the solar system. Crater size and geometry depend on many factors, among them the size and velocity of the impactor, the materials of the impactor and target, local gravity, and impact angle. The strength of the target material can affect geomorphology of impact craters. These properties must be considered for some impacts. Early stages of crater formation are driven by thermodynamic properties, while later stages are governed by additional factors such as internal friction and local gravity. The role of material strength depends on the mass and velocity of the impactor. Hydrocode simulations have been used to model impact cratering, but these methods are often unable to capture the solid mechanics necessary to understand crater formation. The FLAG hydrocode, developed at Los Alamos National Laboratory (LANL), allows for the incorporation of various strength models that can be applied to solid materials. We show verification of FLAG by simulating an aluminum projectile impacting an aluminum target, and we compare these results to those found using other hydrocodes and to analytical solutions. We show validation of FLAG by simulating laboratory impacts and comparing to experimental data. Our results show that FLAG can be used to model impacts of solid materials as well as the craters formed from those impacts.

Wendy K. Caldwell
Los Alamos National Laboratory
Arizona State University
wkcaldwell@lanl.gov

Abigail Hunter, Catherine Plesko
Los Alamos National Laboratory
ahunter@lanl.gov, plesko@lanl.gov

PP1

Thin Interface Asymptotic for Diffusion Controlled Transformation Poster

The Phasefield method is most accurate in the presence of high driving forces, whereas in the case of diffusion control systematic errors are inevitable. To guarantee accuracy and numerical efficiency, spurious effects associated with the diffusivity of the interface need to be corrected. This was done by Karma and Rappel in 1996 with their thin-interface approach. Here we propose an alternative approach to derive a spatially heterogeneous mobility correction and test it with numerical simulations.

Stephan Hubig
ICAMS, Ruhr-Universität Bochum
Universitätsstr. 150, 44801 Bochum
stephan.hubig@rub.de

PP1

Characteristic Distribution: An Application to Material Bodies

Let $\overline{\Gamma} \subseteq \Gamma$ be a subgroupoid of a Lie groupoid $\Gamma \rightrightarrows M$. We can construct a generalized distribution $A\overline{\Gamma}^T$ over Γ called the *characteristic distribution of* $\overline{\Gamma}$ which divide $\overline{\Gamma}$ into transitive Lie subgroupoid over a foliation of M. As an example of groupoid, associated to each simple material body $\mathcal{B}$ there exists a groupoid $\Omega(\mathcal{B})$ (not necessarily a Lie groupoid) consisting of all the material isomorphisms connecting the points of $\mathcal{B}$. The uniformity character of $\mathcal{B}$ is reflected in the properties of $\Omega(\mathcal{B})$: $\mathcal{B}$ is uniform if, and only if, $\Omega(\mathcal{B})$ is transitive. Smooth uniformity corresponds to a Lie groupoid and, specifically, to a Lie subgroupoid of the groupoid $\Pi^1(\mathcal{B}, \mathcal{B})$ of 1-jets of $\mathcal{B}$. So, as an application of the general development we finally have that any simple body $\mathcal{B}$ can be covered by a foliation of some kind of smoothly uniform "subbodies".

Víctor M. Jiménez Morales
ICMAT - CSIC
victor.jimenez@icmat.es

Manuel De Leon
ICMAT - CISIC
mdeleon@icmat.es

Marcelo Epstein
University of Calgary
Calgary, AB, Canada.
mepstein@ucalgary.ca

PP1

Computational Mining and Characterization of

Low Dimensional Heterostructures

Of all the low dimensional materials, single-topology 2D materials are the best studied. However, low dimensional materials encompass a number of other experimentally observed structures with many combinations of 0D, 1D, 2D and 3D components. Well-known examples include graphite with intercalated lithium ions (a 0D-2D structure) or intercalated nanowires (1D-2D), zeolites containing organic molecules (0D-3D), and bulk tunnel structures with inserted polymeric sulfur (1D-3D). Such materials exhibit a variety of promising mechanical, electronic, and catalytic properties. Here, I present a topological algorithm for 'mining' mixed-dimensional materials from large databases. By representing a crystalline structure as an incremental periodic graph, a topological algorithm can be used to consider possible dimensionalities of the graph components. A simple statistical descriptor is then used to determine the most likely configuration. Results of the mining are validated using Density Functional Theory calculations. I will describe a selection of low dimensional materials with interesting electronic properties, as well as limitations of the method.

Peter M. Larsen, Mohnish Pandey, Karsten Wedel Jacobsen
Technical University of Denmark
peter.mahler.larsen@gmail.com, mohpa@fysik.dtu.dk, kwj@fysik.dtu.dk

PP1

Period Evolution in the Occupation Probabilities in a Laser-Driven Three-Level System

The Schrdinger Equation is solved for a three-level system with energy levels Ei. The two driving lasers have a positive energy ratio R equal to (E3-E2)/(E2-E1). The occupation probabilities show a dominant and constant periodicity for R from above 2 down to about 1.05. Lower R leads to pronounced structure and the loss of periodicity. But a shorter period starts to develop at small times and covers more time as R gets closer to 1.

James P. Lavine
Department of Physics
Georgegtown University
jpl62@georgetown.edu

PP1

A MathematicalModelforElectrostaticSprayinganOptimizationofPorousMicrospheres

Electrostatic spraying is widely used for fabricating porous microspheres, and there is no effective way to control the size of microsphere and its porosity. This paper establishes a one-dimensional fluid mechanical model to describe the spraying process, and the main factors affecting the morphology of the microspheres are theoretically revealed and experimentally verified. The model can be used to optimally adjust the spraying process.

Yan-Qing Liu, Ning-Bo Peng, Chan-Juan Zhou, Ji-Huan He
Soochow University
1289341071@qq.com, 773576399@qq.com, 767816562@qq.com, Hejihuan@suda.edu.cn

PP1

A Mean-Field Model for Parallel Computing of Hydrogel Behavior

Hydrogels have attracted attention as smart materials for their ability to respond to environmental stimuli. In this poster, we explore the potential for a mean-field model to capture the properties of hydrogels using massively parallel computation. This approach uses stochastic differential equations derived from the physical properties of underlying gel network segments to reproduce macroscale behavior. In particular, we compare results from small amplitude oscillatory shear flow simulations of a mixture formed by two copolymers.

Erik Palmer
Department of Mathematics
University of South Carolina
etpalmer@math.sc.edu

Paula A. Vasquez
University of South Carolina
paula@math.sc.edu

PP1

Topological Methods for Polymeric Materials: Characterizing the Relationship Between Polymer Entanglement and Viscoelasticity

We draw on mathematical results from topology to develop quantitative methods for polymeric materials to characterize the relationship between polymer chain entanglement and bulk viscoelastic responses. We generalize the mathematical notion of the Linking Number and Writhe to be applicable to open (linear) chains. We show how our results can be used in practice by performing fully three-dimensional computational simulations of polymeric chains entangled in weaves of a few distinct topologies and with varying levels of chain densities. We investigate relationships between our topological characteristics for chain entanglement and viscoelastic responses by performing Lees-Edwards simulations of the rheology over a broad range of frequencies. Our topological measures of entanglement indicate the global topology is the dominant factor in characterizing mechanical properties. We find an almost linear relation between the mean absolute Writhe Wr and the loss tangent and an almost inverse linear relation between the mean absolute Periodic Linking Number LK_P and the loss tangent. These results indicate the potential of our topological methods in providing a characterization of the level of chain entanglement useful in understanding the origins of mechanical responses in polymeric materials.

Eleni Panagiotou
University of California Santa Barbara
lnpanagiotou@yahoo.com

PP1

Quantitative Representation of Solvation Shell Structure Via Molecular Dynamics Simulations

The solvation behavior of C_{60} fullerene has received much attention due to its exceptional electronic properties. Even with the heightened interest caused by the prospect of printable flexible electronics, our understanding of C_{60} in solvents is quite limited. The fullerene molecule, balanced in size between the colloidal regime and that of the surrounding solvent molecules, complicates traditional descriptors of solvation behavior. Herein, we use all-atom molecular dynamics (MD) simulations to gain an insight into the little-understood structural and dynamic proper-

ties of the solvation shell surrounding C_{60} and some of its popular derivatives. Taking advantage of the resolution and length scales afforded by MD, we developed a novel analytical method for visualizing the dynamic solvation shell structure in three dimensions. We then quantify the regularity of this structure as a single descriptor which is shown to correlate with experimentally measured solubility values of C_{60} and phenyl-C_{61}-butyric acid methyl ester (PCBM) for a range of aromatic solvents. Moreover, our analysis of the solvation shell structure at the nanoscale reveals further insights into previously unexplained macroscopic phenomena in C_{60} derivative behavior and suggest mechanisms for C_{60} solvate phase transformations. Our use of atomic scale MD thus allows us to investigate solvent structural regularity that has direct consequences to the device macroscale.

James S. Peerless, Hunter Bowers, Albert Kwansa, Yaroslava Yingling
North Carolina State University
peerless.j@gmail.com, ghbowers@ncsu.edu, alkwansa@ncsu.edu, yara_yingling@ncsu.edu

PP1

Fractal Approach to Wetting Property of a Nanofiber Membrane

It is found that the micro/nano scale surface morphology of a nanofiber membrane affects greatly its wetting property. The fractal geometry is adopted to describe the surface property, and an experiment is designed where porosity is adjusted by different layers of nanofibers, finally a mathematical model is established to predict contact angle by the fractal dimensions, which agrees well with the experimental data.

Ning-Bo Peng, Dan Tian, Chan-Juan Zhou, Ji-Huan He
Soochow University
773576399@qq.com, 931741262@qq.com, 767816562@qq.com, Hejihuan@suda.edu.cn

PP1

Computational Efficiency for Transient Networks of Fene Dumbbells

In this poster the effects of intramolecular forces in transiently networked fluids are explored via a mesoscale mathematical model, represented by a stochastic differential equation. The macroscale behaviors of these transiently networked surfactant or polymeric fluids include shear thinning, shear thickening, shear banding and non-exponential relaxation. We consider first an elastic dumbbell model under simple shear stress and compare results for different elastic spring forces such as a classical Hookean spring, a Finitely Extensible Nonlinear Elastic (FENE), and a modified FENE spring. We then consider a mixture of chains of attached dumbbells, Rouse chains all of length N, and then a polydisperse mixture of Rouse chains of varying lengths. The macroscale stress responses are compared both transiently and in steady state for each type of spring connector at varying shear rates. Our goal is to determine a numerical scheme that has the highest accuracy but also a scheme that is computationally efficient to be used for FENE springs in attaching and detaching, transient, networks.

Lucas E. Quintero
University of Delaware
Mathematical Sciences
quintero@udel.edu

L. Pamela Cook
University of Delaware
Department of Mathematical Sciences
cook@udel.edu

Lin Zhou
Mathematics Department, New York City College of Techonology
Brooklyn, NY 11201, USA
lzhou@citytech.cuny.edu

PP1

A Matrix-Free Numerical Implementation of a Vertex Model with a Stored Energy Term

We adapt a 2D stochastic vertex model into a dynamical system of equations with a matrix-free approach. This model differs from classical vertex model due to the inclusion of a stored energy term associated to each grains. A comparison with a classical 2D vertex model will be included. We will discuss in detail a novel and fast matrix-free implementation of this model and the numerical challenges overcome to obtain a working code. An open-source GPU-code will be provided to the community for comparison and study.

Alejandro H. Sazo
Departamento de Informática
Universidad Técnica Federico Santa María
asazo@alumnos.inf.utfsm.cl

Claudio E. Torres
University of Delaware
ctorres@inf.utfsm.cl

Dmitry Golovaty
The University of Akron
Department of Mathematics
dmitry@uakron.edu

Maria Emelianenko
George Mason University
memelian@gmu.edu

PP1

On the Atomistic Underpinnings of the Burton-Cabrera-Frank Model of Crystal Growth

Recent works show that microscale models of crystal surface evolution, when appropriately coarse grained, result in mesoscale equations resembling the Burton-Cabrera-Frank (BCF) model of step motion. The form of these BCF equations depends on details of the microscale descriptions from which they are derived. In this talk, we consider the extent of the dependence of coarse-grained BCF-like equations on rules for atomistic transitions in a solid-on-solid-type model of a single step. Starting from the master equation governing our microscale model, we estimate discrete corrections to the BCF model analytically and via kinetic Monte Carlo simulations in terms of atomistic rates for external deposition, desorption, and surface hopping. It is shown that seemingly minor changes in microscale rates may have a significant impact on ensuing corrections to mesoscale evolution equations.

Joshua P. Schneider

Gallaudet University
Joshua.schneider@gallaudet.edu

Dionisios Margetis
University of Maryland, College Park
dio@math.umd.edu

PP1

Effect of Nozzles Size on Fibers Morphology and Mechanical Properties in Electrospinning Process

Electrospinning is influenced by many factors, among which the nozzle's size is the main factor. This paper establishes a one dimensional mathematical model to describe the jet motion in the spinning process, fiber's morphology and mechanical properties can effectively controlled by the nozzle's size. Experiment was carefully designed to verify the theoretical prediction. The model also reveals a possible hidden mechanism in the spider spinning, and canbe used for bio-mimic design of nozzles.

Dan Tian, Dan-Ni Yu, Yan-Qing Liu, Ji-Huan He
Soochow University
931741262@qq.com, 448032577@qq.com, 1289341071@qq.com, Hejihuan@suda.edu.cn

PP1

Detecting Cracks with Ultrasonic Waves, a Model-Based Approach

This talk focuses on modeling scattered waves from cracks emanating from a cylindrical hole in thin plates. This class of damage is a topic of great interest among structural health monitoring and non-destructive evaluation communities. Accurate modeling of damage is a prerequisite for reliable model-based detection algorithms. The first part focuses on modeling simulating Lamb wave signals in damaged plates. The second part focuses on signal processing and statistical methods applied to detect the damage.

Richard P. Uber
Air Force Institute of Technology
Department of Mathematics and Statistics
richard.uber@afit.edu

PP1

Nanofiber Membrane for An Ion Sensor

Nanofiber membranes were prepared by electrospinning, which can produce current when they contact a copper sulfate solution, revealing the membrane can be used for an ion sensor. A mathematical model is established in this paper to theoretically study the main factors affecting the current-voltage relationship, and a series experiments are carried out to verify the theoretical prediction. The mathematical model can be used for optimal design of a ion sensor.

Dan-Ni Yu, Yan-Qing Liu, Ning-Bo Peng, Ji-Huan He
Soochow University
448032577@qq.com, 1289341071@qq.com, 773576399@qq.com, Hejihuan@suda.edu.cn

PP1

The Number of Layers in a Cocoon Speaks for Itself

A cocoon is of hierarchical structure with multiple layers. The number of layers plays an important role for its bio-functions. This paper studies the effect of number of layers on vapor permeation. An undamaged cocoon sees the highest permeability among all stripped ones. A fractional model is established, revealing there is optimal value for the number of layer .

Chan-Juan Zhou, Dan Tian, Dan-Ni Yu
Soochow University
767816562@qq.com, 931741262@qq.com, 448032577@qq.com

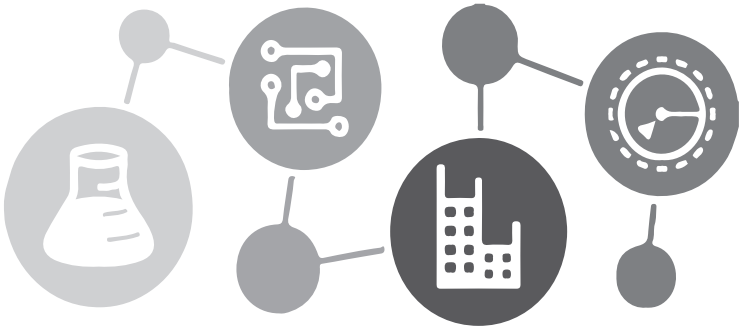
PP1

A New Model for Interface Motion by Interface Diffusion

We shall first present a new model for interface motion by interface diffusion formulated by Alber and myself, which may be applied to Sindering, powder metallurgy, etc. Then a new concept of weak derivatives is proposed, and weak solutions to an initial-boundary value problem of this model are defined. Next An approximate problem for the IBVP is constructed. Finally making use of a classical theorem (the Egorov theorem) we prove the existence of weak solutions to the IBVP.

Peicheng Zhu
University of Basque Country, Spain
pczhu@t.shu.edu.cn

ED18 Abstracts



SIAM Conference on
Applied Mathematics Education (ED18)
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SP1

The AWM-SIAM Sonia Kovalevsky Lecture: Learning and Efficiency of Outcomes in Games

Selfish behavior can often lead to suboptimal outcome for all participants, a phenomenon illustrated by many classical examples in game theory. Over the last two decades our community developed good understanding on how to quantify the impact of strategic user behavior on the overall performance in many games by analyzing Nash equilibria of these games (including traffic routing as well as online auctions). Learning outcomes emerged in recent years as an attractive alternative to Nash equilibrium, modeling players who havent reached a stable equilibrium, but rather use algorithmic learning. We propose that learning is a good model of behavior in games where the systems has high economic value overall, but where stakes of individual items are low, which makes exploring and learning a good behavior. Such games include both Internet packet routing as well as online auctions. In this talk we consider a few closely related questions: What are broad classes of learning behaviors that guarantee high social welfare in games, are these results robust to situations when the game or the population of players is dynamically changing, and does data from such games suggest that learning is indeed a good behavioral model of the participants.

Eva Tardos
Cornell University
Department of Computer Science
eva@cs.cornell.edu

SP2

The John Von Neumann Lecture: Untangling Random Polygons and Other Things

Suppose we are given a random polygon $\mathcal{P}_0$ with vertices $(x_1, y_1), \ldots, (x_n, y_n)$ that have centroid (0,0). If we connect the midpoints of its edges, then we obtain a new polygon. Assume that the x-values and y-values are scaled after each update so that we always have $\|x\|_2 = 1$ and $\|y\|_2 = 1$. This update process can obviously be repeated to produce a sequence of polygons $\{\mathcal{P}_k\}$. No matter how "criss-crossy' the initial polygon $\mathcal{P}_0$, the $\mathcal{P}_k$ eventually "untangle' and their vertices head towards an ellipse with a 45-degree tilt. Why? It turns out that the sequence of x and y vectors that are produced by this iteration are the result of a power method process that involves a shifted version of the n-by-n downshift matrix S_n. That fact plus a slick SVD analysis of a certain 2-by-2 matrix explains everything. In this talk I will step through the matrix computations that explain the untangling. I will also discuss how I came across this problem and why it is a great metaphor of matrix-based computational science.

Charles F. Van Loan
Cornell University
Department of Computer Science
cv@cs.cornell.edu

SP3

Julian Cole Lectureship: Modeling of Complex Fluids: Wormlike Micellar Solutions, Polymers and Mucins

Complex and viscoelastic fluid properties arise due to immersed mesoscale structures. These structures may be small particles, long chain molecules, or transiently connected networks. This talk will cover elements of macroscale, and of stochastic mesoscale, modeling and simulation of transiently networked fluids; fluids typified by wormlike micellar solutions, polymers and mucins.

Pamela Cook
University of Delaware
cook@udel.edu

SP4

W.T. and Idalia Reid Prize Lecture: Modeling, Simulation, and Control of Differential-Algebraic Port-Hamiltonian Systems

Complex multi-physics, multi-scale systems are at the heart of almost all modern technology developments. A highly relevant example is the real time control of modern energy systems that have to integrate different energy sources (fossil and renewables) and large networks of producers and comsumers. To obtain a systematic approach for modeling, simulation, optimization and control of such complex systems, the concept of port-Hamiltonian systems is ideal. The structure is close to the underlying physics, the interconnection, Galerkin discretization and model reduction preserves the structure and there are nice algebraic properties of the equations and geometric properties of the resulting flow. When such systems contain constraints (such as e.g. Kirchhoff's laws in networks) then the resulting model is best described by (partial) differential-algebraic systems of port-Hamiltonian structure. The analysis, numerical solution, and control of this class of systems will be discussed, new mathematical and computational challenges will be described and the success of the approach will be demonstrated for the synchronization of power networks.

Volker Mehrmann
Technische Universität Berlin
mehrmann@math.tu-berlin.de

SP5

I.E. Block Community Lecture: How Paradoxes Shape Mathematics and Give Us Self-Verifying Computer Programs

A paradox is a seeming contradiction. The liar's paradox is one of the best known: "This statement is a false." If the statement is true, then it is false; if it is false, then it is true. Paradoxes can be so amusing that we might think that paradoxes are nothing more than a game. However, paradoxes triggered a crisis in math a century ago when a paradox similar to the barber paradox was found: a barber named Bertie shaves exactly those who do not shave themselves. Does Bertie shave himself? If he does, then he doesn't; if he doesn't, then he does. Other clever paradoxes show us the disturbing limits of computation and mathematics. These results are mathematical bombshells. Today, we design computer programs that check that other computers programs have no bugs. Can computer programs be fed into themselves to check their own correctness? Or does paradox stop us in our tracks? And can we know that beneficial artificial intelligence will not turn evil when it starts to modify its own computer code?

Thomas Hales
University of Pittsburgh

hales@pitt.edu

JP1

The Mathematics of Wrinkles and Folds

The wrinkling and folding of thin elastic sheets is very familiar: our skin wrinkles; a crumpled sheet of paper has folds; and a flat sheet stretched over a round surface must wrinkle or fold. What kind of mathematics is relevant? The stable configurations of a sheet are local minima of a variational problem involving its elastic energy – which consists of a nonconvex membrane energy (favoring isometry) plus a small coefficient times bending energy (penalizing curvature). The bending term is a singular perturbation; its small coefficient is the sheet thickness squared. The patterns and defects seen in thin sheets arise from energy minimization – but not in the same way that minimal surfaces arise from area minimization. Rather, the analysis of wrinkles and folds involves the asymptotic character of minimizers as the sheet thickness tends to zero.

Robert V. Kohn
Courant Institute of Mathematical Sciences
New York University
kohn@cims.nyu.edu

JP2

Applied and Computational Mathematics: A New Curriculum for 21st Century Discovery and Innovation

We present BYU's undergraduate Applied and Computational Math program, which provides students with a rigorous foundation in mathematics, statistics, and computation. This program was designed from the ground up with the hopes of attracting top employers and graduate programs and thus becoming a national model for applied math education. This program runs as a two-year upper-division lockstep curriculum consisting of 32 credit hours, spread out evenly over four semesters. In addition, students select an area of specialization in one of over 25 areas in the pure and applied sciences and take additional coursework to fulfill a concentration requirement. The first year of the program is devoted to the design, analysis, and optimization of algorithms, and gives students an arsenal of mathematical and statistical tools to explore the performance, complexity, and accuracy of algorithms. The second year focuses on the art and science of mathematical modeling, which gives students the ability to connect the real world with abstract mathematics and numerical simulation. At every stage of the program, students integrate theory with application and computation and data-enabled discovery. At the close of its 5th year in service, we have learned a lot about how to build a program, how to adapt to the needs of the students and the changes in technology, and how to adjust the program in real time to serve the needs of employers and other stakeholders.

Jeffrey Humpherys
Brigham Young University
jeffh@math.byu.edu

CP1

Mathematical Modeling with Undergraduates

This talk is a reflection on my successful experience designing and implementing a mathematical modeling course for undergraduate students majoring or minoring in mathematics. Course materials, implementation of open-ended projects, and preparation of students for problem solving will all be discussed.

Shelley B. Rohde
University of California, Merced
srohde2@msudenver.edu

CP1

An Undergraduate Mathematical Modeling Capstone

We will share our success story of a well-established capstone course in mathematical modeling. Student-chosen (and supervisor-approved) projects have included "flower sticks" (a form of juggling), simulation of the games of War and Mancala with statistical analysis of the results, musical tuning systems, baseball ranking using a chess system, and much more.

Therese Shelton
Southwestern University
Southwestern University
shelton@southwestern.edu

CP1

Preparing Students with Minimal Modeling Experience for a Math Modeling Contest: Augusta University Math Departments First (and Second) Attempts at Mcm

For each of the past two years, two different teams of students at Augusta University have participated in COMAPs Mathematical Contest in Modeling/Interdisciplinary Contest in Modeling [MCM/ICM]. These teams were comprised of not only math majors, but also math education, computer science and physics majors. Although Augusta Universitys Math Department is developing more of an applied math and math modeling emphasis, it does not currently have a math modeling course nor much of an emphasis on math modeling in the lower-level math major courses such as Calculus. The concern of the faculty advisors then has been how to prepare students who have potentially minimal modeling experience to participate in (and enjoy) the modeling competition. We will discuss our initial efforts to encourage and support the students who participated. We will also present feedback from some of the students who participated each year along with suggestions for future improvements based on student feedback.

Anastasia B. Wilson
Augusta University
Department of Mathematics
anawilson@augusta.edu

CP2

Implementation of the Generic Solution of Transparent Thinking Approach (tta) in Mathematics Education

Humanity is overburdened by an overwhelming challenges, problems and failures. TTA is developed in response to these multi scale and multi domain problems. Transparent Thinking Approach (TTA) is a newly developed value-engrained and thinking-based educational reform approach (Aliedeh, M. A., 2015 a, b, c, 2016, 2017 and 2018). TTA generic features enables it to easily diffuse in all domains. The main goal of this Curriculum Exemplar session is to

help the participants to taste the real fruits of TTA by grasping the ability to employ different TTA tools in producing a new mathematical instructional materials. The method of delivery of the basic skills in this Session will be the hand-on and mind-on activities that is structured in an innovated sequence to create a coherent and integrated whole. This session will be enhanced by the following interactive features: (A) Creating a Living Example, (B) Specifying the starting and end points, (C) Connecting the Dots. The connection will be accomplished through the four SRBF framework stages : Seeds, Roots, Branches, and Fruits Activities. TTA-Based enhanced writing style is characterized by text serving graphics, visible communication, extended modeling tools, creation of an entertaining storyline and a convincing line of argument, and innovative combination of simplicity and depth. The participants at the end of the session will carry with them a real sample of a TTA-based mathematical instructional material.

Mohammad Aliedeh
Chemical Engineering Department, Mutah University
aliedeh@hotmail.com

Ahmad Aliedeh
Mathematics Department
Mutah University, Jordan
a.aliedeh@gmail.com

CP2

OHMint: An Online Mathematics Course and Learning Platform for Engineering Students

The project oHMint (oHMint stands for online higher mathematics for informatics, natural sciences and technology) is an ongoing initiative with the goal of providing an online self-study course and learning platform for higher mathematics, mostly aimed at all students of engineering degree programs at German universities. Its kickoff is organized and funded through the Hamburg Open Online University, with the technical implementation being handled by integral-learning GmbH. The oHMint project was initiated by members of the OMB+ consortium, a group of 14 German universities offering an online mathematics bridging course for those interested in a STEM university degree program. This bridging course is being used extensively at around 50 German institutions, and oHMint benefits significantly from the expertise gained through its development. Currently, one chapter of oHMint is being produced in a pilot project as a prototype for the future development of the entire course spanning four semesters. This serves as an opportunity to test the implementation of new didactical approaches for delivering content as well as innovative types of exercises, taking into account the specific needs of young people today when it comes to learning mathematics. The full oHMint course will provide freshmen and students of higher semesters with a modern way of transitioning smoothly from a high school level of knowledge in mathematics to a bachelor degree level.

Helena Barbas
Universität Hamburg
helena.barbas@uni-hamburg.de

Ingenuin Gasser
University of Hamburg
Department of Mathematics
ingenuin.gasser@uni-hamburg.de

Franz Konieczny
integral-learning GmbH
franz.konieczny@integral-learning.de

Alexander Lohse
University of Hamburg
alexander.lohse@uni-hamburg.de

Ruedi Seiler
integral-learning GmbH
ruedi.seiler@integral-learning.de

CP2

What Makes a Successful Experience in a First Vector Calculus Course

This work focuses on students' ability to perform on a multi-step applied problem in vector calculus. Assessments have shown that students have difficulties solving an inverse problem in the context of a vector initial value problem (IVP). In particular, we assess a projectile motion problem where students are asked to solve for the initial speed. We identify problems with setting up the IVP, solving the differential equation and solving the resulting nonlinear systems of equations. Following this initial assessment, we adopt a long-term implementation of teaching the separate steps involved in such a problem over a full course. We provide assessments of each step throughout the course using WeBWorK problems, quizzes, in class projects, take-home assignments and tests. We anticipate future collaborations with professors in engineering and physics that emphasize common strategies for successfully solving an IVP regardless of the context. The results of a follow-up assessment to these changes in pedagogy will be presented. Recommendations for future teaching strategies will be included.

Cristina Negoita
Arizona State University
cristina.negoita@oit.edu

James Fischer
Oregon Tech
jim.fischer@oit.edu

CP2

Flipping Math Classes to Promote a Smooth Transition from High School to College in Brazil

The Brazilian higher education system is undergoing a fast growth of social and racial inclusion polices. Teenagers from low income families, whose parents did not attend the university, are now becoming undergraduate students of hard sciences and engineering courses. The diversity and inclusion policies, however, present a challenge to professors: the students' lack of mathematical skills. In the state of Sao Paulo, 85% of the high-school graduate students attended public schools. Official math exams show that 48% of these students are below the "basic" level, while 47% are at the basic level and only 5% have "adequate" mathematical skills. In fact, most of the students have difficulties summing fractions and dealing with the distributive property. The University of Campinas has a general 2-year education program, called ProFIS, aimed to bring public high-school students to the undergraduate courses of the university. The most demanding and feared subject of the ProFIS curriculum is mathematics. In 2011, about 50% of the students failed math courses. Since then, these courses evolved from the traditional classroom model to the flipped

classroom model, where the instructional content is delivered outside the classroom, by books and online videos, and the class time is spent on practical activities, where the students work in a collaborative way. In this talk, we present this new teaching strategy, as well as its impact on the students' performance.

Francisco M. Gomes
University of Campinas - Brazil
Department of Applied Mathematics
chico@ime.unicamp.br

CP2

Let Your Students Do the Talking: Using Student Videos As An Assessment Tool in a Linear Algebra Class

My goal for this talk is to share how I have used video to assess student understanding in an introductory sophomore linear algebra course. The course is built around 3 units, each with challenging tasks that assist students to develop an understanding of key linear algebra concepts. To promote student interactions during the activities, the groups write out their solutions on large white boards. Upon completion, the group members are required to shoot a short video with an explanation of the group work. These videos usually are 1 2 minutes long and provide a wealth of information on student thinking. At the same time, they give students a chance to practice using the language of linear algebra. I will discuss the logistics of the process and provide examples of student videos.

Susan Hagen
Virginia Tech
hagen@math.vt.edu

CP3

Teaching Calculus for Biology and Medicine

Almost all higher education institutions have a separate calculus sequence designed with biology and pre-med students in mind. I will describe our efforts in teaching this group of students how to connect abstract mathematical concepts taught in calculus courses to 'real life" biology and chemistry examples.

Korana Burke, Tim Lewis
UC Davis
kburke@ucdavis.edu, tjlewis@math.ucdavis.edu

Sam Walcott
University of Caliornia, Davis
swalcott@math.ucdavis.edu

CP3

A Model for a 100-level Course on Programming and Computer Algebra

This talk describes a model for a 100-level course on programming and computer algebra. Calculus I serves as a prerequisite for the class and may be taken concurrently. The choice of programming language and computer algebra system can vary by semester to serve the needs of different students in the mathematics major, including those with interests in applied mathematics, statistics, pure mathematics, and education. Assignments include explorations, exercises, student presentations, programming homework, computer-algebra homework, a programming application assignment, a computer-algebra application assignment, and exams. The application assignments require the students to connect programming and computer algebra to material from other courses in the mathematics major. In this talk, we provide an overview of materials and resources for the course in programming and computer algebra, as well as links to the documents and sites in question.

Laura K. Gross
The University of Akron
Department of Theoretical and Applied Mathematics
laura.gross@bridgew.edu

CP3

Writing Projects for Applied Mathematics Courses

A primary attraction of an applied mathematics course is the promise of applying mathematics to the real world. However, this task is often challenging (if not impossible) to accomplish within the confines of the standard 50-minute class period. In this presentation, we will discuss out-of-class writing projects, one solution to this challenge. This discussion will include a particular format of writing project that emphasizes teamwork, writing skills, and critical thinking. We will also discuss potential sources of such projects, as well as assessment methods.

Catie Patterson
Austin College
cpatterson@austincollege.edu

CP3

Bringing Authentic Modeling to College Algebra and Calculus Through Collaboration with Partner Disciplines

Mathematicians from a consortium of ten institutions have been working with partner disciplines to improve mathematics courses in the first two years of higher education. One of the themes among the variety of institutions, courses, and partner disciplines is authentic mathematical modeling experiences. In this talk, we will share a framework for our collaboration along with examples of modeling activities that are being implemented in college algebra and calculus courses. In addition, we will share how these modeling activities are being integrated into the courses offered by the partner disciplines.

Victor Piercey
Ferris State University
victorpiercey@ferris.edu

CP3

Teaching Linear Algebra with Applications

In this talk, I will discuss teaching an introductory linear algebra class with an emphasis on applications. The class is an upper level undergraduate class aimed primarily at STEM majors. The discussed applications range from image processing to data grouping and clustering. These applications are incorporated into teaching in a form of weekly computer-based projects. The projects provide a hands-on opportunity for students to work with real data while using linear algebra concepts they simultaneously learn in lectures.

Anna Zemlyanova
Department of Mathematics
Kansas State University

azem@ksu.edu

MS1

Mathematical Modeling in Secondary Teacher Preparation

In secondary teacher preparation programs, undergraduate students have to learn mathematical content as well as pedagogical methods for teaching that content. In the context of mathematical modeling, this means that students must simultaneously develop familiarity and proficiency with the mathematical modeling process as well as effective ways of teaching mathematical modeling. The latter includes selection of modeling tasks, flexibility in accepting student solution approaches, assessment of student-created models, and pedagogical methods for facilitation of presentation of models and ways to compare and contrast peer-created models with their own. I will discuss some experiences developing curricular materials in mathematical modeling for secondary mathematics teacher preparation through the Mathematics of Doing, Understanding, Learning and Educating for Secondary Schools (MODULES) Project, funded by the National Science Foundation (NSF).

Cynthia Anhalt
University of Arizona
Department of Mathematics
canhalt@math.arizona.edu

MS1

A Course in Mathematical Modeling for Pre-Service Secondary Teachers

The Common Core State Standards for Mathematics elevated the status of Mathematical Modeling (MM) in the K-12 curriculum. This is surely a welcome change for the SIAM community, but it raises questions about how the preparation of K-12 teachers for engaging students in authentic MM. The few studies that exist indicate that preparation in MM is very limited. At California State University Long Beach, a course in MM for Mathematics Education majors was co-developed and co-taught by an applied mathematician and a mathematics educator. The development and teaching of the course was approached as a design experiment. We have collected and partially analyzed data from two iterations of the course. The goals of this session are to: 1. describe the motivation for and content of the course, 2. report on preliminary findings and emergent hypotheses from our MM course, and 3. open up a discussion about teacher preparation in MM.

Joshua Chesler
California State University, Long Beach
California State University, Long Beach
josh.chesler@csulb.edu

MS1

Introducing Basic Research Skills through Agent-Based Modeling

Agent-based modeling plays a pivotal pedagogical role in the entry level mathematical modeling course at Amherst College. By focusing on agent-based modeling in NetLogo, rather than differential equation-based modeling, the course is accessible to nearly all of our students and attracts students from a broad array of majors. The course is centered around three large modeling projects (schooling/swarming, infectious spread, and artificial societies, with a mix of group and individual work), in which students formulate a focused question and work through the modeling process, with the emphasis on developing and implementing a model that has sufficient complexity to address the targeted question of interest, yet simple enough to analyze thoroughly and produce insightful results. Through student-led discussions of modeling articles from the research literature, they learn to critically read research papers and experience a wide range of agent-based modeling topics. Through this combination of modeling projects and literature review, students develop and practice essential research skills.

Tanya Leise
Amherst College
tleise@amherst.edu

MS1

Weak Inertial Lift of Rotating Colloidal Wheels Near a Plane

Recent experimental work has investigated the motion of aggregated, superparamagnetic, colloidal particles immersed in a fluid. The particles in these experiments are driven by a magnetic field, which effectively applies an external torque on the particles that causes them to move. The particles under investigation are not neutrally buoyant and thus they sink towards the bottom of the laboratory assembly. It is observed that shortly after torque is applied, a particle resting on a surface will lift up and translate until it reaches some equilibrium height from the surface. In this talk we investigate the origin and magnitude of this lift. While it is tempting to apply Stokes equations because the radius of the particles is on the order of microns, it is known that no net lift is possible in Stokes flow for agreggates with the symmetry considered in the experiments. We consider approaches in the so called weak inertia regime that take advantage of having a small, but non-zero, Reynolds number, to estimate lift forces on various configurations of particles and external torques.

Forest O. Mannan
Tulane University
fmannan@mines.edu

MS3

Biomathematics Workshops: a Model for Interdisciplinary Collaboration and Undergraduate Research

In this age of big data, providing students with authentic opportunities to analyze real data and create data-informed mathematical models is of critical importance. To that end, the Mathematics Program at Pacific University, and the NSF Science and Technology Center for Coastal Margin Observation & Prediction (CMOP) at Oregon Health and Science University (OHSU), embarked on a unique collaboration resulting in a pair of so-called Biomathematics Workshops. These Biomathematics Workshops held in January 2014 and in May 2015, provided Pacific University undergraduate students with foundational training in elements of mathematical modeling, computational science, and statistical analysis, as well as intensive tutorials on the biogeochemistry of the Columbia River estuary. Then using field and simulation data from the SATURN collaboratory (http://www.stccmop.org/saturn), students worked in teams of three to design predictive models of various aspects of an annual Red Water Bloom in the Columbia

River Estuary. Each team wrote up their results in formal scientific reports that were evaluated by both a mathematician and a research biochemist. This presentation will discuss the processes involved in the development of this unique educational initiative as well as findings related to the student learning experience.

Ian Besse
Pacific University
besse.ian@pacificu.edu

Vanessa Green, Nievita Bueno Watts
Oregon Health and Science University
greenva@ohsu.edu, buenowat@ohsu.edu

Mark Ward
Purdue University
mdw@purdue.edu

Antonio Baptista
Oregon Health & Science University
baptista@ohsu.edu

MS3

Bringing Data into Mathematical Modeling Courses

Mathematical modeling is a natural course for students to begin working with data in the classroom. In this talk, some resources for data sets relevant to commonly taught topics in modeling will be provided. In addition, ideas for effectively bringing data into the modeling curriculum will be discussed.

Jakob J. Kotas
University of Portland
kotas@up.edu

MS3

Integrating Data into a First Course in Differential Equations

In this talk, I will highlight several examples of data collection, parameter identification, and model validation that are easily accessible to students in a first-course in differential equations.

Katie Oliveras
Seattle University
Mathematics Department
oliveras@seattleu.edu

MS3

Using Hands-on Experimentation to Introduce Differential Equations

Differential equations is frequently a college sophomore level course for a mathematics or other STEM major. However, the concepts of differential equations are intuitive and easily visualized. Furthermore, differential equations are universal in application and are often cited as an eye-opening subject for future mathematics and applied mathematics majors. For this reason, I believe differential equations can and should be introduced in a qualitative sense to students earlier in their mathematical careers. In this talk, I will describe how hands-on experiments with physical pendulums can be used to motivate a discussion of topics from differential equations in a week-long applied mathematics laboratory suitable for high school students. I will reflect on the strengths and weakness of this curriculum and discuss how it could be adapted for other settings.

Jacob Price
University of Washington
jrp14@uw.edu

MS4

Promoting Culture Change, One Turtle at a Time: Undergraduate Research in Agent-Based Modeling of Violence Prevention

Interpersonal violence on college campuses has received much attention in recent years, and when you see the numbers, you can understand why. It has been reported that many as 1 in 4 women and 1 in 30 men will experience sexual violence at least once during their four years in college. These numbers are both outrageous and unacceptable. But what can be done? At the University of Portland, and other colleges across the nation, we have adopted the Green Dot bystander violence prevention program, which challenges the culture of interpersonal violence and trains students to take a stand for one another. In the Mathematics Department at the University of Portland, students are creating models of this program to further investigate the philosophies of the Green Dot program and seek additional mechanisms to strengthen its effectiveness on campus. Here I will provide background on how this research began, how it has opened doors for students, and how agent-based modeling can not only be a tool for investigating issues of social justice, but also how its use in the classroom and in undergraduate research has the potential to level the playing field for students of diverse backgrounds.

Hannah L. Callender
University of Portland
callende@up.edu

MS4

Whose Math and For What Purpose? A Community Seminar on Identity, Culture, and Mathematics

In the spring of 2018, the Pomona mathematics department hosted a community seminar on identity, culture and power in the discipline and education of mathematics. The seminar was open to all students, faculty, and staff of the college as well as any members of the local community. In this talk I describe the specifics of the seminar, what types of issues we discussed, what a typical seminar session looked like, and what we all gained from the experience.

Gizem Karaali
Pomona College
gizem.karaali@pomona.edu

MS4

Answering the Question "When Are We Ever Going to Use This?"; Arming Our Students with the Tools Needed to Change the World for the Better

"We all use math everyday," begins the show Numb3rs. We really do. Mathematics has the power to change the world for the better by informing us of systemic injustice and helping us to develop solutions. In this talk, we will present two course modules developed for upper division

classes that enable students to use their mathematical skills to explore questions of racial injustice in the allocation of public education funds and pollution in the Chesapeake Bay with its implications on livelihoods of watermen. One of the courses features experiential learning and requires students to consult with local non-profit organizations. We will provide course materials to use in the classroom, as well as steps to design a service learning course.

Emek Kose, Allison L. Lewis
St. Mary's College of Maryland
ekose@smcm.edu, allewis@smcm.edu

MS5

The Education for Sustainability Philly Project: Supporting Teachers to Develop Lessons on Sustainability

We discuss the results of a one year pilot program funded by the NSF to develop a model for teacher leadership develop in Education for Sustainability which aims to support implementation of the School District of Philadelphias Green Futures sustainability initiatives. A cohort of 14 high school teachers drawn from STEAM fields participated in a 60 hour professional learning community in which they learned about the Education for Sustainability standards and developed lessons that incorporated these standards and linked with the National Wildlife Federations Eco-Schools Pathways program. These lessons were place based, making use of the rich array of sustainability resources in the Philadelphia region, and included hands on projects in which students could green their schools and communities. The teachers explored ways to build connections in their lessons that between STEM and non-STEM fields.

Victor Donnay
Bryn Mawr College
vdonnay@brynmawr.edu

MS5

Fostering and Sustaining Interdisciplinary Faculty Communities Around Undergraduate Teaching: Insights from the Qubes Project

The Quantitative Undergraduate Biology Education and Synthesis (QUBES) project acts as an online center supporting a diverse community of faculty and projects interested in improving students quantitative reasoning in biological contexts. We provide an online platform for scientific collaboration and computation that is being used by over 70 partner projects representing the life sciences, mathematics, earth science, statistics, computer science, and education research communities. To help our partners share their products and resources we have implemented a system for providing professional development to distributed, heterogeneous groups of teachers called Faculty Mentoring Networks (FMNs). Working across disciplinary boundaries to support communication, planning, delivery, and evaluation of FMNs has required explicit discussions of the differences among academic traditions, particularly as they influence uptake by other disciplines and use in teaching settings. This presentation will focus on several case studies of interdisciplinary collaboration facilitated by the QUBES project and highlight a set of practical lessons learned that inform our ongoing efforts to promote faculty engagement with diverse teaching and learning communities.

Sam Donovan
University of Pittsburgh
sdonovan@pitt.edu

MS5

The Math Modeling Hub: a New Online Community of Practice for Educators

The Math Modeling Hub (MMHub) serves as a repository of information related to mathematical modeling education. Resources supported by the MMHub include materials for classroom use, professional development for people who are new to math modeling, and "sandbox" areas where educators can collaboratively develop, edit, and test instructional materials. The MMHub also promotes and sustains a community of practice by hosting forums and online subgroups (such as mentoring networks) and facilitating communication among members about events outside the hub. The MMHub allows for extensive and varied levels of discussion and collaboration, and helps connect people beyond the barriers of geographical distance. This summer marks the initial public rollout of the MMHub; everyone with an interest in math modeling education, from experts to novices, is welcome to join the community. This presentation will introduce the audience to the purpose, features, early activity, and future plans for the new Math Modeling Hub.

Jason Douma
University of Sioux Falls
jason.douma@usiouxfalls.edu

MS5

My Experiences in a Faculty Mentoring Network for Mathematical Modeling

Faculty mentoring networks are online groups, usually including 10-15 faculty members focused on a specific topic, that typically meet every two weeks over a period of several months. They allow colleagues across the country to discover new teaching materials and pedagogical techniques and incorporate them into their courses. The Mathematical Modeling Faculty Mentoring Network (MMFMN) brings together faculty to learn about, discuss, and implement math modeling instructional approaches and materials. In its inaugural online meetings during the fall of 2017, fellow master math modeling teachers shared, developed, and refined modeling activities as well as teaching strategies. In the spring, these teachers committed to helping at least one other colleague to incorporate math modeling into their curriculum. In this session, I will share some of the benefits I gained from collaborating with these master teachers in the fall and some of the observations and challenges I faced in bringing these materials back to my school colleagues less familiar with mathematical modeling in the spring.

Lauren Shareshian
Oregon Episcopal School
shareshian@oes.edu

MS6

Exploring Ways to Support Stem Learning and Math Modeling in the Early Grades

When elementary school teachers are designing or selecting mathematical modeling tasks, it is possible to choose

an engaging, fun task that does not yield rich mathematical discourse. This talk will present several examples of tasks developed in the IMMERSION elementary school math modeling program and provide both guiding principles and cautionary tales.

Marka Carson
Pomona Unified School District, USA
mkacarson@yahoo.com

MS6

Affordances of Mini-Modeling Tasks in the Elementary Grades

Where is the math? Elementary mini modeling tasks can show kids where the math is in any subject area. Modeling helps kids go beyond computation and engage in quantitative explorations that will be relevant in their lives and their jobs. This talk will share tasks from a 5th grade classroom that engaged students in answering modeling questions that arose from their reading.

Nicki Lew
Pomona Unified District
Nicki.Lew@pomona.k12.ca.us

MS6

Mathematical Modeling with Cultural and Community Contexts in Elementary Grades

Abstract Not Available At Time Of Publication.

Padmanabhan Seshaiyer
George Mason University
pseshaiy@gmu.edu

MS6

Mathematical Modeling in Kindergarten

In this talk I will share reflections from my kindergarten classroom over the past year. In particular I will focus on the classroom culture, habits of mind and questioning techniques that prepare kindergarteners to engage in mathematical modeling.

Robin Stankiewicz
Pomona Unified District
Robyn.Stankiewicz@pomona.k12.ca.us

MS7

Developing Mathematical Modeling Skills in Graduate-Level Courses

Mathematical modeling is the science of formulating application field phenomena mathematically; analyzing the formulated problems mathematically; using computers to solve the equations that express the phenomena; and integrating these elements to gain insight into the application field. In this talk, we will explain our philosophy for teaching first-year graduate students the art of mathematical modeling. The year-long sequence of two semester courses is structured around a series of guiding principles for mathematical modeling and engagement in practice of the process of mathematical modeling.

Kara Maki, David S. Ross
Rochester Institute of Technology
klmsma@rit.edu, dsrsma@rit.edu

MS7

The Mathematical Modeling Process As a Value-Added Experience for Graduate Students

For over 30 years, a small but motivated group of faculty across several universities have organized and hosted the Mathematical Problems in Industry (MPI) workshop. This Oxford-style workshop brings together industrial presenters and academics to solve contemporary problems that arise outside of the academy. The energetic style of the study-group has been known to intimidate graduate students (and some faculty as well). To attend to the special needs of graduate students who are seeking an industrial experience, the MPI organizing committee created a successful modeling camp aimed at preparing students for the rigors of the work-shop. The MPI workshop serves as the capstone experience for these students. These experiences have driven change within the applied mathematics curriculum at the University of Delaware (UD). The course focuses students more on modeling principles, such as mass-action or conservation principles, across a variety of application domains rather than traditional methods and techniques. In this presentation, I will discuss the curriculum along with the challenges and benefits of this approach.

Louis F. Rossi
University of Delaware
rossi@math.udel.edu

MS7

The IMA Math-to-Industry Boot Camp

The speaker will describe the IMA Math-to-Industry Boot Camp which was first offered in the Summer of 2016. The program provides training and experience to prepare Mathematics PhD students for internships and employment in industry. The training includes 'hard skills' such as computing and modeling, it also provides students with 'soft skills' such as teamwork, communication. Now in its third session, the speaker will point out lessons learned – what works and what does not, to-do's and not-to's – for institutions considering offering such activities to their students.

Fadil Santosa
School of Mathematics
University of Minnesota
santosa@math.umn.edu

Daniel Spirn
University of Minnesota
spirn@umn.edu

MS8

Assessment/Evaluation Plans and Results on Simiode Programs Workshops and Scudem - Student Competition

We present assessment/evaluation results from several years of SIMIODE workshops (MAA-PREP, JMM, MathFest) and Minicourses (JMM, MathFest) in which we show the effectiveness and resulting commitment of participants to using modeling in their differential equations courses and contributing their own ideas. We also present results on the assessment of SCUDEM 2018, an undergraduate

competition of modeling with differential equations.

Barbara Edwards
Oregon State University
edwards@math.oregonstate.edu

Jennifer Czocher
Texas State University
czocher.1@txstate.edu

MS8

Engaging in Pedagogical Development, Applied Scholarship, and Professional Service with SIMIODE

This talk will give personal examples of the many opportunities available to instructors in engaging with the SIMIODE community. These include being trained in and developing a modeling-first (inquiry-based) pedagogy to improve student learning, incorporating applied mathematics research into teaching, student mentorship, and curriculum creation, and opportunities to share in and shape resources for others through professional service.

Corban Harwood
George Fox University
rharwood@georgefox.edu

MS8

SCUDEM 2018 - Student Competition Using Differential Equations Modeling Organization, Activities, Participation

The Student Competition in Undergraduate Differential Equations Modeling (SCUDEM) is an annual international week-long competition designed to give students experience using differential equations to model real-world scenarios. Each team has a faculty coach, and at each regional competition host site the faculty coaches meet to for a faculty development program on the opportunities for modeling in the classroom. We will give details on the 2018 competition, specifically its impact on student creativity and understanding of differential equations and its effectiveness in promoting intercollegiate faculty discussion on the roll of modeling in the classroom.

Corban Harwood
George Fox University
rharwood@georgefox.edu

Philip Nosler, Laura Nosler, Alexandra Hanson
Clackamas Community College, USA
philnosler@gmail.com, nosler.laura@student.clackamas.edu, alexandra.hanson@gmail.com

MS8

SIMIODE Community and Purpose - Supporting Modeling in Teaching Differential Equations

We present an overview of SIMIODE Systemic Initiative for Modeling Investigations and Opportunities with Differential Equations, its purpose and possibilities with attention to activities the attendees could engage in such as use of Modeling Scenarios in their teaching; publication of their own teaching activities; finding sources for ideas on modeling in their coursework; collegial exchange of ideas, videos, and data sets; organizing student modeling teams for competitions, and more.

Brian Winkel
Director of SIMIODE
BrianWinkel@simiode.org

MS9

Promoting Cultural Diversity Through Mathematical Modeling

Abstract Not Available At Time Of Publication.

Ricardo Cortez
Tulane University
Mathematics Department
rcortez@tulane.edu

MS9

Broadening Engagement by Extending the Classroom to Conferences

Abstract Not Available At Time Of Publication.

Mary Ann E. Leung
Sustainable Horizons Institute
mleung@shinstitute.org

MS9

Transforming Institutional Best Practices Through Inclusive Education and Global Engagement

Abstract Not Available At Time Of Publication.

Padmanabhan Seshaiyer
George Mason University
pseshaiy@gmu.edu

MS9

Promoting Diversity in STEM Through Research Activities

Abstract Not Available At Time Of Publication.

Mariel Vazquez
University of California, Davis, USA
'mrlvazquez@ucdavis.edu'

MS10

On the Role of Optimization Algorithms in Deep Learning

Learning with deep neural networks has been very successful recently in a wide variety of machine learning tasks. Even though the training loss is a complex non-convex objective, simple methods such as stochastic gradient descent (SGD) are able to find a global minimum. More surprisingly, the solutions found by SGD have small test error, even though the problem is generally over-parametrized (model has more parameters than the number of samples). This is a result of the implicit regularization of the optimization algorithm (SGD), that results in picking a global minimum with a smaller test error. In this talk, I will discuss our recent work towards understanding this generalization behavior and its relation to the optimization methods for neural networks.

Srinadh Bhojanapalli
Toyota Technological Institute at Chicago

srinadh@ttic.edu

MS10

An Informal Approach to Teaching Calculus

I believe that the common approach to teaching calculus devotes too much attention to detail and formalism. As a result, the central ideas of this beautiful subject are often obscured. I'd like to propose an alternative approach to teaching calculus that accentuates the essential ideas and treats the concept of the infinite and infinitesimal in a natural and approachable fashion.

Pavel Grinfeld
Drexel University
pg77@drexel.edu

MS10

Applications of Deep Learning in the Classroom

Today, there is tremendous demand for deep learning expertise across industries. Education is rising to this challenge. In this talk we will highlight examples of courses successfully empowering students with deep learning skills and the tools available to support this. Join us for a conversation to further these objectives.

Loren Shure
MathWorks, USA
loren.shure@mathworks.com

MS10

The Structure of a Deep Neural Net

We begin with the matrices of weights that connect each layer of neurons to the next layer. There is also the crucial nonlinear "activation function' to be applied to the input at each neuron — to produce the output that is multiplied by new weights and sent forward. The choice for this function is often ReLU $(x) = \max(0, x)$. Then the overall learning function from all the layers is continuous and piecewise linear. We describe the key algorithms: (stochastic) gradient descent and backpropagation. to optimize weights. And we report on the experience of teaching a new MIT course 18.065 on Linear Algebra and Learning from Data (`math.mit.edu/learningfromdata`).

Gilbert Strang
Massachusetts Institute of Technology
Mathematics Department
gilstrang@gmail.com

Gilbert Strang
Massachusetts Institute of Technology
Department of Mathematics
gilstrang@gmail.com

MS11

The Introductory Math Program at the University of Michigan

In the early 1990s, the University of Michigan Introductory Math Program reformed its approach to teaching calculus (and 'Data, Functions and Graphs,' which serves as a precalculus course), and much of the structure created at that time remains to this day. The program is characterized by active learning methods (especially group-work) in small sections, with a focus on conceptual understanding, communicating mathematics, and mathematical modeling. I will discuss the structure, philosophy, and operation of our program.

Hanna Bennett
University of Michigan
hbennett@umich.edu

MS11

Teaching Calculus: Then and Now

For close to a hundred years, and especially since George Thomass seminal textbook from the early 1950s, the content of the freshman calculus sequence has remained essentially unchanged. The calculus reform movement beginning thirty years ago brought about welcome changes in pedagogy which included graphical and numerical approaches facilitated by new technologies. But the MAAs recent study of practices in calculus instruction, and current calculus texts, suggest that, with a few exceptions, the traditional order of topics has remained static. Particularly when a large proportion of college calculus students have already studied calculus in high school, new and different approaches are needed. These may include such things as active engagement in modeling authentic real-world problem situations, data-driven explorations of rates of change and accumulation, and creative methods of assessment. This symposium seeks to reveal and publicize novel examples of restructuring of the first year of college calculus.

Gary Simundza
Wentworth Institute of Technology
simundzag@wit.edu

MS11

Applying Cognitive Science to the Classroom

We will present two examples of our work in applying current work in cognitive science to the college calculus classroom. In the first case, we followed up on work redesigning homework in a signals and systems class (Butler, et al, 2014, "Integrating cognitive science and technology improves learning in a STEM classroom") with a multiyear study looking at the effects of reordering homework problems on student learning in a first course in calculus. Our second project is inspired by Jerome Epstein's Calculus Concept Inventory as well as the misconceptions literature in cognitive science including Durkin & Rittle-Johnson's 2014 paper "Diagnosing misconceptions: Revealing changing decimal fraction knowledge". We are working on identifying and diagnosing the most common misconceptions in calculus. Expert instructors can do this from experience, but many sections of calculus are taught by novice instructors and we are working on developing tools to help them.

Emma Smith Zbarsky
Wentworth Institute of Technology
smithzbarskye@wit.edu

Andrew Butler
Washington University in St. Louis
andrew.butler@wustl.edu

MS12

The S-Stem Program: Funding Opportunities for

Broadening Participation By Low-Income Students in Applied Mathematics

Abstract Not Available At Time Of Publication.

Ron Buckmire
National Science Foundation
rbuckmir@nsf.gov

MS12

Insights from the Siam Workshop Celebrating Diversity

Abstract Not Available At Time Of Publication.

Erica J. Graham
Bryn Mawr College
ejgraham@brynmawr.edu

MS12

The Affordances and Challenges of Teamwork in Mathematical Modeling

Abstract Not Available At Time Of Publication.

Rachel Levy
Harvey Mudd College
levy@hmc.edu

MS12

The Msri-Up Model: Cultivating Mathematical Talent in Summer+ Programs

Abstract Not Available At Time Of Publication.

Herbert A. Medina
Mathematics Department
Loyola Marymount University
hmedina@lmu.edu

MS13

Developing and Mathematics and Climate Themed Bridge Course to Upper Level Math

This talk will describe a mathematics course, aimed at second-year undergraduate students with a background in calculus and ordinary differential equations, that introduces some of the mathematics involved with climate, on urban and global scales. The educational objective is to motivate more advanced courses in linear algebra, partial differential equations, and numerical analysis in terms of a compelling contemporary application. In this respect, the course serves as a model for a "bridge" course in applied mathematics, just as the usual introduction to proof course is for pure mathematics. (A sister course, Mathematics and Cancer, develops similar concepts.) Modeling topics start with simple "box" models of the ocean and include extensive discussion of the heat equation, with applications to urban climate.

Eric J. Kostelich
Arizona State University
School of Mathematical and Statistical Sciences
kostelich@asu.edu

MS13

The Diume Project: Developing and Implementing Computer-Based Calculus Modules Using Environmental Data

The Data Integration in Undergraduate Mathematics Education (DIUME) is an NSF funded project to design technology-integrated in-class modules based on real-world data sets for undergraduate mathematics courses ranging from Calculus I through Linear Algebra. Thematically, the modules largely focus on the environment and sustainability. The modules are designed to fit naturally into those classes, simultaneously reinforcing student learning of the mathematical content and increasing students ability to work computationally with real-world data. We will discuss the modules and share results from the first year of implementing them in Calculus courses.

Carl Lutzer
Rochester Institute of Technology
cvlsma@rit.edu

MS13

Mentoring Undergraduate Math Research on the Reversibility of Sea Ice Loss

I will present an example of an undergraduate math research project at the intersection of mathematics and climate. In this University of Minnesota math capstone project, then-senior Sarah Pierro explored the question "How soon must atmospheric greenhouse gas concentrations be reduced, in order to avoid irreversible sea ice loss?" Pierro used Ian Eisenman's single-column sea ice model with nonlinear ice-albedo feedback dynamics and seasonal forcing terms as a simplified setting for answering this question. The project wove together physical concepts (e.g. enthalpy, conservation of energy) with mathematical concepts (e.g. time-periodic systems, Poincare maps, bifurcations, and hysteresis). It also required simulating the system numerically in MATLAB, optionally by adapting code that Eisenman shares publicly. The societal relevance of the research question, along with the range of skills required to address it, made for an engaging research project.

Katherine Meyer
University of Minnesota
meye2098@umn.edu

MS13

Undergraduate Research in Conceptual Climate Modeling

We discuss a yearlong undergraduate research project using low-dimensional mathematical models to understand current climate, historical climate, and the drivers of climate change. Energy balance models present a relatively easy approach for students to dive into the field of climate science without requiring too much background. They also feature many standard topics from dynamical systems (e.g., bifurcations, stability analysis). We explore the Budyko-Widiasih model for the global average surface temperature of the Earth as a function of latitude, coupled with the movement of the ice-line (the border between ice and no ice). The number and stability of equilibria is investigated as a function of several parameters. A slightly amended model to include the effect of CO2 in the atmosphere provides some evidence for the theory of Snowball Earth and a subsequent ice-free state in the Neoproterozoic Era.

Gareth E. Roberts

Dept. of Mathematics and C.S.
College of the Holy Cross
groberts@holycross.edu

Cara Donovan
College of the Holy Cross
cmdono18@g.holycross.edu

MS14

An Alternative Calculus Sequencing for An Undergraduate Core Mathematics Program

We will discuss a calculus sequencing where an introductory ordinary differential equations course is introduced immediately after a single variable calculus course. This is a slight variation of the usual sequencing of calculus courses, but we propose that the benefits are great especially when modeling real-world phenomena is integrated into the course. We will highlight these benefits which give students an early understanding of the power of mathematics in the academic and professional world with hope to create more math majors and in general, more STEM graduates.

Ivan Dungan
United States Military Academy
gregory.dungan@usma.edu

Randy Boucher
United States Military Academy
West Point
randy.boucher@usma.edu

MS14

Integrating First-Year Calculus and Physics Through Project-Based Learning

Modeling the Physical World is a year long project-based integrated Mathematics and Physics course aimed at advanced incoming first-year students. The core of the course is a collection of open-ended modeling projects worked on in groups throughout the semester. In this talk we discuss the structure of the course, finding compelling modeling problems, and the positives and negatives of building a course around modeling projects

Nathan Pennington
Creighton University
nathanpennington@creighton.edu

MS14

Rethinking Calculus for Engineers

Exercises for an introductory calculus class are designed to engage students in active learning with a focus on understanding concepts. Students collect (or work with previously collected) data and compute average rates of change. They then explore instantaneous rates of change, differentiation and integration. This approach also provides a different, less computationally-oriented experience for those students who have already studied calculus in high school. A newly developed text book complements this approach. Many of these exercises use a common theme so that students working in later exercises already have a familiarity with the context and can focus on each lessons learning objective. One such theme explores an oscillating cantilevered spaghetti noodle. Students initially gather data for the position of the tip of the noodle, plot these data and fit an appropriate function to the data, ignoring damping. They then calculate the average velocity, plot these new data points and postulate an instantaneous velocity function. In later exercises they refine the position function to include damping, explore the use of the product rule to get a damped velocity function, and explore accumulation by using the velocity function to reconstruct the original position function. Students empirically explore their function models and the effect of various function parameters using the online graphing application Desmos as they adjust their functions to best fit the data.

Mel Henriksen, Gary Simundza
Wentworth Institute of Technology
henriksenm@wit.edu, simundzag@wit.edu

MS15

Real Career Readiness

Abstract Not Available At Time Of Publication.

Solomon Garfunkel
COMAP
Sol@comap.com

MS15

Needed Math

Abstract Not Available At Time Of Publication.

Michael Hacker
Hofstra University
michael.hacker@hofstra.edu

MS15

Real Problems from the People Who Hire

Abstract Not Available At Time Of Publication.

Eric Robinson
Ithaca college (ret.)
robinson@ithaca.edu

MS16

Mentoring Undergraduate Researchers in Industrial Mathematics: Challenges and Results

In this talk, we will discuss the challenges of mentoring undergraduate students in research projects. We highlight several different several undergraduate research opportunities and student training in computational mathematics at ERAU, including the PIC Math program (Preparing Students for Industrial Careers in Mathematics) projects and individualized projects. We will discuss getting students involved in these projects and share ideas for successfully designing and mentoring such projects. The outcomes of the projects and lessons learned from these research experiences will be presented.

Mihhail Berezovski
Embry-Riddle Aeronautical University
mihhail.berezovski@erau.edu

MS16

Creating Partnerships with People in Industry and

Getting Research Problems for Students to Solve

Suppose you wanted to develop partnerships with people in business, industry, or governments (BIG) to get research problems for your students to work on and be better prepared for careers in BIG. How would you make these partnerships? How would you get research problems from industry? What would those problems look like? Answers to those questions can come through the PIC Math program. PIC Math is a MAA/SIAM supported program funded by NSF to prepare mathematical sciences undergraduate students for industrial careers by engaging them in research problems from industry. In this talk, we will discuss how faculty members many of whom have no experience in applied math or in BIG develop partnerships with people in industry, get research problems for their students as a result of these partnerships, and what these problems look like.

Michael Dorff
Brigham Young University
mdorff@math.byu.edu

Suzanne L. Weekes
Worcester Polytechnic Institute (WPI)
sweekes@wpi.edu

MS16

Student Research Projects and Programs in the National Nuclear Security Administration

The National Nuclear Security Administration (NNSA) is a semiautonomous agency within the U.S. Department of Energy whose mission is maintaining the U.S. nuclear weapons stockpile, nuclear nonproliferation, counterterrorism and counterproliferation, emergency response, and powering the nuclear navy. It is also one of the largest research and development enterprises in the world, encompassing 3 national laboratories and the Nevada National Security Site. There is a wide range of opportunities for mathematicians to build vibrant careers across the entire mission space, having a daily impact on national security. In this presentation, we will introduce the stockpile stewardship and nuclear nonproliferation mission spaces by featuring student research supported by the National Science Foundations Mathematical Sciences Graduate Internship program, PIC Math, and Nevada National Security Site internships. We will show how student projects developing multilayer network models for wireless sensors and designing new mathematical approaches for near-field seismic measurements are contributing to nuclear nonproliferation research, and how student collaborations to construct new mathematical models for laser measurement systems for dynamic material studies are helping to guide future experiments in support of the nations nuclear weapons stockpile.

Aaron B. Luttman
National Security Technologies, LLC
luttmaab@nv.doe.gov

MS16

Lenati's Data Science Interview and How Students Can Get the Skills to Pass It

With the rise of data science as a field, more and more mathematics students are getting data science jobs after undergrad. Unfortunately, students are often confused as to what data science employers are looking for in their candidates. The interview process is foreboding, and its hard to find out what it will be like. In this talk, I will walk through what Lenati looks for in our data science hires, and how we go about interviewing candidates. I will give examples of real interview questions and why we ask them. This is shine light on what skills candidates need, and how students can start getting those skills during school through projects like PIC Math. I will also discuss how students can reach out to professionals to have more resources to ask questions to.

Jonathan Nolis
Lenati
jnolis@outlook.com

MS17

Supporting Mathematics Students and Colleagues: Be An Active Bystander

Many of us have been a witness to a microaggressions, or been on the receiving end of one, this in our departments, conferences and workshops, etc. We may wish we had stepped in at the time, or wish someone had stepped in for us. This talk is about being an "active bystander": what it is, what are the barriers for action, what are the potential benefits and pitfalls for all involved of being an active bystander, whether people might be trained to become better active bystanders, etc. As time permits, we will discuss a few hypothetical scenarios

Rosalie Belanger-Rioux
Harvard University
Department of Mathematics
rbr@math.harvard.edu

MS17

The Need for a Revolution in Mathematics (Education): How Math Bolsters Whiteness

Abstract Not Available At Time Of Publication.

Rochelle Gutierrez
University of Illinois at Urbana-Champaign
Department of Curriculum and Instruction
rg1@illinois.edu

MS17

Being Human in STEM: a flexible collaborative course model for enhancing your campus STEM community

In response to concerns voiced by students during a November, 2015 sit-in at Amherst College in support of Black Lives Matter, a chemistry professor collaborated with students to develop a project-based course focused on diversity and inclusion in STEM, titled Being Human in STEM. In the course, students drive the academic inquiry, investigating both the local experience and the literature on diversity in STEM, and use that research to design their own interventions to share with and engage their own STEM community. This model for collaboratively developing a framework to understand and navigate diverse identities in the classroom and beyond can be adapted to any institution. The course is already being replicated in the Physics department at Yale University and will be implemented in the Chemistry department at Skidmore College next year.

Sheila Jaswal
Amherst College

Biochemistry and Biophysics Program
sjaswal@amherst.edu

Mylinh Le
Amherst College
n/a

MS17

A Course on "Race and Gender in the Scientific Commnuity"

We will discuss the goals and ideas behind a course on race and gender in the scientific community that was designed by a team of undergraduate students at Brown and is now offered as a regular course. This course examines disparities in representation in the scientific community, issues facing different groups in the sciences, and paths towards a more inclusive scientific environment. The course explores these topics through texts dealing with the history, philosophy, and sociology of science, and also addresses specific problems faced by underrepresented and well-represented racial minorities, women, and LGBTQ community members. The target audience are students majoring, or interested in majoring, in the life and physical sciences, including the mathematical sciences. The format consists of assigned readings that are then discussed in class in small and large groups.

Zofia Stanley
University of Colorado, Boulder
Department of Applied Mathematics
zofia.stanley@colorado.edu

Bjorn Sandstede
Division of Applied Mathematics
Brown University
bjorn_sandstede@brown.edu

MS18

Exploring Differential Equations Using Chebfun

Introductory courses in differential equations have to combine modeling, theory, analytical techniques, and computation for students who are often comfortable with little besides pattern matching and symbol manipulation. The open-source software project Chebfun offers the opportunity to interactively explore the connection between ODEs and their solutions, and to investigate different types of ODE problems, such as eigenvalue problems, that are not usually in the standard syllabus. Most problems can be solved in a GUI without learning coding syntax. More sophisticated programmatic investigation is possible by piggybacking on automatically generated code templates.

Tobin Driscoll
University of Delaware
Mathematical Sciences
driscoll@udel.edu

MS18

Matrices and the Complex Plane

Linear algebra and complex analysis are usually taught as two completely separate courses. They are brought together in a course on operator theory, which most students never take. But the fundamental uses of complex analysis in matrix theory can easily be covered in a linear algebra course, assuming that students have had basic complex analysis, or in a complex analysis course, assuming that students are familiar with matrices. Since even real matrices may have complex eigenvalues, it is generally assumed that students are at least familiar with complex numbers. If they know the Cauchy integral formula, then it is trivial to extend this formula to diagonalizable matrices and it requires just a little more work to extend it to all square matrices. Another important concept is the field of values, or, numerical range of a matrix: A set in the complex plane consisting of all Rayleigh quotients q^*Aq/q^*q. With these concepts in hand interesting discussions can take place about norms of functions of a matrix, such as powers A^k, $k = 1, 2, \ldots$, or the matrix exponential e^A.

Anne Greenbaum
University of Washington
greenbau@uw.edu

MS18

Numerical Stability of Linear System Solution Made Easy

We consider the numerical solution of systems of linear equations $Ax = b$, with a complex (real) nonsingular coefficient matrix A. Direct methods, such as Gaussian elimination with partial pivoting, QR decomposition, or Cholesky decomposition for Hermitian (symmetric) positive-definite matrices compute the solution x in three steps: First they factor $A = S_1S_2$ into a product of "simpler" square matrices S_1 and S_2, and then they solve two linear systems, one with S_1 and one with S_2. A direct method is numerically unstable if the elements of S_1 or S_2 have much larger magnitude than those of A. We present simple perturbation bounds for the computed solution, that feature a growth factor $\|S_1\|\|S_2\|/\|A\|$ in addition to the condition number of A. Instead of accounting for individual roundoff errors, we set up a compact perturbation model that represents the errors accumulated in each of the three steps. Then we bound the residual norm in terms of these perturbations. The resulting bound can be inserted into any existing residual bound for the computed solution. Thus, a short and intuitive derivation can capture the element growth without recourse to an unwieldy roundoff error analysis.

Ilse Ipsen
North Carolina State University
Department of Mathematics
ipsen@ncsu.edu

MS18

Perturbation Theory for Eigenvalues and Eigenvectors

Eigenvalues and eigenvectors are of crucial importance throughout applied mathematics, but their behavior under perturbation is not nearly as well known as it should be. This topic goes back to Rayleigh, but many of the most important results date from the mid and late 20th century. There are two broad streams of research. The first is classical analytic perturbation theory, where one considers the behavior of eigenvalues of a matrix or linear operator that is an analytic function of one or more parameters. The second concerns perturbation bounds rather than expansions, describing how to bound the perturbation of eigenvalues and associated eigenvectors or invariant subspaces when a nominal matrix is subjected to a perturbation with a given norm and structure. In this talk we will focus on the first

stream.

Michael L. Overton
New York University
Courant Instit. of Math. Sci.
mo1@nyu.edu

Ren-Cang Li
University of Texas - Arlington
rcli@uta.edu

MS19

2D Projects: Reinforcing Connections Between Subjects

Students begin to make connections across subjects within the same term and apply them in interdisciplinary design projects called 2D Designettes (or 2D projects). This talk will describe several projects that integrate various subjects: Chemistry, Biology, Physics, Mathematics, Programming in a selection of 2D projects that ran at SUTD from 2012 to 2013.

Sergey Kushnarev
Singapore University of Technology and Design
sergey_kushnarev@sutd.edu.sg

MS19

Curriculum Organization and the Cohort Classroom Model

The academic structure of SUTD is designed to support a curriculum that develops technically-grounded leaders who will contribute to society through technology and design and make an impact on the world. The SUTD undergraduate programme is divided into two distinct portions, Freshmore (Terms 1 to 3) and Pillar (Terms 4 to 8). The Freshmore terms provide students with the fundamentals which prepare them for a specialisation in any of the four pillars. During the three Freshmore terms, students take common classes together in a cohort-based learning format. They are grouped into cohorts that serve to foster collaborative learning and a sense of teamwork, ownership and belonging. Cohort-based learning incorporates hands-on activities such as simulations, demonstrations and problem sets where students are challenged to devise solutions in context. Upon completing the Freshmore terms, students select to specialise in one of the four pillars, graduating with the respective degrees. Design is another critical element in our curriculum. In addition to providing a strong technical-grounding, through the Freshmore terms and in the pillars, and cultivating creativity and a perceptive mind through humanities, design is literally everywhere at SUTD. The 5th Row is made up of co-curricular activities that add considerably to the learning experience of students by providing opportunities for them to develop their leadership, communication and teamwork skills.

Kin Leong Pey
Singapore University of Technology and Design
peykinleong@sutd.edu.sg

MS19

Design Thinking and Engineering Education

The talk presents the collaborative design teaching in the early years of engineering and architecture education. The problem of teaching design at the freshman and sophomore levels is that, from a constructivist approach, design is the summit of the learning curve: therefore, it is challenging because the technical background to back design decisions is lacking. This talk analyses this perceived difficulty and presents a case of design teaching in which both project based and process based design education models are hybridized and adapted to the specific design education in the context of Singapore University of Technology and Design.

Christine Yogiaman, Arlindo Silva
Singapore University of Technology and Design
christine_yogiaman@sutd.edu.sg, arlindo_silva@sutd.edu.sg

MS20

Epidemic Modeling to Inform Decisions @ Los Alamos National Laboratory

Abstract Not Available At Time Of Publication.

Sara Del Valle
Los Alamos National Laboratory
sdelvall@lanl.gov

MS20

The Role of a Professional Society in Facilitating Industry-Academia Partnerships for Operations Research and Analytics Careers

INFORMS, a global professional society of more than 12000 members from academia, industry, and government, is focused on promoting and supporting the use and practice of operations research, management science, and analytics. Research and applications of these fields are making significant contributions in the real world through the use of quantitative decision-making. Due to the nature of the fields supported by INFORMS, we are in a prime position to facilitate collaborations between industry and academia. In this talk, I will explore and discuss various models for implementing these collaborations.

Tasha Inniss
INFORMS
tinniss@informs.org

MS20

Students in the Bausch & Lomb/RIT Contact Lens Research Collaboration

The Center for Applied and Computational Mathematics (CACM) at RIT has a research collaboration with Bausch and Lomb. We develop and apply models of the mechanics of contact lenses, the eye, and the tear film in order to improve comfort. Math students, engineering students, and computer science students have worked on this research with members of the CACM faculty. Some have done so as summer employees at B and L Research Labs; some have worked as summer research students at RIT; some have been part-time employees paid through the research contract; others have made parts of the project into research courses for credit. One software engineering student began by writing code for this project and became a paid consultant to a specialty contact lens firm. In this talk we will discuss how students have advanced this research, and how involvement with this research has affected students' educations and their careers.

David S. Ross

Rochester Institute of Technology
dsrsma@rit.edu

MS20

Research Experiences on Industrial Math Problems

There is great benefit for university faculty, students, and mathematical scientists working in industry and government to collaborate. In this talk, we make clear these benefits, share our experiences, and point out opportunities that exist for industry/government-university partnerships. The speaker has been involved in the WPI REU Program in Industrial Mathematics and Statistics, the Preparation for Industrial Careers in Mathematical Sciences (PIC Math) program, and the Math Problems in Industry workshops among others, and she will highlight these and other initiatives.

Suzanne L. Weekes
Worcester Polytechnic Institute (WPI)
sweekes@wpi.edu

MS21

Teaching Data Science with Awareness

Abstract Not Available At Time Of Publication.

Tim Chartier
Davidson College
Dept. of Mathematics and Computer Science
tichartier@davidson.edu

MS21

Community Partnership" in Undergraduate Mathematics

Abstract Not Available At Time Of Publication.

Ami Radunskaya
Pomona College
Mathematics Department
ami_radunskaya@pomona.edu

MS21

Ethics in Mathematics - An Undergraduate Education Imperative

Abstract Not Available At Time Of Publication.

Joseph Skufca
Clarkson University
jskufca@clarkson.edu

MS21

Ethics Across the Curriculum As Applied to First Year Mathematics

Abstract Not Available At Time Of Publication.

Lizette Zietsman
Virginia Tech
Interdisciplinary Center for Applied Mathematics
lzietsma@vt.edu

MS22

Teaching Networks to Graduate Students Using CHUNKS and Network Profile Summary

We overview the method used for teaching network science to graduate students in sciences at the Naval Postgraduate Schools. The CHUNKS are into innovative adaptive learning modules that incorporate varying levels of disciplinary knowledge using a variety of delivery methods, to include demos, videos, interactive applications, TED talks, webinars, programming concepts (personalized to the skill of the student), and data manipulations. The instructor facilitates the learning experience by presenting the state of the art of the subject, together with how it can be used, while guiding the students through a web of the aforementioned demos and videos. The Network Profile Summary is a then used by students to present their knowledge, instead of quizzes and tests.

Ralucca M. Gera
Naval Postgraduate School
rgera@nps.edu

MS22

Reconstructing Networks with Heterogeneous and Unknown Errors

The vast majority of network datasets contains errors and omissions, although this is rarely incorporated in traditional network analysis. Recently, an increasing effort has been made to fill this methodological gap by developing network reconstruction approaches based on Bayesian inference. These approaches, however, rely on assumptions of uniform error rates and on direct estimations of the existence of each edge via repeated measurements, something that is currently unavailable for the majority of network data. Here we develop a Bayesian reconstruction approach that lifts these limitations by not only allowing for heterogeneous errors, but also for individual edge measurements without direct error estimates. Our approach works by coupling the inference approach with structured generative network models, which enable the correlations between edges to be used reliable error estimates. Although our approach is general, we focus on the stochastic block model as the basic generative process, from which efficient nonparametric inference can be performed, and yields a principled method to infer hierarchical community structure from noisy data. We demonstrate the efficacy of our approach in a variety of empirical and artificial networks.

Tiago de Paula Peixoto
University of Bath, UK
t.peixoto@bath.ac.uk

MS22

Understanding the Global Structure of Networks

Over the past decade, social network analysis has emerged as an important field, allowing for better understanding of huge complex systems of interactions. This talk focuses on two important areas of social network analysis- collecting data (sampling) and characterizing network structure- and discusses opportunities for involving students in research.

Sucheta Soundarajan
Department of Computer Science
Rutgers University

ssoundarajan@gmail.com

MS22

Teaching Networks to Undergraduate Students Without Prerequisites

Network science is an exciting area of applied mathematics with tremendous relevance in todays connected world. Following the model (and textbook) of a very successful course at Cornell, I have been teaching a lower-level undergraduate course at Stanford without any pre-requisites for the past three years. The modal student has been a sophomore majoring in engineering, but the full range has run from undeclared freshman to math major seniors, with the occasional MBA student mixed in. Younger students walk away excited to learn more advanced mathematics, while more advanced students walk away excited by new applications. I will discuss my experiences teaching this class, which I describe as an engineering perspective on network systems, focusing on intuitions.

Johan Ugander
jugander@stanford.edu
Stanford University