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SIAM Annual Meeting (AN22)

July 11–15, 2022

SIAM Conference on Applied Mathematics Education (ED22)

July 11–12, 2022

SIAM Conference on the Life Sciences (LS22)

July 11–14, 2022

SIAM Conference on Mathematics of Planet Earth (MPE22)

July 13–15, 2022

This document was current as of June 27, 2022. Abstracts appear as submitted.

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Annual Meeting

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IP1

Opening Remarks and Presentation: Probability, Sports, and Public Policy

Recent advances in data collection have made sports an attractive testing ground for new analyses and algorithms, and a fascinating controlled microcosm in which to explore social interactions. In this talk I will describe two studies in this arena: one related to public health and the pandemic and one related to the role of skill and chance in everyday activities. In the first, I will discuss what can be learned from the natural experiments that were (fortuitously) run in America football stadiums. During the 2020 National Football League (NFL) season, teams collaborated with local communities to determine whether or not to allow fans in the stadiums during the pandemic. These policy decisions were made based on local guidelines, local prevalence of the virus, community risk tolerance, and other localized considerations; some stadiums ultimately decided to allow fans at the games while others remained closed, providing perhaps the first set of natural experiments that can be analyzed to investigate the impact of opening stadiums on public health. The second topic I will discuss centers on fantasy sports which have experienced a surge in popularity in recent years. One of the consequences of this recent rapid growth is increased scrutiny surrounding the legal aspects of the games, which typically hinge on the relative roles of skill and chance in the outcome of a competition. While there are many ethical and legal arguments that enter into the debate, the answer to the skill versus chance question is grounded in mathematics. In this talk I will analyze data from daily fantasy competitions and propose a new metric to quantify the relative roles of skill and chance in games and other activities.

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IP2

Machine Learning Frameworks for Discovering Biophysical Signatures in 3D Shapes and Images

The recent curation of large-scale databases with 3D surface scans of shapes has motivated the development of tools that better detect global patterns in morphological variation. Studies which focus on identifying differences between shapes have been limited to simple pairwise comparisons and rely on pre-specified landmarks (that are often known). In this talk, we present SINATRA: a machine learning pipeline for analyzing collections of shapes without requiring any correspondences. Our method takes in two classes of shapes and highlights the physical features that best describe the variation between them. We develop a rigorous simulation framework to assess our approach, which themselves are a novel contribution to 3D image and shape analyses. Lastly, as case studies with real data, we use SINATRA to (1) analyze mandibular molars from four different suborders of primates and (2) facilitate the visual identification of structural signatures differentiating between the trajectories of two protein ensembles resulting from molecular dynamics simulations. Together, these results highlight a promising future for interpretable machine learning to facilitate the non-trivial task of pattern recognition in evolutionary and structural biology with substantially increased resolution.

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IP3

Living With Complexity: Pragmatic Approaches to Performance

The end of Dennard or frequency scaling has forced computer architects to find performance through innovation and specialization. Many HPC systems today have compute nodes with multiple GPUs, others depend on vector instructions integrated into the processor. In all cases, performance comes from specialized computing elements. These complex elements are often combined with complex memory, I/O, and internode networking systems. This complexity offer many ways to achieve performance, but at a price. This great complexity means that it is hard for humans to obtain good performance. And because these systems are not only complex but are hard to model the performance accurately, it is hard to automate the process of obtaining good performance. This also assume that the algorithm is fixed, but the best performance may require algorithm and/or data structure changes, further complicating the goal of achieving performance. The most practical approach is a man-machine or augmented human approach. This talk will describe some of the challenges and some current work that leverages both state-of-the-art compilers and source-to-source transformation techniques to provide a pragmatic approach to achieving good performance with reasonable effort by combining the strengths of humans and machines.

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IP4

High Dimensional Data Completion: Models, Algorithms and Applications

In recent years, high dimensional data completion has been extensively studied and analyzed, which can be applied to many data science applications such as recommendation, image recovery and one-bit data statistical estimation. In this talk, we present several variants of data completion models and their applications using linear algebra techniques. We provide theoretical insight to create a rigorous scientific basis for solving such data completion problems. Numerical examples are also given to demonstrate the usefulness of these models.

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IP5

Blumberg Talk Title TBA

Abstract will be posted here when it becomes available.

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IP6

Mathematical Analysis of Atmospheric and Oceanic Dynamics Models: Cloud Formation and

Sea-Ice Models

In this talk we will present rigorous analytical results concerning global regularity, in the viscous case, and finite-time singularity, in the inviscid case, for oceanic and atmospheric dynamics models. Moreover, we will also provide a rigorous justification of the derivation of the Primitive Equations of planetary scale oceanic dynamics from the three-dimensional Navier-Stokes equations as the vanishing limit of the small aspect ratio of the depth to horizontal width. In addition, we will also show the global well-posedeness of the coupled three-dimensional viscous Primitive Equations with a micro-physics phase change moisture model for cloud formation. Eventually, we will also present short-time well-posedness of solutions to the Hibler's sea-ice model.

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IP7

Finite Dimensional Approximations of Hamilton-Jacobi-Bellman Equations in Spaces of Probability Measures and Stochastic Optimal Control of Particle Systems

Hamilton-Jacobi-Bellman (HJB) equations in spaces of probability measures is a relatively new area with many applications. It has recently attracted more attention because of its connections with mean field games and mean field control problems. In this talk we will discuss how a class of HJB equations in spaces of probability measures can be approximated by finite dimensional equations. This class of equations contains HJB equations that arise in the study of stochastic optimal control problems for systems of n particles with common noise, interacting through their empirical measures, and similar deterministic particle systems. We will present a procedure to show that the value functions u_n of n particle problems, when converted to functions of the empirical measures, converge as $n \to \infty$ uniformly on bounded sets in the Wasserstein space of probability measures to a function $\mathcal{V}$, which is the unique viscosity solution of the limiting HJB equation in the Wasserstein space. The limiting HJB equation is interpreted in its "lifted" form in a Hilbert space, a technique introduced by P.L. Lions. The proofs of the convergence of u_n to $\mathcal{V}$ use PDE viscosity solution techniques. An advantage of this approach is that the lifted function V of $\mathcal{V}$ is the value function of a stochastic optimal control problem in the Hilbert space.

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IP8

Optimization and Learning with Zeroth-Order Stochastic Oracles

An especially challenging regime in data-driven science and engineering is when one can only query a noisy oracle. From learning controls to designing systems to calibrating models, such problems arise in many domains and are underserved by approaches that presume complete availability of first-order information. We highlight optimization methods for such problems, including methods that employ randomization to increase scalability and methods that exploit other structure outside of the oracle. Coauthors: Raghu Bollapragada, University of Texas; Tyler Chang, Kwassi Joseph Dzahini, Argonne; Cem Karamanli, University of Texas; Xiaoqian Liu, NC State University and Matt Menickelly, Argonne National Laboratory.

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IP9

How Mathematics Enables Science: A Theoretical Biologist's Experience

The data from which we derive much of our understanding of Nature are frequently generated by measurement. Measurement maps unknowns onto observables, whose relationship to the unknowns of interest is seldom self-evident. Scientific understanding requires reconstruction of this mapping. Mathematics is important both for enabling such reconstruction and for designing measurement methods that induce mappings with knowable functional forms. I will describe two exciting examples of such uses of mathematics. The first one involves a long-standing problem in influenza sero-surveillance, where poorly understood measurements were a basis for vaccine design. We reconstructed a mapping underlying these measurements, thus revealing insights that were independently experimentally validated and have important implications for influenza vaccine design. The second example concerns our design of methods for optimizing use of the limited resources available for COVID-19 testing. Access to the underlying mappings made possible the derivation of performance guarantees for these methods, enabling their prudent deployment to support COVID-19 surveillance in Rwanda. I will summarize some lessons learned from this experience. Based on joint work, particularly, with N. Turok.

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IP10

Closing Remarks and Invited Presentation: Physics-Informed Machine Learning

Machine learning is emerging as an essential tool in many science and engineering domains, fueled by extraordinarily powerful computers as well as advanced instruments capable of collecting high-resolution and high-dimensional experimental data. However, using off-the-shelf machine learning methods for analyzing scientific and engineering data fails to leverage our vast, collective (albeit partial) understanding of the underlying physical phenomenon or models of sensor systems. Reconstructing physical phenomena from indirect scientific observations is at the heart of scientific measurement and discovery, and so a pervasive challenge is to develop new methodologies capable of combining such physical models with training data to yield more rapid, accurate inferences. We will explore these ideas in the context of inverse problems and data assimilation; examples include climate forecasting, uncovering material structure and properties, and medical image recon-

struction. Classical approaches to such inverse problems and data assimilation approaches have relied upon insights from optimization, signal processing, and the careful exploitation of forward models. In this talk, we will see how these insights and tools can be integrated into machine learning systems to yield novel methods with significant accuracy and computational advantages over nave applications of machine learning.

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SP1

AWM-SIAM Sonia Kovalevsky Lecture: Two of my Favorite Problems

I will discuss two problems on which I have worked extensively and the many remaining open questions. The first involves the Lanczos algorithm for constructing an orthonormal basis for the Krylov space corresponding to a Hermitian matrix A and a given vector b. The vectors produced can be used to solve linear systems, compute eigenvalues/vectors, evaluate matrix functions $f(A)b$, etc. And while this algorithm is very widely used, it is, in the most intuitive sense, dramatically **unstable**. Behavior of the best implementations using the best computer arithmetic have been explained to some extent, but with implementations being developed for single and half precision and with computations being rearranged to make better use of parallelism, etc., it is important to know what will and will not work. The second has to do with nonsymmetric matrices and operators. It is known that eigenvalues alone provide no information about the behavior of Krylov space methods such as GMRES; the field of values, or, numerical range provides some information, but it is too large a set. I will discuss K-spectral sets and what they can tell us about the behavior of Krylov space methods and other problems in numerical analysis.

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SP2

John Von Neumann Prize Lecture: Patterns, Waves, and Bifurcations in Single and Collective Cell Migration

Biology presents fascinating challenges to applied mathematicians. For several decades my interests have focused on the biology of cell migration. A blend of modeling, dynamical systems, partial differential equations, bifurcations, and computational methods can be brought to bear on intriguing questions like How does a white blood cell navigate to a site of infection? and How do cells migrate together in a sheet to seal a wound?. In this talk, I will survey some of my work, highlighting promising scientific and mathematical questions available for young researchers. I will also describe more recent research at a higher scale, where cells interact with one another, leading to new emergent behavior at the collective level.

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SP3

Past President's Address: ¡br¿Complex Environments and Complex Shapes: Perspectives on Biofluid Models at the Microscale

Using a waving flagellum, a mammalian sperm must swim to and penetrate an extracellular matrix surrounding the egg for fertilization. Choanoflagellates, a microorganism that is an important predator on bacteria in aquatic ecosystems, also swim by waving a flagellum. Moreover, this flagellum creates a water current that carries bacteria to the microbe's prey-capturing collar. In addition to these biological examples, helical nanorobots have been engineered to penetrate tissue for targeted drug delivery or to break apart blood clots. Performance of each of these functions - fertilization, feeding, and transport - depends upon the hydrodynamics of filaments (rigid or flexible) in a fluid that may have embedded microstructures. In this talk we will discuss modeling choices that capture some of the complexities in a given system. We will demonstrate how computational models, coordinated with lab experiments, have probed the effect of prey capture on the swimming and feeding performance of choanoflagellates. We will also explore the dynamics of helical microswimmers that penetrate a polymeric network and have the ability to change the material properties of the network as they move through it.

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SP4

W. T. and Idalia Reid Prize Lecture: Control and Machine Learning

In this lecture we shall present some recent results on the interplay between Control Theory and Machine Learning, and more precisely, Supervised Learning and Universal Approximation. We adopt the perspective of the simultaneous or ensemble control of systems of Residual Neural Networks (ResNets). Roughly, each item to be classified corresponds to a different initial datum for the Cauchy problem of the ResNet, leading to an ensemble of solutions to be driven to the corresponding targets, associated to the labels, by means of the same control. We present a genuinely nonlinear and constructive method, allowing to show that such an ambitious goal can be achieved, estimating the complexity of the control strategies. This property is rarely fulfilled by the classical dynamical systems in Mechanics and the very nonlinear nature of the activation function governing the ResNet dynamics plays a determinant role. It allows deforming half of the phase space while the other half remains invariant, a property that classical models in Mechanics do not fulfill. The turnpike property is also analyzed in this context, showing that a suitable choice of the cost functional used to train the ResNet leads to more stable and robust dynamics. This lecture is inspired in joint work, among others, with Borjan Geshkovski (MIT), Carlos Esteve (Cambridge), Domnec Ruiz-Balet (IC, London) and Dario Pighin (Sherpa.ai).

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SP5

I. E. Block Community Lecture: Artificial Intelligence and Cryptography: Privacy and Security in the AI Era

How is Artificial Intelligence (AI) changing your life and the world? How can you expect your data to be kept secure and private in an AI-driven future? AI is the science of machine learning, or the use of data and computation to build mathematical models capable of making predictions. AI may improve our lives, but without adequate safeguards, AI may also jeopardize the security of our private data. This talk will explain Private AI and the dynamic relationship between cryptography and AI. Cryptography is the science of protecting the privacy and security of data. A new form of encryption based on the mathematics of lattices secures data while still enabling AI.

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SP6

Julian Cole Lectureship: ¡br¿Strong Localized Perturbation Theory for the Analysis of Localized Solutions to Some Nonlinear Diffusive Systems

Localized spatial patterns for various classes of linear and nonlinear diffusive processes arise in a wide variety of physical and biological applications. We will highlight some problems in this area and outline a singular perturbation method, known as strong localized perturbation theory (SLPT), that is designed specifically for analyzing diffusive problems with small localized features in multi-dimensional domains. Applications of this methodology to a mean first capture problem for a Brownian particle, to collective quorum-sensing dynamics triggered by small signalling compartments, and to localized patterns in a reaction-diffusion system relevant to spatial ecology will be illustrated.

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JP1

Joint Plenary with the SIAM Conference on Applied Mathematics Education (ED22):¡br¿ Building Mathematical Communities of Students, Faculty, and the Public to Create Pathways from K-12 to Graduate Programs

Given the large percentage of Latino and first-generation college students in the Rio Grande Valley, the University of Texas Rio Grande Valley serves as a vital pipeline for preparing the nations leadership in STEM disciplines from underrepresented groups. In this talk, we describe efforts to build communities in mathematics involving public schools, universities, students and faculty, and the UTRGV Center of Excellence in STEM Education (C-STEM). We will discuss how we have built communities of undergraduates and K-12 students through summer camps and mobile STEM labs through the C-STEM. Additionally, we will discuss how communities of faculty through university collaborations have created pathways to graduate programs via REUs, team-teaching of advanced math courses and boot camps aimed at preparing students to effectively apply for graduate programs. At the departmental level, we will describe how we have built communities within our student population through collaborative problem-solving sessions. A crucial component in many of these programs is the inclusion of professional development workshops to guide students along the path to success in graduate school.

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JP2

Joint Plenary Speaker with the SIAM Conference on the Life Sciences: ¡br¿ Machine Learning and Sparse Modeling for Scientific Discovery, with Examples in Fluid Mechanics

Accurate and efficient reduced-order models are essential to understand, predict, estimate, and control complex, multiscale, and nonlinear dynamical systems. These models should ideally be generalizable, interpretable, and based on limited training data. This work describes how machine learning may be used to develop accurate and efficient nonlinear dynamical systems models for complex natural and engineered systems. We explore the sparse identification of nonlinear dynamics (SINDy) algorithm, which identifies a minimal dynamical system model that balances model complexity with accuracy, avoiding overfitting. This approach tends to promote models that are interpretable and generalizable, capturing the essential physics of the system. We also discuss the importance of learning effective coordinate systems in which the dynamics may be expected to be sparse. This sparse modeling approach will be demonstrated on a range of challenging modeling problems, for example in fluid dynamics, and we will discuss how to incorporate these models into existing model-based control efforts.

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JP3

Joint Plenary Speaker with the SIAM Conference on Mathematics of Planet Earth (MPE22) ¡br¿ How Machine Learning can Improve Projections of Future Climate

Abstract will be posted here when available.

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CP1

The Jones Polynomial in Systems with Periodic Boundary Conditions

The entanglement of collections of filaments is a problem that arises in many contexts, such as polymers and textiles. Measuring entanglement in such systems is a challenge. In addition,many systems of filaments are modeled using Periodic Boundary Conditions (PBC). Studying entanglement in such systems is even more complex. In this paper we propose a definition for the Jones polynomial of open or closed curves in systems employing periodic boundary conditions. This is a one variable Laurent polynomial of a finite link in

3-space. For closed curves, this gives a topological invariant upto density constraint and the initial choice of the base cell that captures the grain of entanglement in this infinite periodic system. In fact, we show that for systems of closed chains in 1 PBC, the periodic Jones polynomial is a repetitive factor of the Jones polynomial of the infinite component link. For open curves, this gives a polynomial with real coefficients which are continuous functions of the chain coordinates. We show with some illustrative examples that the periodic Jones polynomial is a useful tool for measuring knotting in periodic systems.

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CP1

Randomized Methods for Accelerating Spectral Graph Partitioning

Graph partitioning is important for load balancing and other applications in high-performance computing. We study two randomized methods for accelerating eigensolvers in the Trilinos parallel spectral partitioning library Sphynx. We evaluate a randomized Cholesky preconditioner [Chen, Liang, Biros] for LOBPCG. Our results include performance of the preconditioned eigensolver for graph Laplacians arising from both meshes and highly irregular graphs. We also evaluate an eigenvector approximation technique using a randomized projection method. These methods are then applied to sample graph partitioning problems in Sphynx.

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CP1

Quasi-Triangularization of Matrix Polynomials over Arbitrary Fields

It is a well known fact that every square matrix over an algebraically closed field can be triangularized by similarity (even unitary when a definite scalar product is present) transformations. In 2013, Taslaman, Tisseur, and Zaballa, showed that any regular polynomial matrix $P(\lambda)$ over an algebraically closed field can be triangularized by unimodular transformations (the polynomial matrix analogue to similarity) such that the triangularization has the same degree as $P(\lambda)$. A classical but much less known fact is that every square matrix over an arbitrary field is similar to a k-quasitriangular matrix, block triangular matrix with square blocks along the diagonal whose sizes are bounded by k, the highest degree among all the irreducible factors of the characteristic polynomial. This talk focuses on recent work that generalizes this fact to regular polynomial matrices. That is, we show that every regular polynomial matrix over an arbitrary field is unimodularly equivalent to a k-quasitriangular, polynomial matrix of the same degree, where k is the highest degree among all the irreducible factors in the Smith form of $P(\lambda)$.

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CP1

The Topology of the Meiotic Splindle

The meiotic spindle undergoes significant changes during cell division, using a complex mechanism that involves changes in the conformations of microtubules. In this talk will use tools from Topology to rigorously characterize the 3-dimensional conformation of microtubules in 3 stages of meiosis using experimental data obtained through electron tomography. Our results show that the geometry/topology and entanglement of microtubules changes throughout cell division and it depends on the location of the microtubules from the chromosomes and center of the spindle.

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CP1

Topological Metrics of Biopolymer Structure and Function

Proteins and other biopolymers can be represented by mathematical curves in space. Understanding the structure of such macromolecules is at the core of very important problems in biology, such as protein folding, protein aggregation and cell nucleus organization and function. The single, pairwise, or multi-chain characterization of entanglement complexity becomes rigorous in the context of mathematical topology. In this talk we will introduce a novel and general topological approach to analyze the structures of macromolecules. We will apply our methods to proteins and show that these enable us to create a new framework for understanding protein folding, which is validated by experimental data. When applied to the SARS-CoV-2 spike protein, we see that topology can predict residues where mutations can have an important impact on protein struc-

ture and possibly in viral transmissibility. These methods can thus help us understand biopolymer function and biological material properties in many contexts with the goal of their prediction and design.

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CP2

Algorithmic Market Making in Foreign Exchange Cash Markets with Hedging and Market Impact

In OTC markets, one of the main tasks of dealers / market makers consists in providing prices at which they agree to buy and sell the assets and securities they have in their scope. With ever increasing trading volume, this quoting task has to be done algorithmically. Over the last ten years, many market making models have been designed that can be the basis of quoting algorithms in OTC markets. Nevertheless, in most (if not all) OTC market making models, the market maker is a pure internalizer, setting quotes and waiting for clients. However, on many markets such as foreign exchange cash markets, market makers have access to liquidity pools where they can hedge part of their inventory. In this paper, we propose a model taking this possibility into account, therefore allowing market makers to externalize part of their risk by trading in a liquidity pool. The model displays an important feature well known to practitioners that within a certain inventory range the market maker internalizes the flow by appropriately adjusting the quotes and externalizes outside of that range. The larger the market making franchise, the wider is the inventory range suitable for internalization.

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CP2

Bayesian Calibration of Models for Block Copolymer Self-Assembly: Likelihood-Free Inference and Expectation Information Gain Computation via Measure Transport

With the growing impact of model-based predictions in the nanolithography application of block copolymer (BCP) self-assembly, it is increasingly important to ensure the reliability of the models. In this work, we consider the Bayesian calibration of models for BCP self-assembly, with data produced by microscopy or X-ray scattering characterization. In particular, the aleatory uncertainty represented by the long-range disordering in BCP equilibrium structures is accounted for in the calibration. The uncertainties in characterization data lead to intractable integrated likelihood evaluations and we propose to tackle this challenge with likelihood-free inference via a measure transport approach. For effective inference with high-dimensional images, we advocate constructing summary statistics that quantitatively describe image features related to features of latent material structures. We also show that the expected information gain can be computed with no significant additional cost via the proposed inference approach. Lastly, we present a numerical case study based on the Ohta–Kawasaki model for diblock copolymer thin film self-assembly and top-down microscopy characterization. Several energy-based and Fourier-based summary statistics are introduced. We demonstrate the power of the proposed approach for model calibration and understanding the effects of summary statistics choices, image corruptions, and experimental designs on the calibration results.

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CP2

Long-Term Analysis of Numerical Methods for Stochastic Hamiltonians

In this talk, we focus our attention on providing long-term estimates of the Hamiltonian deviation computed along numerical approximations to the solutions of stochastic Hamiltonian systems, both of Itô and Statonovich types. It has been demonstrated that the expected Hamiltonian of an Itô Hamiltonian system with additive noise exhibits a linear drift in time, while the Hamiltonian function is conserved along the exact flow of a Stratonovich Hamiltonian system. Here, the investigation leads to providing modified differential equations associated to suitable discretizations for the aforementioned problems, in the direction of a weak backward error analysis. Then, long-term estimates are provided both for Itô and Stratonovich Hamiltonian systems, revealing the presence of parasitic terms affecting the overall conservation accuracy. Finally, a numerical evidence is provided to confirm the theoretical analysis.

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CP2

Rare Events Simulation in Bacterial Genetic Evolution Model

Rare events refer to the extreme events with low occurrences. These events might disturb the dynamics of the systems dramatically, despite their low frequencies. Major earthquakes and heat waves in nature; economic crisis and terroristic attack in humane society; pandemic disease

spread in the system where nature and humane society interact. It is crucial to study the possible paths leading to the happening of these rare events in order to avoid the the potential widespread damages. We focus on the rare events that the percentages of certain intermediate-strength genotypes become unusually large in a stochastic model of genetic evolution of bacteria population. Based on importance sampling method and the large deviations theory results of this stochastic model from [R. Azencott, B. Geiger, I. Timofeyev, Rare Events Analysis in Stochastic Models for Bacterial Evolution.], we introduce a numerical algorithm to force random trajectories to realize the rare fixations by following most likely paths through thin tubes. Moreover, we are able to estimate the small probabilities of fixations by estimating the probabilities of forced trajectories that realize the fixations.

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CP3

Study of a Supersonic-Sonic Patch Arising in 2-D Relativistic Transonic Flows with General Equation of State

We prove the existence and regularity of a global smooth solution for a supersonic-sonic patch arising in modified Frankl problem in the study of two-dimensional steady isentropic relativistic transonic flows with a general equation of state over a symmetric airfoil. Such type of patches appears in many transonic flows over an airfoil and flow near the nozzle throat. Using the characteristic decompositions method and a well-known partial hodograph transformation in terms of angle variables, we prove the existence and regularity of solutions in partial hodograph plane first and then obtain the global solutions in physical plane by using an inverse transformation.

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CP3

Long-Time Behavior of a Hyperbolic PDE Model for Natural Selection at Multiple Levels of Organization

In many biological systems, natural selection acts simultaneously on multiple levels of organization. This scenario typically presents an evolutionary conflict between the incentive of individuals to cheat and the collective incentive to establish cooperation within a group. To study this conflict, we consider a hyperbolic PDE model of a group-structured population, in which members within a single group compete with each other for individual-level replication; while the group also competes against other groups for group-level replication. We derive a critical threshold for the relative strength of between-group competition such that defectors take over the population below the threshold while cooperation persists in the long-time population above the threshold. We further establish long-time bounds on the time-average of the collective payoff of the population, showing that the long-run population cannot outperform the payoff of a full-cooperator group even in the limit of infinitely-strong between-group competition. When the group replication rate is maximized by an intermediate level of within-group cooperation, individual-level selection casts a long shadow on the dynamics of multilevel selection: no level of between-group competition can erase the effects of the individual incentive to defect.

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CP3

Shock Polars for Ideal and Non-Ideal Gas

In a compressible flow, varying the angle of an oblique steady shocks turns a given upstream state into a curve of possible downstream states called shock polar. For ideal gas with polytropic (calorically perfect) equation of state (eos) it is a classical result that there is a unique "critical' shock turning the velocity by a maximal "critical' angle, and that the critical shock is transonic. For shock reflection problems such as flow onto a solid wedge, any smaller turning angle is realized by two possible shocks, one weaker and one stronger than the critical shock. The weak-type shock is generally considered stable and usually observed. Recent results show that for ideal gas with non-polytropic eos (thermally but not calorically perfect), the shock polar still has a unique and transonic critical shock, assuming that the eos is convex, meaning pressure is a convex function of volume, at constant entropy. Moreover the Mach number is decreasing on the subsonic part of the polar. The same can be shown for compressible potential flow. For barotropic (isentropic) Euler flow the shock polar is convex in the velocity plane, so that critical shocks are still unique, but they may be supersonic in some cases. Finally, for the van der Waals eos, the simplest and most important model of non-ideal gas, examples near the thermodynamic critical point show that critical shocks may not only be supersonic but not even unique, raising interesting new non-uniqueness questions.

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CP3

Numerical Methods for the Time-Dependent Quantum Hydrodynamic Model

Numerical methods are developed for the time-dependent smooth quantum hydrodynamic (QHD) model by solving the gas dynamical part of the equations with a positivity-preserving third-order WENO method, treating the quantum mechanical terms as source terms; the parabolic heat conduction part using the TRBDF2 method; and the elliptic Poisson equation using Chebyshev SOR. These are the first time-dependent simulations of the smooth QHD model. Time-dependent simulations of the resonant tun-

neling diode using the smooth QHD equations are presented, which show realistic negative differential resistance (the experimental signal of quantum resonance) in the current-voltage curve.

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CP3

A Stability Result for a Nonlinearly Damped Suspension-Bridge

In this work, we investigate the following weakly damped nonlinear suspension-bridge problem

$$\begin{cases} u_{tt}(x,y,t) + \Delta^2 u(x,y,t) + \alpha(t) g(u_t(x,y,t)) = 0, \ in\ \Omega \times (0,\infty) \\ u(0,y,t) = u_{xx}(0,y,t) = u(\pi,y,t) = u_{xx}(\pi,y,t) = 0, \ (y,t) \in (-d,d) \times (0,\infty) \\ u_{yy}(x,\pm d,t) + \sigma u_{xx}(x,\pm d,t) = 0, \ (x,t) \in (0,\pi) \times (0,\infty), \\ u_{yyy}(x,\pm d,t) + (2-\sigma) u_{xxy}(x,\pm d,t) = 0, \ (x,t) \in (0,\pi) \times (0,\infty), \end{cases}$$

where $\Omega = (0,\pi) \times (-d,d)$, $g : \mathbb{R} \to \mathbb{R}$ and $\alpha : [0,+\infty) \to (0,+\infty)$ are functions such that α is non-increasing and differentiable, u is the vertical displacement of the bridge, and σ is the Poisson ratio. We use the multiplier method and the properties of the convex and establish an explicit and a general decay result for the solution energy of the problem. This decay result depends on the functions α and g and is obtained without any restriction growth assumption on g at the origin.

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CP4

Optimal Time-Dependent Classification for Diagnostic Testing

Antibody tests can identify past infection by quantifying the immune response of an infected individual, thereby providing guidance for decisions about public health measures. The relative antibody measurements change with time due to the variation in an individuals antibody levels and prevalence in the population as the pandemic progresses. We use optimal decision theory to develop a time-dependent, probabilistic classification scheme which takes both the personal and the population-level effects into account. These classification domains change with time and suggest a natural adaptive scheme for estimation of prevalence, taking into account the progression of the pandemic through the use of publicly available data. We demonstrate the results by using a combination of SARS-CoV-2 and synthetic data sets, and detail the type of data needed to execute this scheme in real-world settings.

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CP4

The Expected Utility Model on Hub Capacity Allocation for Time-Definite LTL Carriers

The time-definite express freight delivery common carriers publish tariffs and deliver express parcels door-to-door with guaranteed delivery times. The small shippers are charged with full fares who generally are lack of bargaining powers. On the other hand, the carriers may also offer bids with discounts to big accounts shippers in order to fill up otherwise unused hub capacity. In this study, we assume that the carrier is risk-averse, that it would accept a guarantee payoff rather than join the bidding game for big accounts and possibly receiving nothing. As the result, its utility function is concave. Collectively, the carrying capacity allocation model under dual markets for the carriers is to determine tariffs for small shippers and also to decide whether or not to joining the bid games for big accounts so that their expected profits are maximized while fully utilizing the available hub capacity. We modeled this integral-constrained concave program in link formulation and demonstrated computationally using Taiwans largest time-definite LTL freight carrier.

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CP4

Stackelberg Risk Preference Design: Quantification of Randomness As the Decision

Recently, risk measures have been of great interests for studying decision-making under uncertainty. Various analysis and applications of given risk measures have been discussed in the literature. In reality, however, risk preferences can be influenced by various factors, such as past experience or information regarding the uncertainty. In this work, we propose a Stackelberg risk preference design problem to study decision-making under uncertainty when individual risk preferences are controllable. In particular, we endow an individual in a population with a risk preference type, which leads to a risk measure capturing her quantification of randomness. We consider the population's averaged response towards an underlying stochasticity as the follower's action. The leader designs the distribution of the types so that the follower's action is in her favor. To fit stochastic decision problems, we consider an extended approximate Stackelberg solution, where both of leader's and the follower's actions can be suboptimal. We introduce the primitive perception gap measuring the discrepancy between the original and the anticipated distributions of types to derive bounds on the approximate solution. Leveraging the coherency and law-invariance property of risk measures, we derive a single-level reformulation to solve our problem. We describe the concept of risk preference design in contract problems and connect our problem formulation with meta learning problems.

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CP4

Automated Compound Discrimination Using Mass Spectra and the Min-Max Test

Compound discrimination is a ubiquitous task in several science and engineering applications, and mass spectrometry is one of the fundamental analytical chemistry tools towards this end. The datum generated through mass spectrometry summarizes the relative counts of ions generated during analysis of the compound and can be thought of as a general signature of a compounda signature is distinctive but rarely identical across multiple instances. Traditionally, compounds are discriminated based on the dissimilarity of their mass spectral signatures as determined by a trained analyst, but developing automated discrimination methods is desirable for applications requiring higher throughput analysis (e.g., drug identification). In this presentation, we describe a simple mathematical method that leverages replicate mass spectral signatures to automate compound discriminationthe min-max test. We also explore how these simple ideas can be applied in other industrial applications requiring high-throughput discrimination of signature-type data.

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CP4

Probability Distribution-Based DART-MS Compound Discrimination

Direct Analysis in Real Time Mass Spectrometry (DART-MS) is a new technology for chemical identification where an important application is screening for illegal compounds in seized drug evidence. In DART-MS, heated gas molecules are used to both desorb and ionize an analyte. This procedure rapidly produces multiple spectral measurements of an analyte at various fragmentation levels. DART-MS is not performed in a vacuum, so resulting spectra have a greater tendency to vary due to contamination. Distinguishing structurally similar compounds using DART-MS is often accomplished using the cosine similarity measure. We present an alternative method of peak matching using probability distributions in two dimensions that takes advantage of the replicate measurements coming from DART-MS. To demonstrate the efficacy of our method we will present numerical results for identifying Fentanyl derivatives and compare the results to those from using cosine similarity.

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CP4

Bayesian Routing Games with Information Obfuscation

Smart vehicles are enabled to receive, process, and exchange information in a real-time manner to choose routes that maximize their individual optimality. This leads to profound challenges in network traffic congestion control in the presence of inconsistency between the individual optimality and network optimality. This work proposes a dynamic routing recommendation mechanism with intentionally obfuscated traffic information, aiming to balance the individual optimality and the network optimality by shaping the vehicles selfish adaptive routing decisions. We consider a dynamic routing game over a transportation network. Each vehicle is a self-interested Bayesian player who partially observes the state of the network and updates its routing at each node of the network. The planner privately observes the state of the transportation network while each vehicle privately possesses its observation. A dynamic design regime is obtained to incentivize the vehicles to behave in the planners interests.

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CP5

Dynamic Tipping in the Non-Smooth Stommel-Box Model of Thermohaline Circulation

In this talk I will describe the behaviour at tipping points close to non-smooth fold bifurcations in stochastically forced non-autonomous systems. The focus is the Stommel-Box, and related climate models, which are piecewise-smooth continuous dynamical systems, modelling thermohaline circulation.We obtain explicit asymptotic expressions for the behaviour at tipping points in the settings of both slowly varying freshwater forcing and rapidly oscillatory fluctuations. The results, based on combined multiple scale and local analyses, provide conditions for the sudden transitions between temperature-dominated and salinity-dominated states. In the context of high frequency oscillations, a multiple scale averaging approach can be used instead of the usual geometric approach normally required for piecewise-smooth continuous systems. The explicit parametric dependencies of advances and lags in the tipping show a competition between dynamic features of the model. We make a contrast between the behaviour of tipping points close to both smooth Saddle Node Bifurcations and the non-smooth systems studied on this paper. In particular we show that the non-smooth case has earlier and more abrupt transitions. This result has clear implications for the design of early warning signals for tipping in the case of the non-smooth dynamical systems which often arise in climate models.

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CP5

An Energy Conserving Mechanism in Space-Time Metamaterials

Changing the microstructure properties of a space-time metamaterial while a wave is propagating through it, in general requires addition or removal of energy, which can be of exponential form depending on the type of modulation. This limits the realization and application of space-time metamaterials. We resolve this issue by introducing a novel mechanism of conserving energy in non-linear space-time media. The idea is first demonstrated by considering a wave-packet propagating in a discrete medium of 1-d chain of springs and masses, where using our energy conserving mechanism we show that the spring stiffness can be incremented at several time interfaces and the energy will still be conserved. We then consider an interesting application of time-reversed imaging in 1-d and 2-d spring-mass systems with a wave packet traveling in the homogenized limit. Our numerical simulations show that, in 1-d, when the wave packet hits the time-interface two sets of waves are generated, one traveling forward in time and the other traveling backward. The time-reversed waves re-converge at the location of the source and we observe its regeneration. In 2-d, we use more complicated initial shapes and even then, we observe regeneration of the original image or source. Thus, we achieve time-reversed imaging with conservation of energy in a non-linear regime. The energy conserving mechanism can be easily extended to continuum media.

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CP5

New Extremum Seeking Control System with Multi-Agent Application

Extremum Seeking Control (ESC) is an adaptive control method that steers a given dynamical system to the extremum (min/max) of an objective function, usually assumed to exist but is unknown - expression wise. Control-affine ESCs (in the form $\dot{x} = f(x,t) + \sum_{i=1}^{m} g_i(x,t)u_i(t)$, x is the state space, f, g_i are vector fields, and u_i are control inputs) have been developing for about a decade in their stability characteristics and applicability to different systems, especially Multi-agent ones. In this presentation, we summarize these developments but also introduce our novel ESC system which (i) have attenuating oscillations, (ii) characterized by a simpler stability condition, and (iii) works with systems many significant ESC approaches could not solve. Moreover, we present a numerical simulation results of a multi-agent vehicle system in direct comparison with literature.

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CP5

Renormalisation of the Two-Dimensional Border-Collision Normal Form

Piecewise-linear maps arise from mathematical models in diverse applications. Families of such maps readily exhibit chaos in a robust fashion and this was popularised by Banerjee, Yorke, and Gregobi in their 1998 Phys. Rev. Lett. paper. In this talk, I will show how the powerful technique of renormalisation can be applied to their map to reveal its bifurcation structure. Broadly speaking renormalisation involves showing that, for some member of a family of maps, a higher iterate or induced map is conjugate to a different member of the family.

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CP6

A Modified Preconditioned Conjugate Gradient Method for Approximating the Scattering Amplitude

In this paper, we present a new iterative method (Nonsymmetric Saddle Point Preconditioned Conjugate Gradient (NspPCG)) for approximating the scattering amplitude that involves solving two linear systems: a forward system ($A\mathbf{x} = \mathbf{b}$) and an adjoint system ($A^T\mathbf{y} = \mathbf{g}$). Once these two systems are solved, the scattering amplitude, defined by $\mathbf{g}^T\mathbf{x} = \mathbf{y}^T\mathbf{b}$ is easily obtained. We derive a conjugate gradient-like iteration for a nonsymmetric saddle point matrix that is constructed to have a real positive spectrum. We investigate the use of Schur Complement preconditioners with block-diagonal factorization to speed up the convergence of our method and compare the results to the generalized least squares residual (GLSQR) and quasi-minimal residual (QMR) methods with preconditioning.

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CP6

Active Control of Scalar Helmholtz Fields in the Presence of Obstacles

In this paper, we consider the problem of actively manipulating scalar Helmholtz fields by using a source D_a in the presence of coupling sound-soft and sound-hard obstacles. We prove the existence of and characterize a necessary input on the boundary ∂D_a such that the radiated field satisfies desired control constraints in near field exterior regions and prescribed far field directions.

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CP6

High Resolution Reconstruction of the Shape and Impedance Function of An Obstacle Using Acoustic Scattered Field Measurements

In this talk, we consider the problem of reconstructing up to high resolution the shape and the impedance function of an obstacle from measurements of the scattered field at multiple frequencies. This problem have several applications in medical imaging, non-destructive testing, radar, and etc... We will present a method based on the recursive linearization algorithm (RLA). In the RLA, we solve a sequence of inverse scattering problems using increasing single frequency measurements. Since each of those problems is ill-posed and nonlinear, we apply the damped Gauss-Newton method using a band-limited representation for the shape of the obstacle and of the impedance function. At each frequency, the initial guess is the solution of the previous frequency. Numerical examples are presented to demonstrate that the method can recover the shape and impedance function of the obstacle with high resolution.

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CP6

Numerical Solutions for the Darcy-Jordan Model of Finite Amplitude Acoustic Waves

The complexities of chemical explosions, earthquakes, and lightning can be examined through analysis of propagating waves in compressible matter, where a sudden change occurs known as the moment of "gradient catastrophe". Consider the uni-directional EoM for finite amplitude acoustic waves in relaxing media and dual-phased materials,

$$u_t + (v_0 + \sigma u)u_x + \lambda u = 0.$$

An example of this PDE is the "damped Riemann equation" derived from the Darcy-Jordan Model (DJM),

$$u_t + (1 + \epsilon\beta u)u_x + \frac{1}{2}\delta u = 0,$$

where $\delta \propto X^v/K$ is the dimensionless Darcy coefficient. Applying the method of characteristics, we obtain the exact result

$$u(x,t) = u_0(\xi)\exp(-\delta t/2)$$

$$x - t - \xi = (\alpha^*)^{-1}u_0(\xi)g(t),$$

where $\xi = \xi(x,t)$ is the wave variable, allowing for shock analysis in solitary waves. The hyperbolic and nonlinear nature of this PDE produces an initial value problem with a complicated solution at the moment of gradient catastrophe, physically interpreted as a shock wave with formation beginning at time $t = t^*$, which yields a multi-valued solution. Prior attempts to solve this equation have resulted only in implicit solutions or explicit solutions for certain initial conditions. Here, a coalescence of numerical methods provides an algorithm capable of finding both single- and multi-valued solutions, as demonstrated in numerical experiments.

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CP7

Manipulating Transport Properties of Passive Tracers in Channels via Cross Section

Traditionally, theory developed for dispersion of passive tracers has focused on predicting the effect of anomalous diffusion which occurs as the result of laminar fluid flow. This theory has had success matching with both experiment and numerical simulation. However, precise control of the tracer's distribution is more challenging. Our prior work has established similar agreements between theory, simulation, and experiment in predicting a tracer distribution's skewness. In particular, we developed asymptotic theory which predicts the sign differences seen in skewness depending on cross section – and this showed agreement with experiment. However, these studies relied mainly on idealized cross-sectional shapes, and left an open question about questions of optimality and channel design for specific purposes. Here, I will present a computational framework to extend this work past idealized cross sections and explore questions in shape optimization towards precise control of the tracer distribution.

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CP7

Pore Scale Analysis and Upscaling of a Coupled System of Semilinear Parabolic PDEs and a Nonlinear ODE

We investigate a system of semilinear parabolic PDEs coupled with an ODE in a heterogeneous porous medium. Our goal is to establish the existence and uniqueness of a global-in-time weak solution and further upscale the system from the microscale to the macroscale to study the global behavior. To achieve our goal, we start with the microscopic equations where two mobile species with space-dependent different diffusion coefficients react and precipitate in the form of immobile species on the grain boundary. We model the surface reaction phenomena by using Langmuir isotherm. We take into account a reversible reaction so the immobile species also dissolve to give mobile species in the pore space. The dissolution process is described by a multivalued discontinuous rate term. The main obstacles in the analysis are the space-dependent nonidentical diffusion coefficients, the multivalued discontinuous rate term and the nonlinear surface reaction rate term. We tackle the multivaluedness by introducing a regularization parameter $\delta > 0$. The existence theory relies on Rothes method and to upscale the system we use homogenization tools such as two-scale convergence and boundary unfolding operator. We have also defined a modified version of the extension operator. We will also address an iterative limit problem

in this paper.

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CP7

Dynamics of Spherical Spin Glasses

We determine equations for the limiting dynamics of the spherical spin glass in the large size limit. The spherical spin glass is a paradigm for high-dimensional stochastic processes in a disordered environment - perhaps the most well-known example is stochastic gradient descent in the case of a highly disordered Hamiltonian. Most previous work on spin glass dynamics proceeded from delayed differential equations that describe the dynamics of the correlation function. The main novelty of this work is to determine an autonomous PDE that characterizes the limiting dynamics. This PDE is then used to study the glassy dynamical phase transition.

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CP7

Cyclic Symmetry Induced Pitchfork Bifurcations in the Diblock Copolymer Model

The Ohta-Kawasaki model for diblock copolymers exhibits a rich equilibrium bifurcation structure. Even on one-dimensional base domains the bifurcation set is characterized by high levels of multi-stability and numerous secondary bifurcation points. Many of these bifurcations are of pitchfork type. In previous work, the authors showed that if pitchfork bifurcations are induced by a simple $\mathbb{Z}_2$ symmetry-breaking, then computer-assisted proof techniques can be used to rigorously validate them using extended systems. However, many diblock copolymer pitchfork bifurcations cannot be treated in this way. In the present paper, we show that in these more involved cases, a cyclic group action is responsible for their existence, based on cyclic groups of even order. We present theoretical results establishing such bifurcation points and show that they can be characterized as nondegenerate solutions of a suitable extended nonlinear system. Using the latter characterization, we also use computer-assisted proof techniques to validate these bifurcations. While the methods proposed in this paper are only applied to the diblock copolymer model, we expect that they will also apply to other parabolic partial differential equations. This is joint work with Peter Rizzi and Thomas Wanner.

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CP7

Sobolev Estimates for Non-Uniformly Parabolic PDEs

Sobolev energy estimates are proven for solutions of initial-value-problems for general non-uniformly parabolic second-order PDEs having symmetric coefficients depending on the independent and dependent variables, without any assumption on the location of the non-uniformity. Local-in-time existence of solutions to initial-value problems for such systems and convergence results for singular limits involving such systems are consequences of those uniform bounds. The results can be applied to generalize a variety of results for viscous equations and systems to the case when the viscosity is not strictly positive. Examples include certain geometric optics expansions and eddy viscosity models.

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CP7

Solving a Friction Stir Welding Problem with Reduced Order Models and Neural Networks

The friction stir welding process can be modelled using a system of heat transfer and Navier-Stokes equations with a shear dependent viscosity. Finding numerical solutions of this system of nonlinear partial differential equations over a set of parameter space, however, is extremely time-consuming. Therefore, it is desirable to find a computationally efficient method that can be used to obtain an approximation of the solution with acceptable accuracy. In this talk, we present a reduced basis method for solving the parametrized coupled system of heat and Navier-Stokes equations using a proper orthogonal decomposition (POD). In addition, we apply a machine learning algorithm based on an artificial neural network (ANN) to learn (approximately) the relationship between relevant parameters and the POD coeffiients. Our computational experiments demonstrate that substantial speed-up can be achieved while maintaining reasonable accuracy.

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CP8

Analysis of Bias-Variance Trade-Off in Estimators for Variational Inferencing

Variational inference (VI) is a method that approximates probability densities through optimization. VI has been used in many applications and tends to be faster than classical methods, such as Markov chain Monte Carlo sampling. Traditionally, instead of KL divergence, the evidence lower bound is used as a cost function. We then optimize the parameters of a variational distribution. We explore the technicalities in using KL divergence in such a scenario, synthesizing estimators, and leveraging upon the

delta method to study the bias-variance trade-off. Our objective is to study the gradient space of the KL divergence with respect to the variational parameter and to understand how we can tune the bias and variance by optimizing importance sampling. With lower variance in the gradient information, we can achieve larger optimization steps, lower the number of samples needed, which we compare against the ELBO based optimization.

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CP8

Fantasy Football Machine Learning Algorithm

For the past four years, I had missed the playoffs in my fantasy football league. The other members of my league would not let me forget this for even a moment. I wanted to find a way to use my new knowledge of coding to remedy this cycle of losses. After reading about the creation of WalterPicks, an app that provides sports insights using machine learning and AI, I was inspired to create my own machine learning algorithm to predict fantasy football scores using data from previous seasons. In this talk, I will discuss how we automated the data collection process, the details of feature selection, the model used, and how we trained, tested, and tuned the model. For the 148 players overall, the model overprojected points per game by an average of 2.4225 fantasy points. Thanks to the software we created (and maybe a little bit of luck), I ended up winning my fantasy football league.

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CP8

Informationally Mosaic Multi-Agent Reinforcement Learning

Multi-agent Reinforcement learning (MARL) has shown encouraging successes in addressing the sequential decision-making problem of multiple autonomous agents within a dynamic environment. The key to its successes is that MARL enables agents to adjust strategies based on their perceptions of the surroundings and the feedback from the environment. We refer to the structure of feedbacks and perceptions as the information structure of MARL. To achieve a broader deployment in reality, MARL must be able to adapt agents to varying information structures. The issue of learning under unknown, dynamic, and generally amorphous information structures poses a great challenge to current MARL studies. To address it, we propose a novel framework, Informationally Mosaic Multi-Agent Reinforcement Learning (IMMARL), where agents with different information structures coordinate in an unprescribed way to explore and utilize constructive information from the environment. In particular, the agent's exploration operates in a laissez-faire manner, that is, it voluntarily rewards others for discovering and sharing helpful information. The proposed framework brings up flexible interoperability, and increases the modularity in MARL systems. We introduce a novel metric, *Value of Information* (VoI), to quantify the importance of informational exploration during learning. We corroborate on the proposed IMMARL and VoI using experiments conducted in procedurally-generated benchmark environments.

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CP8

Global Index on Financial Losses Due to Crime in the United States

Despite the potential importance of crime rates in investments, there are no indices dedicated to evaluating the financial impact of crime in the United States. As such, this paper presents an index-based insurance portfolio for crime in the United States by utilizing the financial losses reported by the Federal Bureau of Investigation. The objective of our paper is to introduce new risk hedging financial contracts for crime, consistent with dynamic asset pricing. Underlying the index, we hedge the investments by issuing marketable European call and put options and providing risk budgets. These budgets show that real estate, ransomware, and government impersonation are the main risk contributors in our index. Next, we evaluate the performance of our index via stress testing to determine its resilience to economic crisis. Of all the factors considered in this study, unemployment rate has the potential to demonstrate the highest systemic risk to the portfolio. Our portfolio will help investors envision risk exposure in the market, gauge investment risk based on their desired risk level, and hedge strategies for potential losses due to economic crashes. In conclusion, we provide a basis for the securitization of insurance risk from certain crimes that could forewarn investors to transfer their risk to capital market investors.

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CP8

GiantKelpeR: A Webapp for Exploratory Analysis of Macrocystis Pyrifera Population Change in California

On the North American West Coast, giant kelp (Macrocystis pyrifera) population declines have been prevalent with increasing extreme heat waves in sea surface temperature (SST). Individuals typically persist below 22 C and past this quickly die off. Giant kelp is the foundational species of the California coast kelp forest ecosystem. The value of this ecosystems services has led to several kelp cover monitoring programs, most using remote imagery. Input data and output products are mostly formatted for academic use despite stakeholder value. To tackle this, we are developing an RShiny webapp to visualize time series of kelp biomass in Southern-Central California with SST changes and derived statistics (number of consecutive days with SST above 22 C and SST anomalies). Rshiny is a package for webapp development in the R language. RShiny users can program a webapp in R ran with HTML and CSS. In our webapp, users click a location on a map of kelp

biomass and choose a radius around the selection. In this radius, the previous statistics are calculated from average kelp biomass and SST. Our webapp will help stakeholders and non-specialists explore kelp and SST time series data. Eventually we plan to add spatially explicit kelp genetic monitoring records from projects by our team censusing genetic diversity changes in California kelp beds. Currently we are deploying our webapp online and after will incorporate OpenStreetMap software to improve our map interface and interactivity.

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CP8

Weighted Random Cut Forest for Anomaly Detection

Random cut forest (RCF) algorithms have been developed for anomaly detection, particularly for the anomaly detection in time-series data. The RCF algorithm is the improved version of the isolation forest algorithm. Unlike the isolation forest algorithm, the RCF algorithm has the power of determining whether the real-time input has anomaly by inserting the input in the constructed tree network without changing the whole tree structure. There have been developed various RCF algorithms including Robust RCF (RRCF) with which the cutting procedure is adaptively chosen probabilistically. RRCF shows better performance compared to the isolation forest as the cutting dimension is decided based on the geometric range of the data. The overall data structure is, however, not considered in the adaptive cutting algorithm with the RRCF. In this paper, we propose a new RCF, so-called the weighted RCF (WRCF). The proposed WRCF also cuts the tree network adaptively, but with consideration of the denseness of the data. The proposed method is more efficient when the data is more structured and achieves the desired anomaly score more rapidly than the RRCF. We provide theorems that prove our claims with numerical examples.

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CP9

Supervised Learning Using Truth Tables: Convergence Results and Algorithms.

A novel method for combining weak classifiers in supervised learning is described, which fully characterizes the set of weak classifiers by a truth table. Convexification of the risk function (risk of false decision for any combination of the chosen weak classifiers) with any calibrated C^2 classification function ϕ, yields a minimization problem in $\mathbb{R}^M$, whose unique solution is easily studied using a classical minimization algorithm that amounts to iteratively solving equations in $\mathbb{R}$ with a Newton method. The complexity of this method depends only linearly on the number M of weak classifiers and does not depend on the number of examples in the training set or on the dimension of the underlying space where the examples are considered. In the case of two well-known ϕ's, the Boosting function (for all M) or the Logistic function (in the case $M = 3$), the algorithm even leads to an explicit formula for the sequence of points of the sequence that converges to the minimum point. This framework is then used to study the quality of the training set, i.e., how the results are modified if some examples are added or removed from the training set, thus setting criteria for the stability of the results under such operations. This leads to criteria for quasi-separability of two sets (two-class classifiers) or margin analysis. Linear separation of a mixture of 2 Gaussian distributions is used as an illustration of our work and results.

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CP9

Optimal Recovery from Inaccurate Data in Hilbert Spaces: Regularize, But What of the Parameter?

In Optimal Recovery, the task of learning a function from observational data is tackled deterministically by adopting a worst-case perspective tied to an explicit model assumption made on the functions to be learned. Working in the framework of Hilbert spaces, this article considers a model assumption based on approximability. It also incorporates observational inaccuracies modeled via additive errors bounded in l_2. Earlier works have demonstrated that regularization provide algorithms that are optimal in this situation, but did not fully identify the desired hyperparameter. This article fills the gap in both a local scenario and a global scenario. In the local scenario, which amounts to the determination of Chebyshev centers, the semidefinite recipe of Beck and Eldar (legitimately valid in the complex setting only) is complemented by a more direct approach, with the proviso that the observational functionals have orthonormal representers. In the said approach, the desired parameter is the solution to an equation that can be resolved via standard methods. In the global scenario, where linear algorithms rule, the parameter elusive in the works of Micchelli et al. is found as the byproduct of a semidefinite program. Additionally and quite surprisingly, in case of observational functionals with orthonormal representers, it is established that any regularization parameter is optimal.

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CP9

Physics-Informed Neural Networks with Transfer Learning for Time-Dependent Partial Differential Equations

Neural network-based surrogate models are widely applied to solve ordinary differential equations and partial differential equations. By incorporating the governing equations into the loss function to guide the direction of gradient descent, Physics-Informed Neural Networks (PINNs) have attracted significant attention for solving such equa-

tions. However, training deep neural networks usually require big data and a large amount of training time to converge. In this study, we adopted a transfer learning approach to address this problem. The efficacy of transfer learning PINNs is tested on systems of data-driven time-dependent partial differential equations, namely, non-linear Schrodinger equations and non-linear Reaction-Diffusion equations. Highly accurate solutions to these differential equations are acquired with largely reduced training time.

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CP9

Active Learning of Nonlinear Operators via Neural Nets for Predicting Extreme Events

We develop an experimental design framework for predicting extreme events in infinite-dimensional systems using neural operators. Extreme phenomena, such as pandemic spikes, electrical-grid failure, or rogue waves, have catastrophic consequences for society. Extremes are rare, belong to infinite-dimensional systems, and are stochastically excited. Unfortunately, standard training of machine learning models assumes both plentiful data and moderate dimensionality. Neither is the case for extreme events. We navigate these challenges by combining novel training schemes in Bayesian experimental design (BED) with neural operators. The BED scheme actively selects data for quantifying extreme events, while the neural operator approximates infinite-dimensional, nonlinear operators via a specially designed neural network architecture. Our test bed for discovering extremes is a partial differential equation that takes the form of highly nonlinear deep-water waves. We find that BED using neural operators performs similarly as Gaussian Process (GP) regression BED at moderate dimension or data size. When dimensionality or data size increases, only neural operators provide useful BED performance. Specifically, we push our analysis to 20D where standard GP techniques are futile, yet the neural BED framework discovers extreme waves. We also discuss parallel batching of acquisition samples and the generality of the BED neural operator framework for other high-dimensional systems.

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CP9

Physics-Guided Machine Learning Framework for Simultaneous Inverse Design and Optical Response Prediction of Photonic Metamaterials

Optical metasurfaces consist of densely arranged unit cells that manipulate light, which have found increased applications in imaging, sensing, and communication. Viable design prediction for suitable optical response remains challenging for complex metamaterial systems due to high non-linearity and possible non-unique solution to the inverse problem. Recently deep learning (DL) methods have emerged to tackle inverse design problems; however, they are often notorious for being un-interpretable and have high data requirement. Hence, we introduce a physics-guided DL framework to enable accurate and scalable inverse design of metasurfaces. The addition of physics improves generalizability while reducing data burden. To prove the concept, we focus on the inverse design of a representative plasmonic device that consists of metal gratings deposited on a dielectric film on top of a metal substrate. We model a tandem neural network architecture with physics-based constraint in the loss function. The constraint is derived from the physics of a homogenized structure whose addition improves generalizability and interpretability of the model by predicting designs that are scientifically consistent. Our model converges with an accuracy of 97% for the inverse model and reconstructs the desired optical spectrum with 97% accuracy for wavelength spectra in the visible light range; it also has an accuracy of 96% and reconstructs with 99% accuracy for a single wavelength incident.

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CP9

Adaptive Machine Learning Framework for Multi-Scale Coarse-Grained Non-Equilibrium Kinetics

The computationally intensive simulations of non-equilibrium hypersonic flows by relying on high fidelity state-to-state kinetics are impractical in multidimensional CFD applications. The high computational load is associated with the solution of underlying master equations, a

system of ODEs able to model the evolution of the distribution functions of the species quantum states by considering energy exchange and dissociation processes. In this work, a machine learning (ML)-based approach is developed for accelerating numerical simulations of such stiff and high-dimensional thermochemical systems. The present framework leverages a novel hierarchical and adaptive deep learning architecture able to learn the solution operator of multi-scale coarse-grained (CG) kinetic master equations. The recently proposed physics-informed DeepONet (PI-DeepONet), *i.e.* a deep operator network (DeepONet) trained in the physics-informed (PI) fashion, performs as the core structure of the entire deep learning framework. At the same time, a controller-like surrogate is developed to leverage the multi-scale connotation of the problem by executing a novel adaptive predictive technique for non-equilibrium thermochemical processes. This work lays the foundation for constructing an efficient ML- and CG-based surrogate model to be coupled with Navier-Stokes solvers for accurately characterizing the non-equilibrium phenomena.

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CP10

Elastic Scaffolds for Tissue Engineering Applications

Scaffolds engineered for use in tissue regeneration consist of multiple pores which are lined with cells, through which nutrient-rich culture medium flows. Nutrient solution circulates throughout the scaffold pores, promoting cellular proliferation. The proliferation process depends on several factors: scaffold geometry, the nutrient solution flow rate, shear stress effects, and the elastic properties of the scaffold material. These factors significantly influence tissue regeneration rates and capabilities. While scaffold geometry, nutrient flow, and stress effects have been the focus of recent studies, the objective of our work is to determine how scaffold elasticity influences cellular growth under constant nutrient flux. To maintain constant flux conditions as the pore radius shrinks due to cell growth, applied pressure the pore inlet is increased. Increased applied pressure causes expansion of the elastic scaffold pore, permitting an increase in total tissue growth beyond that observed for rigid scaffolds. In this paper, our objectives are as follows: (i) develop a mathematical model for cell proliferation describing fluid dynamics, scaffold elasticity, and tissue growth; (ii) solve the models and then simulate the tissue proliferation process. The simulation can emulate real-life cell growth in a tissue engineering pore and offer a solution that reduces the numerical burdens. The results from our algorithm are in agreement with experimental observations from literature.

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CP10

Computational Framework for Accurate Modeling of Grafts for Optimal Tissue Vascularization

Tissue engineering of skin grafts is a promising tool to aid the bodys healing process through its built-in regeneration mechanisms. A careful selection of graft parameters will ensure the restoration of healthy tissues. One of the promising methods consists of introducing template channels with controllable properties to provide faster microvasculature organization and transport of necessary nutrients to the cells outside these channels. It is critical, both for computational and experimental models, to understand how the biomaterial properties will impact angiogenesis and vasculogenesis in a graft since this situation is different than in native tissue. Essential parameters for modeling include the geometry of channels in the graft and its biomaterial properties, which can considerably alter the influence of swelling, the material degradation time, and the transport of dissolved substances through the grafts contributing positively to the cell viability. This collaboration between mathematicians and bioengineers aims to create a robust computational framework to simulate physical and biological phenomena in the graft material. We will present our first computational results obtained for multiple 2D models and discuss future applications to models using laboratory data.

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CP10

Scalable Simulation of Systems of PDEs for Modeling Tumor Growth

Computing technology is continuously making advancements that establish a framework for higher resolution in mathematical modeling. However, these models are based on well-established numerical methods that become progressively more expensive with increasing resolution. To compensate, researchers must currently simplify models with assumptions, lower resolution, fewer parameter sets, etc. For certain simulations, such as the modeling of solid tumor growth, these can be compromising simplifications. Results are less accurate, time intensive, and overgeneralized for individual patients. In order to provide doctors with valuable, accurate information for prognoses and clinical treatment decisions, greater scalability must be achieved. We hypothesize that the combination of Krylov Subspace Spectral (KSS) methods with exponential Rosenbrock methods, addressing stiffness issues, will produce a new class of numerical methods achieving high-order accuracy and scalability for the modeling of solid tumor growth.

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CP10

Modeling Interaction of Glioma Cells and Car T-Cells Considering Multiple Car T-Cells Bindings

Chimeric antigen receptor (CAR) T-cell based immunotherapy has shown its potential in treating blood cancers, and its application to solid tumors is currently being extensively investigated. For glioma brain tumors, various CAR T-cell targets include IL13R
alpha 2, EGFRvIII and HER2, etc. In our work, we develop a mathematical model of IL13R
alpha 2 targeting CAR T-cells for treating glioma. We focus on extending the work of Kuznetsov et al. (1994) by considering binding of multiple CAR T-cells to a single glioma cell, and the dynamics of these multi-cellular conjugates. Our model more accurately describes experimentally observed CAR T-cell killing assay data than a model which does not consider cell binding. Moreover, we derive conditions in the CAR T-cell expansion rate that determines treatment success or failure. Finally, we show that our model captures distinct CAR T-cell killing dynamics at low, medium, and high antigen receptor densities in patient-derived brain tumor cells.

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CP10

Forced and Spontaneous Symmetry Breaking1 in Cell Polarization

How does breaking the symmetry of an equation alter the symmetry of its solutions? Here, we systematically examine how reducing underlying symmetries from spherical to axisymmetric influences the dynamics of an archetypal model of cell polarization, a key process of biological spatial self-organization. Cell polarization is characterized by nonlinear and nonlocal dynamics, but we overcome the theory challenges these traits pose by introducing a novel, broadly applicable numerical scheme allowing us to efficiently study our model in a wide range of geometries. Guided by numerical results, we discover a dynamical hierarchy of timescales that allow us to reduce relaxation to a purely geometric problem of area-preserving geodesic curvature flow. Through application of variational results, we analytically construct steady states on a number of biologically relevant shapes. In doing so, we reveal nontrivial solutions for symmetry-breaking which defy conventional wisdom on the link between symmetry-breaking and geometry.

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CP10

A Mechano-Diffusion Model of Morphogenesis

Morphogenesis is the biological process that causes cells, tissues, or organisms to develop their shape. The theory of morphogenesis, proposed by Alan Turning, is a chemical model where biological cells differentiate and form patterns through intercellular reaction-diffusion. Reaction-diffusion models can produce a chemical patterning that mimics patterns observed in nature. However, while they provide a prepattern that appears plausible, they do not describe a mechanism in which the pattern is expressed. An alternative model is a mechanical model of the skin, initially described by Murray, Oster, and Harris. This model used mechanical interactions between cells without a chemical prepattern to produce structures like those observed in a Turing model. We derive a modified version of the Murray, Oster, Harris model that incorporates nonlinear deformation effects in this talk. Since it is observed in some experiments that chemicals present in developing skin can cause or disrupt pattern formation, the mechanical model is coupled with a single diffusing chemical. Furthermore, it is observed that the interaction between deformations of the tissue with a diffusing chemical can cause a previously undescribed instability. This instability could describe both the pattern's chemical patterning and mechanical expression without the need for a reaction-diffusion system.

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CP11

An Efficient Hybrid Finite Element Approximation

for Numerical Simulation of Multiphase Flow in Heterogeneous Porous Media

Control volume finite element (CVFE) methods provide a flexible approach for modeling coupled flow and transport in highly heterogeneous porous media characterised by sharp contrasts in material properties across subdomain boundaries (e.g. fractures). The finite element method resolves the elliptic flow model, whereas the finite volume method provides a stable solution for the hyperbolic conservation law. In classical CVFE methods, the control volume mesh is constructed by spanning element boundaries. This continuous control volume approach is robust but in the presence of material property discontinuities it introduces non-physical leakage of CV-defined solution fields. An alternative CVFE approach that circumvents this issue incorporates discontinuous pressure approximations which prevent control volumes from spanning elements. However, the approach has high computational cost per element. In this work, we propose using hybrid finite element pressure approximations to capture flow and transport. The new formulation combines the best of both approaches by exploiting the continuous approach in smooth regions of the domain while the discontinuous approximation is applied locally along material discontinuities. This hybrid formulation combines the unparalleled robustness of continuous methods with the accuracy of discontinuous approximations. The effectiveness of the new scheme is demonstrated with several numerical experiments for heterogeneous subdomains.

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CP11

Numerical Simulation of Gas Migration in a Cement Slurry Column

Gas invasion from well formations into the freshly cemented annulus is estimated to cause 25–30% of the failures of wellbore cementing operations. Previous studies suggested that gas migration can be mitigated by allowing enough time for the cement to develop sufficient gel strength, which describes the phase change from the slurry to a gel-like material. Cement slurries exhibit yield stress with rheological properties which can depend on temperature, pressure, volume fraction, etc. In this work, we look at the rising and the distribution of air bubbles in cement slurries. Our simulations are based on room temperature laboratory scale experiments, representative of wellbore experiments developed at our lab, of a column of cement slurry prepared according to industry recommended practices. The column undergoes continuous air (gas) injection at the bottom. The flow of the slurry and the air bubbles is modeled using a continuum approach, where equations for the volume fraction of the cement, mass, and linear momentum are solved numerically. The cement suspension viscosity is calculated according to the Bingham and the Herschel-Bulkley fluid models. These equations are implemented as customized non-Newtonian viscosity libraries and are solved in OpenFOAM (a CFD code). The results show that gas migration strongly depends on the cement slurry stress model as well as gas injection flow rate.

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CP11

Role of Nematic Strength and Activation Parameter in Active Polar Liquid Crystal Channel Flows

Suspensions of active polar liquid crystalline polymers (APLC) exhibit complex phenomena such as spontaneous flows, pattern formations, and defects. Using the Kinetic Model, which couples the Smoluchowski Equation and the Navier-Stokes Equations, we conduct numerical simulations of APLC in a microfluidic channel to investigate the competitive effect among different material constants, such as the nematic concentration (the strength of the potential for nematic order) and active strength (the individual nano-rods strength of their individual movement) with and without a pressure gradient. Both Dirichlet and Neumann boundary conditions on the mathematical model are employed. Steady states, including isotropic and nematic states, as well as periodic states are observed. Spontaneous flows reveal interesting geometries in polarity vector orientation and nematic director orientation, such as flow reversals and banded structures with multiple regions within the channel boundaries.

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CP11

Solution of the Stokes-Darcy System in 3D Based on Robin-Robin Domain Decomposition and Boundary Integrals

We present a robust and highly accurate numerical solution of the coupled Stokes-Darcy system in three dimensions. The method is based on a Robin-Robin type splitting of the interface conditions and solving separate Stokes and Darcy problems iteratively, and second kind boundary integral equations for the local problems. The integral equations use a smoothing of the kernels that achieves high accuracy on the boundary. We present numerical results for a benchmark problem of viscous flow around a porous sphere, as well as more general surfaces.

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CP11

Inversion for the Basal Sliding Coefficient for the Stokes Ice Sheet Model under Uncertain Thermal Distribution

Ice sheet models play an essential role in understanding the

dynamics of ice sheets and for eventually accurately anticipate future sea level rise. These models however are typically subject to considerable uncertainties and model errors, stemming from uncertain coefficient fields, uncertain constitutive laws, source terms, geometries, model simplifications, etc. Arguably the primary uncertainty parameter of interest is the so-called basal sliding coefficient field, a phenomenological parameter that lives in the Robin boundary condition at the base of the ice sheet. To date, there was significant effort payed towards estimating this high-dimensional field and on quantifying the uncertainty in the reconstruction. More recently there was some push toward incorporating additional uncertainty stemming from uncertain rheology via the Bayesian Approximation Error (BAE) approach. BAE is a sampling-based technique that can be used to compute statistics of the model error. The main drawback of this method is that several samples may need to be drawn to estimate the model error accurately. In this talk, we present a control variate approach that combines a linear Taylor approximation (leading to analytical expressions of the mean and covariance) and BAE (via sampling) to mitigate the computational cost. We apply this approach to an ice sheet inverse problem governed by an uncertain Stokes (forward) model, where the additional uncertainty stems from thermal properties of the ice.

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CP12

Propagation in Excitable Tissue via Gap Junctions

Gap junctions are channels through which ions can pass directly between cells. They connect cells throughout the body, including heart myocytes, neurons, and astrocytes. Propagation mediated by gap junctions can be passive or active. In passive propagation, the membrane potential of one cell influences that of neighboring cells without triggering action potentials (APs). In active propagation, an AP in one cell triggers APs in neighboring cells; this occurs in cardiac tissue and in the nervous system. It is known experimentally that there is an ideal gap junction conductance for AP propagation — weaker or stronger conductance can block propagation. We present a theory explaining this phenomenon and predicting whether APs can propagate through a given network of cells connected by gap junctions, by analyzing an idealized model that focuses exclusively on gap junctional and spike-generating currents. We also find a novel type of behavior that we call semi-active propagation, in which cells in the network are not excitable at rest, yet still propagate action potentials.

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CP12

Mutations Make Pandemics Worse Or Better: Modeling Sars-CoV-2 Variants and Imperfect Vaccination

COVID-19 is a respiratory disease triggered by an RNA virus inclined to mutations. Since December 2020, variants of COVID-19 (especially Delta and Omicron) continuously appeared with different characteristics that influenced death and transmissibility emerged around the world. In this work, we propose and analyze a dynamical model of two strains, namely native and mutant, transmission dynamics with mutation, and imperfect vaccination. It is also assumed that the recuperated individuals from the native strain can be infected with mutant strain. We compute the basic reproduction number for each strain independently. We prove the nonexistence of backward bifurcation using the center manifold theory, and global stability of disease-free equilibrium when the basic reproduction number. Oscillations appear when the endemic equilibrium loses its stability. An intermediate mutation rate leads to oscillations. When mutation rate increases over a threshold, the system regains its stability and exhibits an interesting dynamics called endemic bubble. Furthermore, the model is parameterized using the Indian data of the cumulative number of confirmed cases and deaths of COVID-19 from March 1 to September 27 in 2021, using MCMC method. Our study demonstrates that the COVID-19 pandemic may be worse due to the occurrence of oscillations for certain mutation rates (i.e., outbreaks will occur repeatedly) but better due to stability at a lower infection level with a larger mutation rate.

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CP12

Mathematical Modeling in Cryobiology

In cryobiology, tissue is frozen in a liquid for the purposes of preservation. The liquid contains a cryoprotective agent, or CPA, which mitigates the tissue damage due to ice formation. However, prolonged exposure to the CPA can also cause damage to the tissue. This is the basis of an optimal control problem. We wish to minimize the damage to the tissue. To calculate the damage, we created a PDE model of the temperature, concentrations, and interface dynamics. We solved this model using numerical methods to identify optimal cryopreservation protocols.

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CP12

An Agent-Based Approach to Simulating Neural Activity and Connectivity

We developed an agent-based model (ABM) to understand and predict pain output from the amygdala, a part of the brain involved in stress adaptation, emotional regulation, and pain. In the ABM, agents represent individual neurons that express either protein kinase C delta (PKC) or somatostatin (SOM). Neurons that express PKC are known to increase pain whereas neurons that express SOM are known to decrease pain. During the models initialization, neurons are assigned type-specific parameters based on laboratory data and an arbitrary location in either the right or left amygdala. A network of directed links is established to allow for the transmission of inhibitory signals between neurons. During each model time step, neurons accrue damage and the firing rates all of neurons are updated based on the intensity of the external stimulus and the strength of signals transmitted through the network. The ABM outputs an emergent measure of pain, which is calculated in terms of the cumulative pro-nociceptive activity of the PKC neurons and anti-nociceptive activity of the SOM neurons. Results demonstrate the ability of the model to produce changes in pain that are consistent with published studies and highlight the importance of several model parameters. We will discuss how undergraduate students in biology and mathematics contributed to the development of the ABM and continue to play a key role in our efforts to refine and expand the model.

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CP12

Boundary-Value Problem for Protein Transport Along Inhomogeneous Microtubules

Networks consisting of many microtubules and actin filaments are key to the transport of material to and from the nucleus of a biological cell. It was hypothesized that defects of active transport along microtubules may be related to many neurodegenerative diseases such as Alzheimers disease and Amyotrophic Lateral Sclerosis. One area of need for immediate study is the scenario where the microtubule paths used by motor proteins become congested, obstructed, or defective. In this talk, I will present the agent-based model of motor protein transport with an inhomogeneity describing such defects. First, I will show how mean-field partial differential equation description was derived from the agent-based model using the multi-scale analysis. Next, an analytic approach to solution of the derived boundary-value problem will be presented. Finally, I will compare results of Monte-Carlo simulations with analytic solutions. Overall, the model for an inhomogeneous microtubule can inform motor protein dynamics in rough regimes where transport properties are not consistent along given paths. This work was done jointly with Shawn D. Ryan (Cleveland Stat University) and Zachary McCarthy (York University, Canada).

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CP12

Delay Induced Swarm Pattern Bifurcations in Mixed Reality Experiments

Natural swarms exhibit patterns in a variety of forms and have inspired researchers to understand how simple organisms produce complex, emergent patterns occurring when individual organisms follow simple dynamics and local rules. Our work provides a model for swarming behavior of coupled mobile agents with communication-time-delay which exhibits multiple dynamic patterns in space, which depend on interaction strength and delay. A bifurcation analysis has been carried out, on the mean-field model, to explore parameter regions where various patterns occur. The theoretical results were verified in robotics applications by introducing a mixed-reality framework in which real and simulated robots communicate in real time creating the self-organized states predicted by the theory. The proposed swarm controller was tested on two different robotic platforms: NRLs autonomous air vehicles and UPENNs micro-autonomous surface vehicles on water. New phenomena occurring in the experiments led to the study of the full swarm equations which reveals new bifurcation curves accounting for experimental results that were not captured by the mean-field model. The model was extended to include external perturbations acting on the swarm motion. We considered swarms immersed in flows and analyzed pattern formation and bifurcations among patterns for swarms immersed in a double-gyre flow and the sheared chaotic flow.

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CP13

Mathematics of Floating 3D Printed Objects

We explore the stability of floating objects through mathematical modeling and experimentation. Our models are based on standard ideas of center of gravity, center of buoyancy, and Archimedes' Principle. We investigate a variety of floating two-dimensional shapes and identify analytically and/or computationally a potential energy landscape that helps identify stable and unstable floating orientations. We compare our analyses and computations to experiments on floating objects designed and created through 3D printing.

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CP13

Existence of a Solution to a System of Partial Differential Equations with Nonstandard Initial Data

We study the existence of a solution to a system of nonlinear equations that models the flow of a compressible, inviscid, isentropic fluid. We use nonstandard initial data. The initial value of the density is known at a single point in the spatial domain, the initial value of the velocity is known throughout the spatial domain, and the initial value of the partial derivative of the velocity with respect to time is known throughout the spatial domain. We prove the existence of a unique, classical solution to this system of equations under periodic boundary conditions. The key to the proof lies in using a priori estimates in a Sobolev space norm.

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CP13

Water Wave Interaction with an Elastic Plate of Variable Flexural Rigidity Submerged in a Two-Layer Fluid

Water wave interaction with submerged bodies has been extensively studied over the years due to its numerous applications in marine and coastal environments. But the majority of publications in the literature based on water wave theory are focused on the structures' uniform features. But in reality, the majority of marine structures have non-uniform structural qualities, and the topic of varying structural characteristics has received very little study. Thus, in this paper, we focus on the topic of water wave interaction using a vertical elastic plate with variable flexural rigidity. The plate is submerged in the lower layer of two layers of fluids, each being of uniform finite depth. Using the equation of motion for the flexible plate and the Green's theorem, the problem is solved by reducing it to a system of coupled integral equations for functions related to the unknown normal velocity of fluid and the difference in potential across the plate. To obtain the unknown functions numerically, a collocation method based on a finite series of second kind Chebyshev polynomials has been introduced. The effect of variable flexural rigidity on different hydrodynamic quantities - reflection and transmission coefficients, plate deflection, and hydrodynamic force acting on the plate are illustrated graphically. Also, the validation of the present analysis is done by recovering existing results for a limiting case and through energy balance relations.

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CP13

Linear and Nonlinear Analysis of Rayleigh-Taylor System with Navier-Slip Boundary Condition

In this talk, we are interested in the Rayleigh-Taylor instability for the incompressible Navier-Stokes equations with Navier-slip boundary conditions around a laminar increasing density profile $\rho_0(x_2)$, in an infinite slab $2\pi L\mathbb{T}\times(-1,1)$. The linear instability study amounts to the study of the following ODE on the interval $(-1,1)$,

$$-\lambda^2[\rho_0 k^2\psi-(\rho_0\psi')']=\lambda\mu(\psi^{(4)}-2k^2\psi'+k^4\psi)-gk^2\rho_0'\psi,$$

with the boundary conditions

$$\begin{cases}\psi(-1)=\psi(1)=0,\\ \mu\psi'(1)=\xi_+\psi'(1),\\ \mu\psi'(-1)=-\xi_-\psi'(-1),\end{cases}$$

where λ is the growth rate in time, $k\in L^{-1}\mathbb{Z}$ is the wave number transverse to the density profile. For each k, we define a threshold of viscosity coefficient $\mu_c(k,\xi)$ for which there is linear instability for $\mu>\mu_c(k,\xi)$ (k-supercritical regime). In this regime, we provide a spectral analysis adapting the operator method of Lafitte-Nguyen and prove that there are infinitely unstable eigenmodes for the linearized system. Secondly, we extend a result of Grenier, namely we construct a wider class of initial data for which the nonlinear perturbation problem departs from the equilibrium, due to the above finding of multiple eigenmodes. Hence, we prove nonlinear Rayleigh-Taylor instability in a high regime of viscosity $\mu>3sup_{k\in L^{-1}\mathbb{Z}}\mu_c(k,\xi)$.

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CP13

Drag Force on Particles at a Fluid Interface in Creeping Flows

The problem of particles attached to an interface between two immiscible fluids has been extensively studied and has a wide variety of engineering and medical applications. Here we present an asymptotic/numerical investigation of the fluid motion past spherical particles attached to a deformable interface between two immiscible fluids undergoing uniform creeping flows in the limit of small Capillary number. Under the assumption of a constant three-phase contact angle, we analytically obtain the interfacial deformation around a single particle and numerically the two-particle deformation. Applying the Lorentz reciprocal theorem to the zeroth-order approximation for spherical particles at a flat interface and to the first correction in Capillary number allows us to obtain explicit analytical expressions for the hydrodynamic drag in terms of the zeroth-order approximations and the correction deformations. The drag coefficients are computed as a function of the three-phase contact angle, the viscosity ratio of the two fluids, the Bond number, and the separation distance between the particles.

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CP14

Walking into the Complex Plane to 'Order' Better Time Integrators

Most numerical methods for time integration use real time steps. Complex time steps provide an additional degree of freedom, as we can select the magnitude of the step in both the real and imaginary directions. By time stepping along specific paths in the complex plane, integrators can gain higher orders of accuracy and achieve expanded stability regions. Complex time stepping also allows us to break the Runge-Kutta order barrier, enabling 5th order accuracy using only five function evaluations. We show how to derive these paths for explicit and implicit methods, discuss computational costs and storage benefits, and demonstrate clear advantages for complex-valued systems like the Schrodinger equation.

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CP14

Improved Moore-Penrose Continuation Algorithm for the Computation of Problems with Critical Points

The finite element simulation of very large deformation of hyperelastic material is still a challenging problem. The problems are generally driven by a loading parameter and it is often observed that for some values of this parameter, the solution varies extremely rapidly due to geometric and/or material non linearities, often leading to the break down of the solution process. To improve the solution process, numerical continuation methods are often used and have proved to be a very powerful tool. However, these methods can still lead to undesired results. In particular, near severe limit points and cusps, the solution process frequently encounters one of the following situations : divergence of the algorithm, a change in direction which makes the algorithm backtrack on a part of the solution curve that has already been obtained and omitting important regions of the solution curve by converging to a point that is much farther than the one anticipated. Detecting these situations is not an easy task when solving practical problems since the shape of the solution curve is not known in advance. This paper will therefore present an improved Moore-Penrose continuation method that will include two key aspects to solve difficult problems : detection of problematic regions during the solution process and additional steps to deal with them. Numerical examples will be presented to show the efficiency of the new approach.

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CP14

Numerical Solutions of the Time-Dependent Schrodinger Equation with Position-Dependent Effective Mass

The time-dependent Schrodinger equation with a position-dependent effective mass is challenging to solve numerically due to the presence of non-constant mass. For tackling the problem, we will present a Krylov subspace method based exponential integration and an asymptotic Green's function based time propagator. For the former, the wavefunction is represented by a matrix exponential that can be approximated by Krylov subspace method. For the latter, the wavefunction is represented by an integral with retarded Green's function that will be approximated asymptotically. Both methods will have $O(N \log N)$ complexity per time step after careful algebraic manipulations. Numerical examples will be presented for demonstration.

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CP14

A Spectral Multistep Method for Time-Dependent PDEs

Krylov subspace spectral (KSS) methods are high-order accurate, explicit time-stepping methods for partial differential equations (PDEs) with stability characteristic of implicit methods. Unlike other time-stepping approaches, KSS methods compute each Fourier coefficient of the solution from an individualized approximation of the solution operator of the PDE. As a result, KSS methods scale effectively to higher spatial resolution. This talk will present explicit and implicit multistep formulations of KSS methods to provide a best-of-both-worlds" situation that combines the efficiency of multistep methods with the stability and scalability of KSS methods. The effectiveness of spectral multistep methods will be demonstrated using numerical experiments. It will also be shown that the region of absolute stability exhibits striking behavior that helps explain the effectiveness of these new methods.

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CP14

Accelerating Time-Stepping Methods with Surrogate Models

Many scientific computing applications involve dynamical systems that are so complex and require such high fidelity that they become computationally impractical. Model order reduction, machine learning, and other types of surrogate modeling techniques offer cheaper and simpler ways to describe the dynamics of these systems at the cost of additional approximation errors. In order to overcome the individual limitations of the full and surrogate mod-

els, this talk presents new time-stepping strategies based on Runge-Kutta and linear multistep methods that intelligently combine both models. The inexpensive surrogate model is integrated with a small timestep to guide the solution trajectory, and the full model is treated with a large timestep to occasionally correct for the surrogate model error and ensure convergence. We provide numerical experiments to show that this approach can be significantly more efficient than using only the full or surrogate model for the integration. Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS-831294

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CP14

Operator and Dimensional Splitting with Exponential Time Differencing Schemes For Reaction-Diffusion Systems

Operator and Dimensional splitting formulation for Exponential Time Differencing (ETD) schemes is advantageous for efficient simulation of advection-diffusion-reaction systems. These methods are introduced and analyzed for their effectiveness, including smoothing properties when applied to systems with nonsmooth or mismatched data. Several splitting strategies are presented, with discussion of performance for a variety of types of problems.

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CP15

Effects of Wing Bristles and Wing Flexibility on the Aerodynamics of the Smallest Flying Insects

In this project, the effects of wing bristles and wing flexibility on aerodynamic force production in the smallest flying insects were investigated using numerical simulations. Tiny insects fly at Reynolds numbers (Re) in the range 4 60 and use an unusual mechanism for vertical force production: the clap and fling mechanism. Further, the wings of tiny insects are a combination of bristles and a solid membrane instead of just one solid membrane. To investigate the role of bristles, we utilized the hovering clap and fling kinematics of the tiny wasp Encarsia formosa as the model kinematics and its wings as the model wings for our study. We considered the following three values for the ratio of the bristled to the total wing planform area: 0.25, 0.46, and 0.75. The results of our study suggest that at Re relevant to small insect flight, adding bristles to a solid wing doesnt significantly alter the average vertical force produced by the clap and fling mechanism but significantly attenuates the horizontal force required to fling the wings apart. We also investigated the consequences of adding flexibility to rigid wings on aerodynamic force production in small insects. We considered three different flexibilities. Our results show that like bristles, adding flexibility significantly reduces the horizontal force required to fling the wings apart. However, adding flexibility also results in a considerable decrease in the average vertical force acting on the wings.

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CP15

Autoencoder-Enabled Nonlinear Projection-Based Roms for Fluid Dynamics

Reduced order models (ROMS) have been widely researched to substantially improve the efficiency of solving large-scale dynamical systems that are parameterized. One method of reduced order modeling seeks to project the state vector onto a previously-discover lower dimensional latent space on which the dynamics of the system evolve. In modeling complex and nonlinear equations such as is required for computational fluid dynamics (CFD), these methods have often been avoided as their implementation is very model-intrusive, especially when hyper-reduction is involved; however, they machine-learning formulations have demonstrated good performance for many problems. Traditional methods of projection-based ROMs such as Proper Orthogonal Decomposition (POD) also use a linear projection, which is based upon invalid assumptions for nonlinear systems. This work will seek to use machine learning to discover the nonlinear solution manifold and projection operator for accomplishing a nonlinear projection which is used to numerically integrate the reduced-order dynamical system. We will explore both Galerkin and Petrov-Galerkin projections, as well as various methods of hyper-reduction. The results of this work will be compared to corresponding linear subspace projection methods. Example problems will be evaluated including a viscous Burgers Equation and incompressible Navier-Stokes Equations.

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CP15

Physics-Aware Machine Learning Model for Predicting Coastal Hydrodynamics

Numerical models are commonly used to simulate physical phenomena in coastal and near-shore regions to obtain an improved understanding of hydrodynamic processes. These models are crucial to understanding the effects of human intervention and climate change on these environments. Despite the tremendous progress in computational resources and methodologies over the last two decades, these high-fidelity models are still computationally expensive and require a significant amount of expertise. This study explores the use of deep operator networks (DeepONets) to address these issues. DeepONets are a recently introduced class of neural networks that can learn nonlinear operators, instead of functions, directly from simulation or observational data, thus allowing them to learn solution

operators to partial differential equations like the ones that describe hydrodynamic processes. We study the efficiency and accuracy of DeepONet based approximation models using both benchmark and physically realistic problems in coastal flows. We also explore optimal combinations of input and output variables, as well as perform an extensive hyper-parameter search to formulate design guidelines for future efforts in this area.

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CP15

Embedded Deep Learning for Flow Control

We present the first application of an artificial neural network trained through a deep learning PDE augmentation method (DPM) [Sirignano, MacArt, Freund, DPM: A deep learning PDE augmentation method with application to large-eddy simulation, J. Comput. Phys. 423 (2020)] to perform active flow control. The DPM leverages adjoint-based optimization and automatic differentiation for the update of neural network parameters. This PDE-constrained deep learning method is used to control unknown source terms in PDEs such as the Burgers equation and the NavierStokes equations. An example application to the 1D Burgers equation aligns the controlled field with target fields that satisfy the linear advection equation for a wide range of out-of-sample target solutions. This highlights the robustness and generalizability of the DPM, and PDE-constrained neural networks more generally, for active control. However, optimal control performance with increasing control sparsity still remains a major challenge when the controlled PDE and the target PDE evolve differently in the space-time domain, which we describe with examples. For 2D laminar flow over a cylinder, the controlled source flow rate near the cylinder exhibits significantly reduced lift and drag fluctuations. The generalizability of this controller model is tested for reducing drag for different flow geometries and Reynolds numbers. This is an important milestone toward the practical application of DPM to active flow control.

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CP15

Droplets with Slippery Interfaces

Physical systems such as surfactant laden-droplets or those with polymeric interfaces exhibit interfacial slip at the multiphase fluid interface. This slip can dramatically alter the dynamics of these systems in the presence of fluid flow. In this work the dynamics of such a system is numerically investigated via a novel mixed continuous/discontinuous fluid model, whereby material properties are assumed to smoothly change across the interface while the fluid velocity is discontinuous. After a brief discussion of the numerical methods involved, including the full coupling between the fluid velocity and the velocity slip, the influence of interfacial slip on the resulting dynamics will be explored. Sample systems will include individual droplets in the presence of shear flow, filaments, and interactions between many droplets.

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CP15

On the Immersed Boundary Method in Simulating Liquid-Gas Interfaces and Moving Contact Lines

In this work, we combine the immersed boundary method with several techniques to simulate a moving liquid-gas interface on a solid surface. The first technique defines a moving contact line model and implements an extended Generalized Navier Boundary Condition at the immersed solid boundary. The static and dynamic contact line angles are endogenous instead of prescribed, and the solid boundary can be non-stationary with respect to time. The second technique simulates both a surface tension force and an unbalanced Young force with one general equation that does not involve estimating local curvature. The third technique splices liquid-gas interfaces to handle topological changes such as the coalescence and separation of liquid droplets or gas bubbles. Finally, the forth technique re-samples liquid-gas interface markers to ensure a near-uniform distribution without exerting artificial forces. We demonstrate empirical convergence of our methods on non-trivial examples and apply them to several benchmark cases, including a slipping droplet on a wall and a rising bubble.

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CP16

On a Two-Term Time-Fractional PDE: Theoretical and Numerical Considerations

In this talk, I will present the well-posedness and regularity properties of a two-term time-fractional PDE. A class of numerical schemes will be presented and the error analysis will be discussed. Furthermore, I shall briefly discuss some techniques for accelerating the convergence of the developed schemes.

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CP16

Configurable Unit-Cell Topology Design for Bistable and Super-Elastic Metamaterials

This work develops a metamaterial structure that can change between bistable, super-elastic and constant force. To this end, we create a simple unit-cell topology with a damping effect, which can act as a spring. Moreover, we generate this unit-cell to be dynamically configurable and achieve different mechanical behavior in the same design. Thus, we assemble it into various metamaterial structure forms. These structures have simply optimized geometries to produce accessibility and a high damping effect based on the activity of the prosthetic socket user, which maintains constant pressure. Finally, we analyze our metamaterial structures with a large recoverable stress feature by performing the finite element method in nonlinear continuum analysis and explain the method of this analysis. We determine the most convenient metamaterial structures according to the force-displacement curves obtained in the simulation analysis and implement these structures with a 3D printer. We test the energy absorption and structural strengths of our metamaterial structures and demonstrate performance results in both simulated and experimental datasets. According to these results, we describe our selection procedure for the final metamaterial structure.

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CP16

Statistical Field Theory for the Free Energy of An Electro-Mechanical Polymer Chain: Non-Local Dipole-Dipole Interactions in the Fixed Applied Field Ensemble

Existing theoretical approaches for polarizable polymers subject to a combined applied electric field and stretch are based on discrete monomer models. It is challenging to account for the non-local dipole-dipole interaction in this framework. The prior work typically considers only the interaction between the applied field and dipoles. To go beyond this approximation, we apply the statistical field theoretic framework that is based on a continuous description of the polymer chain in terms of density fields. We introduce a self-consistent formulation that enables us to address the setting of constant applied electric field ensembles that transforms the nonlocal interactions into a PDE constraint corresponding to the Gauss equation. We implement the model in a finite element method to compute the free energy, average density, and average polarization distribution at equilibrium. We find that the presence of dipole-dipole interactions leads to qualitative changes in the dipole distributions, total polarization, and equilibrium electric field in the domain. We further notice a sharp instability leading to a collapse of the chain under the strong electric fields as a consequence of dipole-dipole interactions.

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CP16

Buckling Control in Inhomogeneous Soft Composite Sheets

Elastic plates floating on a fluid substrate, and subjected to axial compression, display a sinusoidal pattern in their vertical displacement, called wrinkles. We examine the wrinkles of inhomogeneous soft composite thin sheets lying on a liquid. In particular, we consider effective medium behaviour theories to predict the bending stiffness of a composite plate consisting of a soft host with liquid inclusions both large and small relative to the elastocapillarity length. By imposing a gradient of the volume fraction or varying the inclusion size, we can devise elastic sheets with a varying stiffness and therefore deliberately manipulate the nature of the emerging wrinkles for different lengths of the plate.

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CP16

Steady Vibration Problems in the Coupled Theory of Double Porosity Thermoelastic Materials

In this talk, the linear model of thermoelastic materials with double porosity is introduced in which the coupled phenomenon of the concepts of Darcy's law and the volume fraction of pore network is presented. The basic internal and external boundary value problems of steady vibrations are investigated. Indeed, the fundamental solution of the system of steady vibration equations is constructed explicitly. The radiation conditions are established. Greens identities are obtained and the uniqueness theorems for the classical solutions of the boundary value problems are proved. The surface and volume potentials are constructed and the basic properties of these potentials are given. The boundary value problems are reduced to the always solvable singular integral equations for which Fredholms theorems are valid. Finally, the existence theorems for classical solutions of the internal and external boundary value problems are proved by means of the boundary integral equation method and the theory of singular integral equations. Acknowledgements: This work was supported by

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CP17

Deep Learning of Systems with Physical Structures

We propose a data-driven method to learn dynamics of systems with physical structures using deep neural networks. We incorporate the physical structures into the design of the networks and show that such models can predict dynamics obeying desired physical laws of the system. To demonstrate our method, we focus on conservation laws in partial differential equations and derive conservative form networks. Numerical results show that models with physical structures outperform models without ones in both accuracy and physical property. Moreover, we found that information contents over time in data affect model performance. Model performance initially improves as more data is available over time, but it can also deteriorate as time becomes too long. We found that the later deterioration is caused by temporal error accumulation. This suggests that we should take time integration errors into account as we pick the time span of data.

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CP17

Multiscale Simulations of the Capillary Thinning of Polymer Solutions

When a viscoelastic material is stretched between two surfaces, the interaction between elastic and capillary stresses leads to the formation of a beads-on-a-string structure where between drops, thin and stable filaments form. Under certain conditions, small satellite drops can form between the main droplets. In application, such as in inkjet printing, the emergence of these satellite drops is cause for concern, thus it becomes important to understand what properties lead to their formation. In this work we consider the capillary thinning of polymer solutions via a thin film approximation, in which the polymer stress is implemented via 1) constitutive equation, and 2) kinetic dumbbell equations. The constitutive equations are derived from kinetic equations describing polymers via elastic dumbbells. For many of these models, the macroscopic equations cannot be derived exactly from the microscopic equations, and closure approximations are required. Such approximations can be avoided by simulating the dumbbell equations directly. The CONFESSIT method for multiscale simulations is thus used, wherein the flow field is computed macroscopically, and the polymer stress is calculated via the solution of Langevin equations. Using this method, we investigate the effects that certain mesoscopic properties, e.g., polymer stretch and anisotropic drag, have on drop formation, ultimately revealing phase diagrams showing conditions under which satellite drops do form.

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CP17

Multiscale Modeling of Membranes with Embedded Thin Filaments

Coupled interaction between membranes with embedded thin filaments is ubiquitous in cell biology and plays a vital role in the proper functioning of the cell. For example, spectrin filaments, which are part of the cytoskeletal network, form a network lining the surface of a cell membrane and provide structure and stability. Another example is the ESCRT (endosomal sorting complex) machinery, which is responsible for initiating cell fission in eukaryotic cells. This complex consists of protein monomers that polymerize as thin filaments on the membrane and apply forces that eventually lead to the cell's cleaving into daughter cells. This talk will present a continuum mechanics model to study such systems. For this multiscale model, we show that equilibrium states are determined by a nonlinear PDE for the membrane coupled to ODEs for the filaments with appropriate jump conditions. We will discuss computational strategies to solve the highly nonlinear problem.

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CP17

A Hybrid Physics-Based and Data-Driven Modeling Approach for Identifying Multi-Physics Systems Utilizing Stochastic Optimization

In this work we propose a hybrid computational framework for model-free system identification. This framework stochastically discovers governing differential equations (partial or ordinary) from a given dataset by utilizing genetic programming, one of the machine learning algorithms. The proposed approach allows the easy incorporation of the users prior knowledge into the identification process (e.g., variables, basis functions, initial and boundary conditions, etc.), while the outcomes (i.e., identified differential equations) reveal the system physics embedded in the dataset. We demonstrate the proposed framework, denoted here as GPfSI, through the use of synthetic as well as real data corresponding to widely-encountered complex phenomena that are associated with various disciplines such as structural mechanics, fluid mechanics, hydrology and soil physics. The results show that the exact reference models are successfully identified even in the presence of noisy measurements. Our results indicate that GPfSI is an effective and versatile framework in modeling and understanding multi-physics systems.

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CP17

Multi-Scale Finite Elements for Transport-Dominant Equations Applied to Canopies

Urban canopies consist of buildings or trees that may be scattered or aligned along roads. Such canopies modulate the local climate in a complex way. However, the surface structures established through canopies cannot be resolved in climate simulations. Climate models strive to represent such subgrid features by parameterizations. Multiscale finite element methods have been applied to various porous media applications, mainly for elliptic or parabolic type equations. Here we present a multiscale finite element method for transport-dominated equations. The multiscale method is composed of two parts: an offline phase that precomputes the multiscale basis functions and an online phase that uses these basis functions to compute the coarse solution. The overhead of precomputing the basis functions in each coarse cell can further be reduced by parallelization. The online phase is approximately as fast as a low resolution standard FEM but still reveals fine scale features of a highly resolved solution and is therefore accurate. This approach is studied in order to modulate the effect of fine scales on the coarse scale dynamics in climate simulation models with canopies. In our approach we use viscosity to represent the canopy structure. We compare our multiscale approach with a standard FEM for accuracy and computation efficiency. Further on, we validate our new model with recently obtained wind tunnel data, comparing tracer transport data from experiment and model.

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CP18

Phase-Field Modeling and Peridynamics for Defect Dynamics, and an Augmented Phase-Field Model with Viscous Stresses

This work begins by applying peridynamics and phase-field modeling to predict 1-d interface motion with inertia in an elastic solid with a non-monotone stress-strain response. In classical nonlinear elasticity, it is known that subsonic interfaces require a kinetic law, in addition to momentum balance, to obtain unique solutions; in contrast, for supersonic interfaces, momentum balance alone is sufficient to provide unique solutions. This work finds that peridynamics agrees with this classical result, in that different choices of regularization parameters provide different kinetics for subsonic motion but the same kinetics for supersonic motion. In contrast, conventional phase-field models coupled to elastodynamics are unable to model, even qualitatively, the supersonic motion of interfaces. This work identifies the shortcomings in the physics of standard phase-field models to be: (1) the absence of higher-order stress to balance unphysical stress singularities, and (2) the ability of the model to access unphysical regions of the energy landscape. Based on these observations, this work proposes an augmented phase-field model to introduce the missing physics. The augmented model adds: (1) a viscous stress to the momentum balance, in addition to the dissipative phase-field evolution, to regularize singularities; and (2) an augmented driving force that models the physical mechanism that keeps the system out of unphysical regions of the energy landscape.

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CP18

A Phase-Field Fracture Model for Complex Loading Across the Crack Face

Regularized models of fracture, such as phase-field fracture models, are emerging as competitive approaches for realistic problems including heterogeneities, interfaces, and crack branching. Phase-field models treat the crack as a second phase and use gradient terms to smear out the crack faces, enabling the use of numerical methods for simulations. However, a shortcoming of existing phase-field models is their inability to accurately model the response of cracks when the crack faces close due to compression. Specifically, idealized sharp cracks have zero normal traction when the crack opens up and the crack faces lose contact, while the response under compression is identical to the intact material; further, the shear traction across the crack face is zero. We address this issue by introducing an effective crack energy density that endows the regularized phase-field crack with the effective properties of an idealized sharp crack. Here, we use QR decomposition of the deformation gradient tensor in the basis of the crack, enabling a transparent identification of the crack deformation modes. We then relax over those modes that do not cost energy, providing an effective energy that has the intact response when the crack faces close and zero energy when the crack faces are open. A highlight of this approach is that it is completely in the setting of finite elasticity, enabling potential application to soft materials and other fracture settings where the rotations can be large.

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CP18

Discontinuous Galerkin Discretization for the Variational Phase-Field Approach to Fracture

Crack propagation in brittle materials was reformulated as an energy minimization problem in Francfort and Marigo [1998]. The variational phase-field approach (Bourdin Francfort Marigo 2000, Bourdin Francfort Marigo 2008) follows the line of AmbrosioTortorelli smoothing to the MumfordShah functional Ambrosio and Tortorelli [1990], extended to the energy functional of Francfort and Marigo [1998]. The regularized functional is usually discretized with $\mathbb{P}^1$-Lagrange Finite Elements because of the low regularity of the expected solution. In this presentation, we introduce a symmetric and a non-symmetric Discontinuous Galerkin discretization of the phase-field equations for fracture and compare them to the standard $\mathbb{P}^1$-Lagrange discretization. The stability and robustness of this approach is illustrated on several numerical examples.

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CP18

An Eulerian Description of Surface Growth in Deformable Solids

Surface growth, or accretion, occurs in different applications including the growth of biological tissues and solidification which mechanical stresses play a key role in the final state of the body. In surface growth, the set of the continuum particles constructing the growing body is time-dependent which is challenging for the standard continuum formulations of solids. An Eulerian description of this problem is developed by the introduction of localized mass sources on the growing surface, enabling side-stepping of the issue of an evolving set of material particles. To determine the stress response of the solid body, the elastic deformation is defined as a kinematic descriptor of the added material which is shown to be evolved by a transport equation. As a result, the model has only density, velocity, and elastic deformation as variables in the Eulerian setting. A numerical method based on this formulation is developed. The equations are solved on a fixed discretization in a computational domain that contains the growing body and ambient medium, with a phase indicator function to track the solid body. The evolution consists, at each timestep, of 1) updating the phase function with contributions from mechanical deformation and accretion; 2) filtering of the phase function to preserve tangential smoothness while changing rapidly in the normal direction; 3) solving for mechanical equilibrium to compute the deformation of the solid body; and 4) updating the density of the body.

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CP18

Transient Response of Collinear Griffith Cracks in a Functionally Graded Strip Bonded Between Dissimilar Elastic Strips under Shear Impact Loading

This article analyses the interaction between a central and two symmetrically placed collinear Griffth cracks subject to transient response under anti-plane shear impact loading. The cracks are situated in a strip constituted by functionally graded material (FGM) bonded between two dissimilar elastic strips of equal thickness. The material properties of FGM are assumed to vary exponentially as a function of thickness. Applying integral transforms, the boundary value problem reduces to a system of singular integral equations in the Laplace transformed domain. These equations are solved numerically using the Lobatto-Chebyshev collocation quadrature approach. The inverse Laplace transform is used to find the approximate expressions of dynamic stress intensity factors (DSIFs). The striking feature of the article is the study of phenomenal changes of shielding and amplification through dynamic stress magnification factor (DSMFs) at the tips of the cracks under the sudden impact loading applied at the upper material surface. The effects of impact load applied at different surfaces, positions of cracks' axis and the thickness of the strips of the composite material on the possibilities of cracks' arrest are depicted graphically for different particular cases.

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CP19

Stabilization of Deep Latent Dynamics with Dissipative Bottleneck Layers

We propose a spectral localization technique that allows us to precisely control the spectral properties of residual layers and their corresponding Lipschitz constants. We use this technique to design dissipative residual layers and show that, when added to a deep neural network, these layers act as identity mappings and do not change the default behavior of the network. When activated, however, these layers act as bottlenecks that expose the intrinsic dimensionality of latent dynamics by reducing irrelevant dimensions. This allows for efficient training by taking advantage of overparameterization and high-dimensional augmentation while significantly improving the stability and robustness of models trained on clean data only.

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CP19

PDE-Constrained Optimization for Multiscale Particle Dynamics

There are many industrial and biological processes, such as beer brewing, nano-separation of colloids and bird flocking, which can be described by integro-PDEs. These PDEs describe the dynamics of a particle density within a fluid bath, under the influence of diffusion, external forces, and particle interactions. They often include nonlinear, non-

local boundary conditions. A key challenge is to optimize these types of processes, which requires tools from PDE-constrained optimization. In this talk I will introduce a numerical method to solve this class of optimal control problems, which combines pseudospectral methods and spectral elements with a Newton-Krylov algorithm. This provides a tool for the fast and accurate solution of the resulting optimality systems. In particular, this framework allows for the solution of (integro-)PDE models and optimal control problems on complex domains, which is a crucial feature in accurately describing various (industry) applications. Finally, some examples of current work and future industrial applications will be given. This is joint work with Ben Goddard and John Pearson.

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CP19

A Stochastic Gradient Method for Nonlinear Pde-Constrained Optimal Control Problems under Uncertainty

In this talk, we will describe a class of optimal control problems for semilinear elliptic partial differential equations with random data. The interest in such problems is motivated by some recent research papers in the area of stochastic optimization. Moreover, we will discuss some convergence results of a stochastic optimization method utilized to solve these non-convex stochastic optimization problems. The application of this method to the aforementioned class of PDE-constrained optimization problems will be addressed in detail. Some numerical experiments will conclude the analysis.

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MS1

The Geometry of Adversarial Training

In this talk I will show that "Adversarial Training"a methodology designed for the training of adversarially robust classifiersis equivalent to a variational regularization problem involving a nonlocal perimeter term. Using this structure one can show that adversarial training admits a convex relaxation which is reminiscent of the Chan-Esedoglu model from image denoising. Furthermore, this allows to prove existence of solutions and study finer properties and regularity. Finally, I hint at how to modify adversarial training to an Almgren-Taylor-Wang like scheme for mean curvature flow.

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MS1

Hamilton-Jacobi Equations on Graphs with Applications to Semi-Supervised Learning and Data Depth

Shortest path graph distances are widely used in data science and machine learning, since they can approximate the underlying geodesic distance on the data manifold. However, the shortest path distance is highly sensitive to the addition of corrupted edges in the graph, either through noise or an adversarial perturbation. In this talk we present a family of Hamilton-Jacobi equations on graphs that we call the p-eikonal equation. We show that the p-eikonal equation with p=1 is a provably robust distance-type function on a graph, and the limiting case in which p goes to infinity recovers shortest path distances. While the p-eikonal equation does not correspond to a shortest-path graph distance, we nonetheless show that the continuum limit of the p-eikonal equation on a random geometric graph recovers a geodesic density weighted distance in the continuum. We show the results of applications to data depth and semi-supervised learning. This is joint work with Mahmood Ettehad.

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MS1

A Variational Approach to Robust Statistics

Widespread application of modern machine learning has increased the need for robust statistical algorithms. One fundamental geometric quantity in robust statistics is known as a data depth, which generalizes the notion of quantiles and medians to multiple dimensions. This talk will discuss recent work which connects certain types of data depths with geometric variational problems. These problems have deep connections with optimal control and Hamilton-Jacobi equations, and rely upon ideas from both convex and metric geometry. Computational considerations and a number of related open problems will also be discussed.

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MS1

On Multiclass Adversarial Training and Multimarginal Optimal Transport Problems

Adversarial training is a framework widely used by machine learning practitioners to enforce robustness of learning models. Despite the development of several computational strategies for adversarial training and some theoretical development in the broader distributionally robust optimization literature, there are still several theoretical questions about adversarial training that remain relatively unexplored. In this talk, I will discuss an equivalence between adversarial training in the context of non-parametric multiclass classification problems and multimarginal optimal transport problems. This is another analytical interpretation of adversarial training that expands recently studied connections to perimeter minimization problems.

One of the implications of the connection discussed during the talk is computational: to solve a certain adversarial problem, we may as well solve a multimarginal optimal transport problem. We will discuss many of the nuances of this interpretation and of its computational consequences.

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MS2

FT-GCR: A Fault-Tolerant Generalized Conjugate Residual Elliptic Solver

With the steady increase in core counts per job in high performance computing facilities, systems and algorithms used for numerical simulations increasingly contend with disruptions caused by hardware failures and bit-level misrepresentations of computing data. In many numerical frameworks exploiting massive processing power, the solution of linear systems represents one of the most computationally intensive algorithmic components. With mean times between failures approaching minutes in HPC facilities, iterative solvers are particularly vulnerable to bit-flips. A new method named FT-GCR is proposed here that supplies the preconditioned Generalized Conjugate Residual Krylov solver with detection of, and recovery from, soft faults. The algorithm tests on the monotonic decrease of the residual norm and, upon failure, restarts the iteration within the local Krylov space. Numerical experiments on the solution of an elliptic problem arising from a stationary flow over an isolated hill on the sphere show the skill of FT-GCR in addressing bit-flips on a range of grid sizes and data loss scenarios. Best returns on fault tolerance and detection rates are obtained for larger corruption events. The computational and memory cost of the method is addressed, and savings in the presence of faults are quantified in terms of time to solution compared to unprotected runs. The simplicity of the method makes it easily extendable to other solvers with monotone convergence in a computable norm and a suitable candidate for algorithmic fault tolerance within integrated model resilience strategies. This is a joint work with M. Gillard, Loughborough University.

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MS2

The Distributed Subgradient Method and Network Independence

Distributed optimization has attracted a lot of attention recently as machine learning methods are increasingly trained in parallel over clusters of nodes. Unfortunately, the performance of many distributed optimization algorithms often suffers from scalability problems, with worst-case performance degrading the size of the network increases. We will describe a distributed version of the subgradient method which, under certain conditions, manages to overcome this. Specifically, we will show that, in a network of n nodes, our method is able to converge to a global minimizer of the objective n times faster as compared to a single node, provided the accuracy to which the problem needs to be solved is sufficiently small depending on the spectral gap of the underlying network.

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MS2

Resilient Algorithmic Building Blocks for Decentralized Iterative Computing in the Skynet Software

In any distributed, network-connected system today, either large or small, computers of various types are present throughout the system, leading to edge computing as an increasingly important paradigm. Often these edge devices are low-powered, inexpensive, and unreliable, either due to harsh physical conditions, the threat of cyber intrusions, or simple cost considerations. Collaborative Autonomy is an emerging class of computational techniques and software that enables these edge devices to self-organize and work together as a collective, without the presence of a single central master computer, to solve computational problems and make decisions. A key principle of Collaborative Autonomy is the focus on inherent algorithmic resilience, so that the collective system can adapt around problems in the computational environment, such as hardware malfunctions, network failures, and cyber intrusions. This algorithmic resilience aims to ensure the system as a whole has a high degree of reliability even when no devices do individually. In this edge computing setting, numerical problems are often best solved through iterative, possibly asynchronous, methods. In this talk, we will present the Skynet software under development at LLNL and its novel approach to enabling algorithmic resilience for decentralized iterative methods. Specifically, Skynet focuses on providing a suite of resilient variants of algorithmic building blocks, such as reduce and averaging methods, that are widespread across iterative algorithms. By implementing an iterative method using this building-block interface, a user can often achieve algorithmic resilience to problems in the computational environment for free with little-to-no additional implementation or algorithm design work. We will present a number of common algorithmic building blocks supported by the Skynet software and will show experiments demonstrating the impact of making these building blocks resilient. This is a joint work with Zachary R. Atkins, Alyson L. Fox , Agnieszka K. Miedlar, Christopher J. Vogl. Funded by LLNL LDRD projects 21-FS-007 and 22-ERD-045. Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS-xxxxxx.

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MS2

Asynchronous Parallel Block-Coordinate Forward-Backward Algorithm

We are going to present our work on the convergence properties of a randomized block-coordinate descent algorithm for the minimization of a composite convex objective function, where the block- coordinates are updated in parallel, asynchronously and randomly according to an arbitrary probability distribution. In that work, we prove that the iterates generated by the algorithm form a stochastic quasi-Fejer sequence and thus converge almost surely to a minimizer of the objective function. Moreover, we prove a general sublinear rate of convergence in expectation for the function values and a linear rate of convergence in expectation under an error bound condition of Tseng type. Under the same condition strong convergence of the iter-

ates is provided as well as their linear convergence rate.

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MS3

Comparing Product Throttling for Zero Forcing, Cops and Robbers, and Power Domination

Product throttling addresses minimizing the product of the resources used to accomplish a task and the time needed to complete that task for various graph searching processes. We are interested in product throttling for graph parameters such as zero forcing, cops and robbers, and power domination. The resources for these graph parameters are the blue vertices in zero forcing, cops in Cops and Robbers, and Phasor Measurement Units in power domination. Given a graph, product throttling minimizes a product of the number of vertices (resources) and the time it takes to observe all the vertices in the graph using a using a graph searching process. In this talk, we discuss and compare product throttling for zero forcing, cops and robbers, and power domination.

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MS3

The Threshold Strong Dimension of a Graph

A set W of vertices of a connected graph G is a *strong resolving set* for G if, for every pair of vertices, one of the vertices in the pair lies on a shortest path from the other vertex to some vertex of W. The smallest cardinality of a strong resolving set of vertices of G is the *strong dimension* of G. The *threshold strong dimension* of G is the smallest strong dimension among all graphs having G as a spanning subgraph, and it is denoted by $\tau_s(G)$. We present a geometric characterization of $\tau_s(G)$, which expresses $\tau_s(G)$ in terms of the smallest number of paths (each of sufficiently large order) whose strong product admits a certain type of embedding of G. We also establish logarithmic bounds on $\tau_s(G)$ for graphs in general, and for trees. This is joint work with Nadia Benakli, Novi H. Bong, Linda Eroh, Beth Novick, and Ortrud Oellermann.

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MS3

Inner Code Impact on Graph-Based Codes

Graph-based codes are an important family of error-correcting codes. They may be used to store information so that erroneous may be repaired and missing data can be recovered. Bipartite graphs form a basis for graph-based code families. One set of vertices is associated with coordinates of a codeword or a received word, and the other set of vertices enforces conditions that must be satisfied in order for an assignment of values to be a codeword. These conditions may be simple parity checks or prescribed by more sophisticated inner codes that together give rise to a graph-based code C. In this talk, we consider the impact of the inner codes on properties of the code C.

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MS3

Symmetry Parameters for Mycielskian Graphs

Vertex colorings can be used to study the symmetries of a graph, whether or not the automorphism group of the graph is explicitly known. A graph G is d-distinguishable if there is a coloring of the vertices with d colors so that only the trivial automorphism preserves the color classes. The smallest such d is the distinguishing number, $\mathrm{Dist}(G)$. Similarly, a set S of vertices is a determining set for a graph G if every automorphism of G is uniquely determined by its action on S. The size of a smallest determining set for G is called its determining number, $\mathrm{Det}(G)$. In this talk we will discuss how distinguishing and determining numbers interact with Mycielskian constructions and cones over graphs.

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MS4

Inducing Point Approximations of Kernel Matrices

Kernel-based approximation methods typically lead to large dense linear systems whose size scales with the number of data points. For kernels that are smooth (or smooth away from some diagonal), these matrices can be approximated by matrices with low rank (or low-rank plus sparse) structure. The low rank approximation is often organized around a set of inducing points that serve as the basis for the approximation. In this talk, we describe several different stories for how these inducing points are chosen, appealing to ideas in linear algebra, approximation theory, and Bayesian statistics, and we describe how these ideas can be combined to obtain new methods for approximating kernel matrices.

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MS4

Data-Driven Low Rank Approaches for High Dimensional Data

Dense kernel matrices play a key role in various disciplines such as machine learning, physics, biology, etc. To reduce the computational cost, low-rank techniques are often used to construct an economical approximation to the original matrix. In this talk, we consider linear complexity subset selection based methods for general m-by-n kernel matrices associated with data in possibly high dimensions. The goal of the talk is two-fold: (1) we perform analysis to provide a straightforward geometric interpretation to answer a central question: what kind of subset is preferable for low-rank approximation; (2) based on the geometric interpretation, we present a fast and robust algorithm in O(m+n) complexity for approximating general kernel matrices with both low and high dimensional data. The efficiency and robustness will be demonstrated through extensive experiments.

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MS4

Data Oblivious Low-Rank Approximation of Kernel Matrices

This talk will overview the random features approach for approximating positive semidefinite kernel matrices in a data oblivious manner. I will describe how this method can be viewed as a column subset selection method, and in turn, how tools from randomized numerical linear algebra can yield improved sampling distributions and theoretical guarantees. Work on such guarantees has uncovered exciting connections between leverage-score-based random features sampling, active kernel regression, and classical notions in approximation theory, such as polynomial Christoffel functions. I will discuss several open research directions in this area.

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MS4

Indefinite Large Scale Kernel Approximation - to Loose Or to Preserve Information?

Matrix approximations are a key element in large-scale algebraic machine learning approaches. Focusing on similarities, a common assumption is to have positive semi definite (psd) kernel functions as the underlying source. This is often a too strong constraint and limits practical applications. The approximation either cannot be validly applied or it changes the underlying similarity function. Approximations could in fact also accidentally lead to non-psd representations. In any case the modifications of the original or approximated similarities can have a severe impact on the encoded information. One may loose information or can introduced disturbances. This is particular important if branch-and-bound approaches or mathematically well principled error minimizers are used, to obtain predictive models. Strategies to correct similarities beforehand or after the approximation are often based on spectral corrections, embeddings or proxy approaches. These corrections do often not scale to large data and counteract with the approximation. We explain the problem setting and detail traditional and recent developments in the domain of indefinite learning to correct symmetric similarities at large scale.

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MS5

Deep Residual Learning via Large Sample Mean-Field Stochastic Optimization

We study a class of stochastic optimization problems of the mean-field type arising in the optimal training of a deep residual neural network. We estimate the training weights of the network as the optimal relaxed control of a sampling problem, where a population risk criterion is minimized. We establish the existence of optimal relaxed controls when the training set has finite size. The core of our paper is to prove, via Γ-convergence, that the minimizer of the sampled relaxed problem converges to that of the limiting optimization problem, as the number of training samples grows large. We connect the limit of the sampled objective functional to the unique solution, in the trajectory sense, of a nonlinear Fokker-Planck-Kolmogorov (FPK) equation in a random environment.

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MS5

Adaptive Robust Optimal Execution with Price Impact

In this project, we study optimal execution of trades and focus on the analysis of book depth. We propose a formulation of optimal execution that is adaptive and robust where the controller dynamically learns price impact parameters based on observations and adjusts the actions according to the worst-case parameters to mitigate model risk. This paper is a joint work with Michael Ludkovski and Moritz Voss.

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MS5

A Game and Stochastic Control Methodology for the Convergence of Gans Training, with Applications in Generating Financial Data

Training generative adversarial networks (GANs) is known to be difficult, especially for financial time series. In this talk, we first introduce the well-posedness problem in GANs minimax games and the convexity issue in GANs objective functions. We then propose a stochastic control framework for hyper-parameters tuning in GANs training. The weak form of dynamic programming principle and the uniqueness and the existence of the value function in the viscosity sense for the corresponding minimax game are established. In particular, explicit forms for the optimal adaptive learning rate and batch size are derived and are shown to depend on the convexity of the objective function, revealing a relation between improper choices of learning rate and explosion in GANs training. Finally, we will demonstrate via some empirical studies that training algorithms incorporating this adaptive control approach outperform the standard ADAM method in terms of convergence and robustness. From GANs training perspective, the analysis in this paper provides analytical support for the popular practice of clipping, and suggests that the convexity and well-posedness issues in GANs may be tackled through appropriate choices of hyper-parameters.

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MS5

Large Dimensional Latent Factor Modeling with Missing Observations

In this talk, we will introduce the inferential theory for latent factor models estimated from large dimensional panel data with missing observations. We propose an easy-to-use all-purpose estimator for a latent factor model by applying principal component analysis to an adjusted covariance matrix estimated from partially observed panel data. We derive the asymptotic distribution for the estimated factors, loadings and the imputed values under an approximate factor model and general missing patterns. The key application is to estimate counterfactual outcomes in causal inference from panel data. The unobserved control group is modeled as missing values, which are inferred from the latent factor model. The inferential theory for the imputed values allows us to test for individual treatment effects at any time under general adoption patterns where the units can be affected by unobserved factors. We apply our method to portfolio investment strategies and find that around 14% of their average returns are significantly reduced by the academic publication of these strategies.

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MS6

Geometry and Mechanics of Intrinsically Curved Folds

Elastic sheets with intrinsically curved folds are ubiquitous in nature and engineering; consider for example, a giant lilly pad, top hat or tin can. Unlike the extrinsic curved folds familiar from origami, such intrinsic folds are strong mechanical features that cannot be removed without stretch. I will derive their basic geometric rules, which permit them to deform isometrically by trading off curvature against fold-angle, making such folds interesting mechanisms. The rules also distinguish folds with negative and positive Gauss curvature, and also between symmetric and asymmetric folds of each sign. Symmetric folds can attain a fully folded book-like state, allowing intrinsically curved surfaces to be flat-packed, and then deployed. In contrast, asymmetric folds have a minimum opening angle and corresponding minimum curvature, giving them strength under load. By definition, intrinsic folds cannot be fashioned from a flat sheet by isometric bending. However, they can form in sheets that undergo active metric changes, for example by growth, swelling or contraction. I will give examples, both theoretical and experimental, of programming folds into liquid-crystal elastomer sheets, such that they form on heating through the nematic-isotropic phase transition. Finally, I will discuss how these folds are not truly sharp, but blunted by a trade-off between stretch and bend, leading to an unusual scaling law where the curvature changes with sheet thickness as $t^{-1/7}$.

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MS6

Multistability Graph Analysis of Reconfigurable Origami Structures

Origami has emerged as a promising platform for morphing structures, programmable materials, reconfigurable robotics, and mechanical computing. Origami structures exhibit novel multistability properties, which can be programmed to target specific stable states and actuation modes between configurations. Here we use stochastic search and gradient-based optimization to map out the stable states of the origami structure; and use minimum energy path methods to characterize the folding paths between states (i.e. actuation paths). Then using concepts from Morse theory and shape metrics, we identify intermediate branching points and bifurcations where folding paths intersect. The interaction and connectivity between various folding paths of the origami naturally leads to a graph theoretic representation where the vertices correspond to folded configurations of interest and the edges correspond to folding paths. The graph representation which

emerges can lead to insights on potential actuation cycles for locomotion, and for robotic reconfiguration strategies more broadly. We study mechanisms for tuning certain structural and energetic properties of the graph which may have important implications for effectively utilizing origami principles in robust deployment of origami structures, robotic locomotion, and mechanical logic gates. Because origami principles are scale invariant, this work has potential impact from the nanoscale to the scale of space applications.

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MS6

Statistical Mechanics of Light-Responsive Glassy Nematic Polymers

Nematic networks with photo-responsive mesogens show spontaneous deformation when illuminated, due to a trans-cis bending of the mesogens. A statistical mechanical model shows a separation of energy scales between entropic elasticity and photoswitching. Consequently, there is the emergence of a broken symmetry in the coupling between light and deformation: to leading order, optics drives mechanics but there is no reverse coupling. The broken symmetry is inherited by the evolution, which shows a complex interplay between the characteristic time scales for photoswitching and polymer relaxation. These features agree with our experimental measurements of photoswitching and shape evolution. Joint work with Mahnoush Babaei, Matthew Grasinger, M. Ravi Shankar.

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MS6

Topological Transformations in Symmetric Higher Order Vertex Origami

An origami structure can have many different stable configurations depending on its crease pattern, its underlying material properties, and the elasticity of its creases. This propertymultistabilitymakes origami an intriguing testbed for metamaterials with reconfigurable properties, deployable structures, and structures that mechanically store and process information. Multistability emerges in origamieven in cases where all of its elastic energy is stored in *linear* torsional springs at its creases. Here multistability is due to constraints on the possible fold angles of the structure. Creases must be folded in such a way that the structure does not tear; that is, they must satisfy *compatibility*. So although the energy is a convex function of the fold angles, the manifold of allowable fold angles is nonconvex. The compatibility condition, therefore, has fundamental importance on the multistability of origami structures; however, it is a formidable system of nonlinear equations. Here we utilize group theory to solve for the allowable kinematics, in closed-form, of symmetric origami vertices with multiple degrees of freedom. We show that certain changes in crease geometry lead to topological changes in the manifold of allowable fold angles. Such topological changes provide potential avenues for programming more or less stable configurations into the structure, as each hole in the manifold provides another opportunity for local minima.

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MS7

A Reduced-Order Method for Electron Transport with Long-Range Interactions

In the study of electron transport, one typical situation is a molecular junction, where single molecules are bound to two semi-infinite leads that are regarded as quantum baths. This necessarily introduces a large number of electronic degrees of freedom to the system. Another challenge is the long-range interactions from Coulomb potential. In the density matrix representation, Coulomb potential introduces a highly non-linear Hamiltonian to the Liouville-von Neumann equation. In this talk, we will introduce a model reduction approach using Petrov-Galerkin projection. In order to recover the global electron density profile as a vehicle to compute the Coulomb potential, we propose a domain decomposition approach, where the computational domain also includes segments of the bath that are selected using logarithmic grids. This approach leads to a multi-component self-energy that enters the effective Hamiltonain.

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MS7

Efficient Stochastic Algorithms for Ab Initio Molecular Dynamics

The focus of this talk is on dynamics problems that are driven by quantum mechanics. Namely, the interactions within the dynamics are not explicitly given. But rather, they are expressed in terms of an underlying large-scale eigenvalue problems. Direct simulations require repeated and extensive computation of the electron structures. We will present a multi-scale model, where the fast dynamics, after averaging, gives rise to the correct dynamics. In addition, the fast dynamics can be simulated using a stochastic algorithm that bypasses the computation of the wave functions.

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MS7

Shock Trace Prediction by Reduced Models for a Viscous Stochastic Burgers Equation

Viscous shocks are a particular type of extreme events in nonlinear multiscale systems, and their representation requires small scales. Model reduction can thus play an important role in reducing the computational cost for an efficient prediction of shocks. Yet, reduced models typically aim to approximate large-scale dominating dynamics, which do not resolve the small scales by design. To resolve this representation barrier, we introduce a new qualitative characterization of the space-time locations of shocks, named as the shock trace, via a space-time indicator function based on an empirical resolution-adaptive threshold. Different from the exact shocks, the shock traces can be captured within the representation capacity of the large scales, which facilitates the forecast of the timing and locations of the shocks utilizing reduced models. Within the context of a viscous stochastic Burgers equation, we show that a data-driven reduced model, in the form of nonlinear autoregression (NAR) time series models, can accurately predict the random shock traces, with relatively low rates of false predictions. The NAR model significantly outperforms the corresponding Galerkin truncated model in the scenario of either noiseless or noisy observations. The results illustrate the importance of the data-driven closure terms in the NAR model, which account for the effects of the unresolved small scale dynamics on the resolved ones due to nonlinear interactions.

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MS7

Optimal Renormalization of Multiscale Systems

While model order reduction is a promising approach in dealing with multi-scale time-dependent systems that are too large or too expensive to simulate for long times, the resulting reduced order models can suffer from instabilities. We have recently developed a time-dependent renormalization approach to stabilize such reduced models. In the current work, we extend this framework by introducing a parameter that controls the time-decay of the memory of such models and optimally select this parameter based on limited fully resolved simulations. First, we demonstrate our framework on the inviscid Burgers equation whose solution develops a finite-time singularity. Our renormalized reduced order models are stable and accurate for long times while using for their calibration only data from a full order simulation before the occurrence of the singularity. Furthermore, we apply this framework to the 3D Euler equations of incompressible fluid flow, where the problem of finite-time singularity formation is still open and where brute force simulation is only feasible for short times. Our approach allows us to obtain a perturbatively renormalizable model which is stable for long times and includes all the complex effects present in the 3D Euler dynamics. We find that, in each application, the renormalization coefficients display algebraic decay with increasing resolution, and that the parameter which controls the time-decay of the memory is problem-dependent.

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MS8

Modeling, Solution and Applications Based on the Brinkman Equation

In this talk, we will firstly introduce a one-domain approach of modeling based on Brinkman to simulate the fluid flow over a porous medium. Then we apply the one-domain approach of modeling in fluid topology optimization. A threshold dynamics method will be introduced and the stability analysis will be shown. Then in order to improve the efficiency of solution of Brinkman equation, the adaptive HDG method for Brinkman equation will be introduced and extended to the Brinkman optimal control problem. Numerical results will be provided to validate the analysis.

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MS8

A Local Discontinuous Galerkin Method for Phase Transition Problems

In this presentation, we will discuss an h-adaptive local discontinuous Galerkin(LDG) scheme for the Navier-Stokes-Korteweg (NSK) equations. The NSK equations are used to model the dynamics of a compressible fluid exhibiting phase transitions between a liquid and a vapor phase. To capture the dynamic interface between the two phases accurately, we used the LDG discretization for the NSK equations and a fully time-implicit method. To save computations, local refinement was applied. Recently, we consider the LDG discretization for the non-conservative form of the NSK equations and prove the stability of the numerical discretization. Numerical experiments show the accuracy, efficiency and capabilities of the adaptive LDG discretizations for the NSK equations.

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MS8

Multirate Partially Explicit Scheme for Multiscale

Flow Problems

For time-dependent problems with high-contrast multiscale coefficients, the time step size for explicit methods is affected by the magnitude of the coefficient parameter. With a suitable construction of multiscale space, Chung et al (2021) proposed a stable temporal splitting scheme where the time step size is independent of the contrast. Consider the parabolic equation with heterogeneous diffusion parameter, the flow rates vary significantly in different regions due to the high-contrast features of the diffusivity. In this work, we aim to introduce a multirate partially explicit splitting scheme to achieve efficient simulation with the desired accuracy. We first design multiscale subspaces to handle flow with different speeds. For the fast flow, we obtain a low-dimensional subspace for the high-diffusive component and adopt an implicit time discretization scheme. The other multiscale subspace will take care of the slow flow, and the corresponding degrees of freedom are treated explicitly. Then a multirate time stepping is introduced for the two parts. The stability of the multirate methods is analyzed for the partially explicit scheme. Moreover, we derive local error estimators corresponding to the two components of the solutions and provide an upper bound of the errors. An adaptive local temporal refinement framework is then proposed to achieve higher computational efficiency. Several numerical tests are presented to demonstrate the performance of the proposed method.

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MS8

Staggered DG Methods for Darcy Flows in Fractured Porous Media

In this talk, we will present a staggered DG method of arbitrary polynomial orders for Darcy flows in fractured porous media on general meshes. A staggered DG method and a standard conforming finite element method with appropriate inclusion of interface conditions will be employed to discretize the bulk region and the fracture, respectively. In particular, the analysis weakens the usual assumption imposed on polygonal meshes, indeed, elements with arbitrarily small edges are allowed. The optimal convergence error estimates for all the variables are proved. Our error estimates are shown to be robust with respect to the heterogeneity and anisotropy of the permeability coefficients. Several numerical experiments will be presented to verify the performances of the proposed method.

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MS9

The Spectrum of Linear Peridynamic Operators

A characterization for the eigenvalues of linear peridynamic operators is provided. The analysis is presented for state-based peridynamic operators for isotropic homogeneous media in any spatial dimension. We provide explicit formulas for the eigenvalues in terms of the space dimension, the nonlocal parameters, and the material properties. The approach we follow is based on the Fourier multiplier analysis developed for nonlocal Laplace operators. It is shown that the Fourier multipliers of linear peridynamic operators are second-order tensor fields, which are given through integral representations. The eigenvalues of the peridynamic operators can be derived directly from the eigenvalues of the Fourier multiplier tensors. We reveal a simple structure for the Fourier multipliers in terms of hypergeometric functions, which allows for providing integral representations as well as hypergeometric representations for the eigenvalues. These representations are utilized to show the convergence of the eigenvalues of linear peridynamics to the eigenvalues of the Navier operator of linear elasticity in the limit of vanishing nonlocality. Moreover, the hypergeometric representation of the eigenvalues is utilized to compute the spectrum of linear peridynamic operators.

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MS9

Fractional Hardy-Type and Trace Theorems for Nonlocal Function Spaces with Heterogeneous Localization

I will present a recent work on the mathematical analysis of a nonlocal equation with variable horizon satisfying a conventional Dirichlet boundary condition. The integral equation is characterized by a nonlocal interaction kernel defined heterogeneously with a special localization feature on the boundary. The associated energy defines a function space that allows functions to be as rough as a measurable integrable function inside the domain but as smooth as a differentiable function near the boundary. As a consequence, we can prove trace theorems as well as a Hardy-type inequality which will lead to establishing stability of the energy functional subject to vanishing Dirichlet boundary condition. This is joint work with Q. Du and X. Tian.

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MS9

Operators and Boundary Conditions in Nonlocal

Models

As nonlocal theories have emerged as successful models for studying phenomena and behaviors in different areas of science (continuum mechanics, biology, image processing), mathematical investigations of integral operators and associated systems of equations have been undertaken in several directions. In this talk I will present some recent results on nonlocal frameworks systems based on some existing, as well as newly introduced, nonlocal operators. An in-depth study of properties of the operators includes a series of results on nonlocal versions of integration by parts theorems, Helmholtz-Hodge type decompositions, the role of boundary conditions (both, Dirichlet type and Neumann) in issues of convergence of operators and solutions to their classical equivalents as the interaction horizon vanishes.

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MS9

Analysis of Localized Limits of Nonlocal Energies Motivated by Peridynamics

We investigate properties of minimizers for a class of nonlocal nonconvex functionals that arise in peridynamics as well as the persistence of these properties in minimizers of the localized limit. We demonstrate geometric rigidity in the spirit of Reshetnyak for these nonlocal nonconvex functionals. This rigidity result states that any minimizing convergent sequence must converge to an affine map with gradient in the set of rotations. However, this result does not hold for any corresponding localized energy obtained from the vanishing horizon limit. In the topology of uniform convergence, the zero-set of the localized functional is infinite-dimensional, and includes non-affine maps. In the topology of Γ-convergence, we prove an integral representation for the localized Γ-limit. We then employ convex integration techniques to show that the localized strain energy density vanishes for any "short map;" that is, any deformation tensor with principal strains less than or equal to 1. These relaxation phenomena further quantify the discrepancy between classical nonlinear hyperelastic stored energy functionals and functionals obtained from the localized limit of nonlinear bond-based peridynamics.

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MS10

Signature Moments to Characterize Laws of Stochastic Processes

The normalized sequence of moments characterizes the law of any finite-dimensional random variable. In this talk, I will describe an extension of this result to path-valued random variables, i.e. stochastic processes, by using the normalized sequence of signature moments. I will show how these moments define a metric for laws of stochastic processes. This metric can be efficiently estimated from finite samples, even if the stochastic processes themselves evolve in high-dimensional state spaces. As an application, I will describe a non-parametric two-sample hypothesis test for laws of stochastic processes. Based on joint work with Harald Oberhauser.

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MS10

Signatures and Functional It Calculus

European option payoffs can be generated by combinations of hockeystick payoffs or of monomials. Interestingly, path dependent options can be generated by combinations of signatures, which are the building blocks of path dependence. We focus on the case of 1 asset together with time, typically the evolution of the price x as a function of the time t. The signature of a path for a given word with letters in the alphabet t,x (sometimes called augmented signature of dimension 1) is an iterated Stratonovich integral with respect to the letters of the word and it plays the role of a monomial in a Taylor expansion. For a given time horizon T the signature elements associated to short words are contained in the linear space generated by the signature elements associated to longer words and we construct an incremental basis of signature elements. It allows writing a smooth path dependent payoff as a converging series of signature elements, a result stronger than the density property of signature elements from the Stone-Weierstrass theorem. We recall the main concepts of the Functional It Calculus, a natural framework to model path dependence and draw links between two approximation results, the Taylor expansion and the Wiener chaos decomposition. The Taylor expansion is obtained by iterating the functional Stratonovich formula whilst the Wiener chaos decomposition is obtained by iterating the functional It formula applied to a conditional expectation.

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MS10

The Signature-Based Generative Models for Financial Time Series

Generative adversarial networks (GANs) have been extremely successful in generating samples, from seemingly high dimensional probability measures. However, these methods struggle to capture the temporal dependence of joint probability distributions induced by time-series data. To overcome these challenges, motivated by the autoregressive models in econometric, we are interested in the conditional distribution of future time series given the past information. In this talk, I will present the generic conditional Sig-WGAN framework by integrating Wasserstein-GANs (WGANs) with mathematically principled and efficient path feature extraction called the signature of a path. In particular, we develop conditional Sig-W_1, that captures the conditional joint law of time series models, and use it as a discriminator. The signature feature space enables the explicit representation of the proposed discriminators which alleviates the need for expensive training. We validate the efficacy of our method on both synthetic and empirical datasets.

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MS10

Randomized Signatures: Proofs, Properties and Applications

Randomized Signature is almost as expressive as signature along one path or on path space, but calculated in a different way. Inspiration stems from reservoir computing, where dynamical systems with random characteristics are applied to approximate generic dynamics. There are several ways how to understand its properties: via Johnson-Lindenstrauss projections of high dimensional dynamics, via representations of free algebras in random vector fields, or via path separation properties. In contrast to signatures randomized signatures can be designed to allow for long term approximations via ergodicity properties. (Joint work with Christa Cuchiero, Lukas Gonon, Lyudmila Grigoryeva, Juan-Pablo Ortega).

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MS11

Optimal Fenestration of the Fontan Circulation

Single ventricle physiologies are congenital heart disorders in which only one side of the heart is properly functioning. Mathematical models can be used to simulate the properties of these physiologies and provide useful information regarding how to treat them. Using zero dimensional blood flow equations, we developed a pulsatile compartmental model of the Fontan circulation to explore the effects of a fenestration added to this physiology. A fenestration is a shunt between the systemic and pulmonary veins that is surgically incorporated either at the time of Fontan conversion or at a later time for the treatment of complications. This shunt increases cardiac output and decreases systemic venous pressure. However, these hemodynamic benefits are achieved at the expense of a decrease in the arterial oxygen saturation. The model developed in this paper incorporates fenestration size as a parameter and describes both blood flow and oxygen transport. It is calibrated to clinical data from Fontan patients, and we use it to study the impact of a fenestration on several hemodynamic variables. In certain scenarios corresponding to high-risk Fontan physiology, we demonstrate the existence of an optimal fenestration size that maximizes oxygen delivery to the systemic tissues. Faculty Advisors: Daniel Penny, Department of Pediatrics, Section of Cardiology, Baylor College of Medicine and Texas Childrens Hospital, penny@bcm.edu; Craig Rusin, Department of Pediatrics, Section of Cardiology, Baylor College of Medicine and Texas Childrens Hospital, crusin@bcm.edu; Charles Peskin, New York University, peskin@cims.nyu.edu; Charles Puelz, Department of Pediatrics, Section of Cardiology, Baylor College of Medicine and Texas Childrens Hospital, charles.puelz@bcm.edu

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MS11

Ensemble Neural Networks

Machine learning has become a common tool within the tech industry due to its high versatility and efficiency with large datasets. Partnering with the Nevada National Security Site, our goal is to improve accuracy of machine predictions by utilizing deep learning, which will enable the power and accuracy of a prediction to grow from the model. To build a deep learning model, multiple neural network architectures were developed and combined to create an ensemble neural network. The projects objective is to determine the comparative differences between the efficiency of the ensemble neural network versus each individual neural network. The data set used to validate and train the networks is 1D regressive/categorical. After testing architecture and determining accuracy of certain networks, the model was updated and tested again to increase accuracy. As model precision is a key aspect of machine learning, emphasis is placed on the efficiency of ensemble neural networks to make valid predictions. Faculty Advisors: Mihhail Berezovski, Embry Riddle Aeronautical University, berezovm@erau.edu

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MS11

Enabling Scalability of Virtual Reality Computational Neuroscience Simulations

My research focused on further developing the Neuro-VISOR software. Neuro-VISOR is a virtual reality real-time interactive simulation of neuron electrical transmissions. Neurons interact in complex networks in the brain, so any simulation must be able to handle a large number of neurons interacting. The defining feature of Neuro-VISOR is its ability to be used in real-time which requires stringent performance requirements. Before my research, only two neurons could be run simultaneously within these restraints. The first step was to conduct a systematic comparison of the softwares computational limits. The key findings were that the CPU was the main performance bottleneck and the computational draw of each component. Based on that study I determined the optimal method of improving performance without loss of capabilities was decoupling the visualization from the numerical analysis, increasing the thread utilization, and decreasing the main thread load. The study revealed that these areas caused the largest draw as the number of neurons increased. Subsequent performance tests revealed that these

modifications enabled the desired scalability and resulted in a substantial performance increase. There was a reduction of more than 50% in time per frame for a single neuron. Eight times as many neurons could be run simultaneously while maintaining real-time functionality. Faculty Advisors: Benjamin Seibold, Temple University, seibold@temple.edu; Gillian Queisser, Temple University, gillian.queisser@temple.edu

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MS11

A Tensor SVD-based Classification Algorithm Applied to fMRI Data

To analyze the abundance of multidimensional data, tensor-based frameworks have been developed. Traditionally, the matrix singular value decomposition (SVD) is used to extract the most dominant features from a matrix containing the vectorized data. While the SVD is highly useful for data that can be appropriately represented as a matrix, this step of vectorization causes us to lose the high-dimensional relationships intrinsic to the data. To facilitate efficient multidimensional feature extraction, we utilize a projection-based classification algorithm using the t-SVDM, a tensor analog of the matrix SVD. Our work extends the t-SVDM framework and the classification algorithm, both initially proposed for tensors of order 3, to any number of dimensions. We then apply this algorithm to a classification task using the StarPlus fMRI dataset. Our numerical experiments demonstrate that there exists a superior tensor-based approach to fMRI classification than the best possible equivalent matrix-based approach. Our results illustrate the advantages of our chosen tensor framework, provide insight into beneficial choices of parameters, and could be further developed for classification of more complex imaging data. Faculty Advisors: Elizabeth Newman, Emory University, elizabeth.newman@emory.edu

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MS11

Numerical Methods for Simulating Protein Chromatography

The demand for protein therapeutics, which have been used to treat and manage chronic conditions, has increased dramatically over the last few decades. Current techniques for separating and purifying protein therapies are insufficient for this increasing demand. This report investigates methods to improve membrane chromatography, a method for separating and purifying proteins. Improved methods must increase efficiency while maintaining the purity of the final product. To mathematically model the membrane chromatography process, we solved the nonlinear Reactive Transport Equation with Finite Difference Methods. Using MATLAB, we compared two explicit solution methods, Forward Euler and Improved Euler, to assess which approach was more effective in simulating the membrane chromatography process. We compared our simulated data with previously-obtained experimental data to make this assessment. With our simulations, we verified our ability to model and test the efficiency and resolution separation of the chromatography model. With our findings, we can update the membrane chromatography process for higher efficiency. Faculty Advisors: Anastasia Wilson, Augusta University, anawilson@augusta.edu

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MS12

Decentralized Payment Clearing on a Blockchain

In this talk, we construct a decentralized clearing mechanism which endogenously and automatically provides a claims resolution procedure. This mechanism can be used to clear a network of obligations through blockchain. In particular, we investigate default contagion in a network of smart contracts cleared through blockchain. In so doing, we provide an algorithm which constructs the blockchain so as to guarantee the payments can be verified and the miners earn a fee. We, additionally, consider the special case in which the blocks have unbounded capacity to provide a simple equilibrium clearing condition for the terminal net worths; existence and uniqueness are proven for this system. Finally, we consider the optimal bidding strategies for each firm in the network so that all firms are utility maximizers with respect to their terminal wealths. We first look for a mixed Nash equilibrium bidding strategies, and then also consider Pareto optimal bidding strategies.

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MS12

Credit Freezes, Equilibrium Multiplicity and Optimal Bailouts in Financial Networks

We analyze how interdependencies in financial networks can lead to self-fulfilling insolvencies and multiple possible equilibrium outcomes. We show that multiplicity arises if and only if there exists a certain type of dependency cycle in the network, and characterize banks' solvency in any equilibrium. We use this analysis to understand how to inject capital into banks so as to ensure solvency of all at minimum cost. We show that finding the cheapest bailout policy that prevents self-fulfilling insolvencies is computationally hard (and hard to approximate), but that the problem has intuitive solutions in specific network structures. Bailouts have an indirect value as making a bank solvent improves its creditors' balance-sheets and reduces their bailout costs, and we show how a simple algorithm that leverages these indirect benefits ensures systemic solvency at a total cost that never exceeds half of the to-

tal overall shortfall. In core-periphery networks, indirect bailoutswhereby the regulator bails out peripheral banks first as opposed to targeting core banks directlyare optimal.

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MS12

Dynamic Contagion Modelling in a Generalized Black-Cox Framework

In this talk we will look at a simple model of solvency contagion in a financial system where institutions take into account the probability of counterparties defaulting on their obligations before the terminal time. That is, we look at the impact of marking to market the interbank liabilities. The model can be seen as a generalization of the classical Black-Cox framework, which leads naturally to an interesting comparison with this no-contagion benchmark. As time allows, we will discuss the impact of systemic risk on the term structure, by looking at multiple maturities for the interbank liabilities.

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MS12

Systemic Risk in Markets with Multiple Central Counterparties

We provide a quantitative framework for modelling risk and quantifying payment shortfalls in cleared markets with multiple central counterparties (CCPs). Building on the stylised fact that clearing membership is shared among CCPs, we show that stress in this shared membership can transmit across markets through multiple CCPs. We provide stylised examples to lay out how this stress transmission can take place, as well as empirical evidence to illustrate that the mechanisms we study could be relevant in practice. Furthermore, we show how stress mitigation mechanisms such as variation margin gains haircutting by one CCP can have spill-over effects to other CCPs. Finally, we discuss how the framework can be used to enhance CCP stress testing. The current Cover 2' standard requires CCPs to be able to withstand the default of their two largest clearing members. We show that who these two clearing members are can be significantly affected by higher-order effects arising from interconnectedness through shared membership.

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MS13

Reaction Networks, Toric Differential Inclusions, and the Global Attractor Conjecture

Key properties of reaction network models (such as polynomial dynamical systems given by mass-action kinetics) are closely related to fundamental results about global stability in classical thermodynamics. For example, the Global Attractor Conjecture can be regarded as a finite dimensional version of Boltzmanns H-theorem. We will discuss some of these connections, and we will focus especially on introducing toric differential inclusions as a tool for proving the Global Attractor Conjecture.

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MS13

Analyzing Steady States of Mass Action Systems Through Network Splitting

The process of network translation corresponds a mass action system to a generalized mass action system with equivalent dynamics. Recent research has shown that, when the generalized chemical reaction network underlying the second network has desirable structure, such as weak reversibility and low deficiency, then we may use the network to establish properties of the steady state set and to explicitly construct a steady state parametrization. In this talk, we will extend this theory by introducing the method of "splitting" networks. In a split network, we allow the original network to be partitioned into subnetworks, called "slices", while imposing that the union of the subnetworks preserves the stoichiometry of the original network. We show that this process expands the scope of mass action systems whose steady states can be characterized by the method of network translation.

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MS13

Dynamic Absolute Concentration Robustness in Biochemical Networks

Biochemical reaction networks, such as the bacterial two-component signaling systems, maintain robustness in their output against a high degree of variation in the protein numbers that constitute the signaling circuit. We discuss the underlying network structure that is necessary for such robustness. Specifically, we define dynamic absolute concentration robustness (dynamic ACR), a property that is related to global system dynamics. A species in a biochemical reaction network has dynamic ACR if its concentration converges to the same positive value independent of the initial conditions and also independent of the dynamics of the other species concentrations. We will discuss structural properties of dynamic ACR networks as well as implications of having this property.

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MS13

Geometry of Embedded Reaction Networks and

Toric Structure

In complex-balanced systems, the toric structure is closely related to the geometry of the reaction network, through its deficiency. Geometrically, deficiency measures the linear dependence of reaction vectors; deficiency zero being the case of the network maximally spanning (as an embedded object in $\mathbb{R}^n$). Algebraically, deficiency is the number of algebraically independent constraints on the rate constants necessary for the system to be complex-balanced. These constraints, written in terms of the Kirchoff tree constants, are binomial. In this talk, we look deeper at the geometry of a network and its algebraic implication. In particular, from the geometry of the network we give a simple derivation of the binomial conditions for complex-balancing.

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MS14

Quasistatic Evolution Problems for Models of Geomaterials Coupling Plasticity and Damage

I will discuss recent results about existence of quasistatic evolutions for a model proposed by Kazymyrenko and Marigo in 2019, which uses a suitable coupling between plasticity and damage to study the behavior of geomaterials under compression. The techniques employed for the proofs borrow something both from previous analysis of other plasticity-damage models and from the study of free discontinuity problems in elasticity.

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MS14

Optimal Reconstruction of the Material Response Spectrum from Noisy Measurements

Effective moduli of composites as a function of the properties of constituent materials can be expressed in terms of complex analytic functions of Stieltjes class. The same is true of the complex dielectric permittivity of materials as a function of frequency. In fact, any passive, linear, time-invariant system can be described by an analytic function in the Stieltjes class. The problem of optimal reconstruction of such functions and their spectral measures from a few noisy measurements is therefore one of the fundamental problems in many areas of material science. This leads to a class of quadratic variational problems, where the minimization is over a convex cone, whose geometry is responsible for effective ill-posedness. In this talk I will present an algorithm that harnesses the special geometry of the cone of admissible functions and delivers the minimizer with a certificate of its optimality.

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MS14

Existence of Solutions Past Collisions in Nonlinear Viscoelastodynamics

In this talk, we will consider the time evolution of a viscoelastic solid within a framework that allows for collisions and self-contact. In the static and quasi-static regimes, corresponding existence results have been shown through variational descriptions of the problem. For the fully dynamical case, however, collisions have so far either been ignored or handled using a simplified model, e.g. repulsive terms. In contrast to this, using a newly developed variational technique for general PDEs of similar type, we are able to prove the existence of solutions for arbitrary times and observe some interesting effects due to the instantaneous change of local momentum at the first instance of contact.

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MS14

A Derivation of Linear Elasticity from Finite Elasticity for All Traction Forces

In this talk I will discuss the rigorous derivation of linear elasticity as the low energy limit of pure traction nonlinear elasticity. Unlike previous results, no restrictive assumptions on the forces are imposed and a full Gamma-convergence result is proved. The analysis relies on identifying the correct reference configuration around which we linearize, and studying its relation to the optimal rotations preferred by the forces. The Gamma-limit is the standard linear elasticity model, plus a term penalizing the fluctuations of the reference configurations from the optimal rotations. However, on minimizers this additional term is zero and the limit energy reduces to standard linear elasticity.

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MS15

Hamilton Paths in Domination Reconfiguration Graphs

Given a problem and a set of feasible solutions to that problem, the associated *reconfiguration problem* involves determining whether one feasible solution can be transformed to a different feasible solution through a sequence of allowable moves, with the condition that the intermediate stages are also feasible solutions. Any reconfiguration problem can be modelled with a *reconfiguration graph*, where the vertices represent the feasible solutions and two vertices are adjacent if and only if the corresponding feasible solutions can be transformed to each other via *one* allowable move. Our interest is in reconfiguring dominating sets of graphs. The *domination reconfiguration graph* of a graph G, denoted $\mathcal{D}(G)$, has a vertex corresponding to each dominating set of G and two vertices of $\mathcal{D}(G)$ are adjacent if and only if the corresponding dominating sets differ by the deletion or addition of a single vertex. We are interested in properties of domination reconfiguration graphs. For example, it is easy to see that they are always connected and bipartite. While none has a Hamilton cycle, we explore families of graphs whose reconfiguration graphs have Hamilton paths.

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MS15

Interesting Open Problems in Saturation Theory

Given a family of (hyper)graphs $\mathcal{F}$ a (hyper)graph G is said to be $\mathcal{F}$-saturated if G is $\mathcal{F}$-free for every but for any edge e in the complement of G the (hyper)graph $G + e$ contains some $F \in \mathcal{F}$. This talk will mention several open problems about saturated graphs.

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MS15

Many Cliques in Bounded-Degree Hypergraphs

In the past few years there has been substantial progress on two related problems: determining the maximum number of cliques in graphs of bounded degree, using either vertices or edges as a resource. In this talk I will discuss recent work about generalizing to hypergraphs.

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MS15

Graphs, Codes, and Compressed Sensing

The Interval-passing algorithm (IPA) used in compressed sensing is an iterative process that is used to recover a k-sparse signal $\mathbf{x} \in \mathbb{R}^n$ from a linear measurement vector $\mathbf{y}$ where $\mathbf{y} = M\mathbf{x}$. The matrix M is called the measurement matrix. Similar to the iterative decoder used in decoding low-density parity-check (LDPC) codes, the IPA may be modeled by a bipartite graph called a Tanner graph. Yakimenka and Rosnes showed that graphical substructures called termatiko sets characterize when the IPA fails. In this talk, we present new results on the structure of different types of termatiko sets that exist in the graphs corresponding to certain classes of measurement matrices. This work gives new insight to designing good graphs (and corresponding measurement matrices) for compressed sensing.

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MS16

A Fast Solver for Linear Systems with Tensor Product Structure via Low-Rank Updates

In this talk we consider the numerical solution of linear systems with a tensor product structure of the form

$$(A_1 \otimes I \otimes \cdots \otimes I + \cdots + I \otimes \ldots I \otimes A_d)\, x = b,$$

where the matrices $A_i \in \mathbb{C}^{n \times n}$ are positive definite and belong to the class of hierarchically semiseparable matrices (HSS). Such linear systems arise in the discretization of Laplace-type differential equations on tensorized grids and in the dimensionality reduction of linear dynamical control systems. We propose and analyze a divide-and-conquer scheme based on the technology of low-rank updates that attains the computational cost $\mathcal{O}(n^d \log(n))$ that is quasi-optimal in the case of unstructured right-hand-sides. In

the case $d = 2$, we show how the presence of hierarchical low-rank structure in b can be exploited to further reduce the complexity to $\mathcal{O}(S\log(n))$ where $\mathcal{O}(S)$ indicates the storage cost of b.

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MS16

Rapid Construction of Hierarchical Low Rank Representation via Data Reduction

In this talk, we present a linear complexity sampling based method for H2 matrix construction. Compared with existing method, the new method can deal with kernel functions arising from solving integral equations as well machine learning applications. We will demonstrate the improved performance of the proposed methods with existing methods on a wide range of kernel functions in terms of the accuracy and computational time.

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MS16

Kernel-Independent Low-Rank Approximations with Applications

We analyze a kernel-independent low-rank approximation method for some kernel matrices. The method uses some proxy points to directly form relevant basis matrices. We show the approximation errors and a nearly optimal choice of the proxy points. We then show the application of the method to some matrices arising from some PDE discretizations and image processing problems. The matrices may be viewed as kernel matrices with unknown underlying kernels. The kernel-independent low-rank approximation provides a convenient way to quickly get rank-structured approximations. This is joint wok with Mikhail Lepilov.

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MS17

Numerical Algorithms for Principal Agent Problems

We investigate numerical methods for solving continuous-time Principal-Agent (PA) problems in dynamic contract theory. Stochastic control theory yields a system of Hamilton-Jacobi-Bellman PDEs characterizing PA problems - one for the best-response of the Agent given a contract, and a second for the optimal contract to be offered by the Principal. We extend the Deep Galerkin Method, in particular its Policy Iteration variant, to solve such nonlinear systems. Our actor-critic approach builds two neural network approximations – for the Principal's value function and for the Agent's optimal control. Along the way we investigate efficient training designs and adaptive training to improve algorithmic convergence and stability. Among illustrations, we consider settings where the agent has multiple controls, leading to an implicitly-defined HJB equation of the Principal that was hitherto intractable. This is joint work with Zimu Zhu (UCSB).

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MS17

Deep Learning of Free Boundaries

To be added.

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MS17

Exploratory Control Problem: Some Convergence Results

We will discuss the exploratory HamiltonJacobiBellman (HJB) equation arising from the entropy-regularized exploratory control problem, which was formulated in the context of reinforcement learning in continuous time and space. We will discuss the well-posedness and regularity of the viscosity solution to the equation, as well as the convergence of the exploratory control problem to the classical stochastic control problem when the level of exploration decays to zero. We then apply the general results to the exploratory temperature control problem to design an endogenous temperature schedule for simulated annealing (SA) in the context of non-convex optimization.

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MS17

Partial Information and Complete Monotonicity: Theory and Examples

We will discuss the exploratory HamiltonJacobiBellman (HJB) equation arising from the entropy-regularized exploratory control problem, which was formulated in the context of reinforcement learning in continuous time and space. We will discuss the well-posedness and regularity of the viscosity solution to the equation, as well as the convergence of the exploratory control problem to the classical stochastic control problem when the level of exploration decays to zero. We then apply the general results to the exploratory temperature control problem to design an endogenous temperature schedule for simulated annealing (SA) in the context of non-convex optimization.

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MS18

Repulsive Curves and Surfaces

Numerous applications in geometric, visual, and scientific computing rely on the ability to nicely distribute points in

space according to a repulsive potential. In contrast, there has been relatively little work on equidistribution of higher-dimensional geometry like curves and surfaces—which in many contexts must not pass through themselves or each other. This paper develops a numerical framework for optimization of curve and surface geometry while avoiding (self-)collision. The starting point is the tangent-point energy, which effectively pushes apart pairs of points that are close in space but distant along the geometry. We develop a discretization of this energy, and introduce a novel preconditioning scheme based on a fractional Sobolev inner product. We further accelerate this scheme via hierarchical approximation, and describe how to incorporate into a constrained optimization framework. Finally, we explore how this machinery can be applied to problems in mathematical visualization, geometric modeling, and geometry processing.

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MS18

Human-in-the-Loop Design Tools for Metamaterials That Can Move, Walk, Compute

Mechanical metamaterials have been shown to incorporate extreme material properties such as volume change, tunable shock-absorption, or locally varying elasticity. We view metamaterials as devices, rather than materials, and explore materials that can receive input from their environment, process that information and produce output or reconfigure themselves. During our investigation of parts of these metamaterial devices, we created structures that embed functionality such as robotic movement, performing computations, or context-dependent material transformation. These structures were often aperiodic, heterogenous and therefore difficult to design. We argue that to accelerate structure discovery, we need efficient tools for their exploration. While data-driven approaches can help find new structures, they require pre-defined objectives and are only a partial solution. To discover structures that are further away from the currently known ones, we involve humans and provide them with fast and simple exploration tools. This enables experts to apply their intuition and novice users to contribute their mass creativity to discover functional structures. The breadth of solutions can create a larger database of cell structures and their properties to provide data for principled characterization enabling deeper insights. Since the design space of metamaterials is virtually infinite, such software tools help foster academic exchange to accelerate the advancement of metamaterials.

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MS18

Continuum Field Theory for the Deformations of Planar Kirigami

Shape-morphing finds widespread utility, from the deployment of small stents and large solar sails to actuation and propulsion in soft robotics. Origami and kirigami–patterns of cuts and folds in a sheet–are versatile platforms for shape-morphing, inspiring the design of many morphing structures and devices. However, it remains a challenge to predict their response to a broad range of loads and stimuli. This talk explores general modeling principles for kirigami structures. We describe a coarse-graining procedure to determine all the slighty stressed (soft) modes of deformation of a large class of periodic and planar kirigami. The procedure gives a system of nonlinear partial differential equations (PDE) expressing geometric compatibility of angle functions related to the motion of individual slits. Leveraging known solutions of the PDE and FEM modeling, we present illuminating agreement between simulations and experiments across kirigami designs. Our results reveal a dichotomy of designs that deform with persistent versus decaying slit actuation, which we explain using the Poissons ratio of the unit cell.

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MS18

Collision-Induced Phase Transformations in Mechanical Metamaterials

Flexible mechanical metamaterials are compliant structures designed to achieve desired mechanical properties via large deformation or rotation of their components. While their static properties (such as Poissons ratio) have been studied extensively, much less work has been done on their dynamic properties, especially nonlinear dynamic properties induced by large movement of internal components. Here, we examine the nonlinear dynamic response arising from impact loading of mechanical materials that consist of 1D and 2D arrangements of rotating squares, which leads to formation of solitons. Permanent magnets are added to the squares, which causes the metamaterial to become multistable. Rotations of the squares can thereby lead to sudden rearrangements of squares into new phases. We experimentally and numerically characterize the collisions of solitons in these flexible mechanical metamaterials, which, depending on their amplitude and chirality, can induce a variety of responses, including phase transitions.

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MS19

Machine Learning Based Non-Newtonian Fluid Model with Molecular Fidelity

A long-standing problem in the modeling of non-Newtonian hydrodynamics of polymeric flows is the availability of reliable and interpretable hydrodynamic models that faithfully encode the underlying micro-scale polymer dynamics. The main complication arises from the long polymer relaxation time, the complex molecular structure, and heterogeneous interaction. We developed a deep learning-based non-Newtonian hydrodynamic model, DeePN^2, that enables us to systematically pass the micro-scale structural mechanics information to the macro-scale hydrodynamics for polymer suspensions. The model retains a multi-scaled nature with clear physical interpretation, and strictly preserves the frame-indifference constraints. We show that DeePN^2 can faithfully capture the broadly overlooked viscoelastic differences arising from the specific molecular structural mechanics without human intervention.

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MS19

A Data-Informed Mean-Field Approach to Mapping of Cortical Parameter Landscapes

Neuronal circuitry in the cerebral cortex are characterized by a high degree of structural and dynamical complexity, and this biological reality is reflected in the large number of parameters in cortical models. A fundamental task of computational neuroscience is to understand how these parameters govern network dynamics. While some neuronal parameters can be measured in vivo, many remain poorly constrained due to limitations of available experimental techniques. Computational models can address this problem by relating difficult-to-measure parameters to observable quantities, but to do so one must overcome two challenges: (1) the computational expense of mapping a high dimensional parameter space, and (2) extracting biological insights from such a map. In this talk, I will report on a recently proposed approach to address these challenges. The proposal is based on a parsimonious data-informed algorithm that efficiently predicts spontaneous cortical activity, thereby speeding up the mapping of parameter landscapes. Time permitting, I will also discuss how lateral inhibition provides a basis for conceptualizing cortical parameter space, enabling us to begin to make sense of its geometric structure and attendant scaling relations. The approach is illustrated on a biologically realistic model of the monkey primary visual cortex.

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MS19

The Approximation of Fokker-Planck Equations Using Deep Learning and Adaptive Sampling

In this work, we present an adaptive deep density approximation strategy based on KRnet (ADDA-KR) for solving the steady-state Fokker-Planck (F-P) equations. F-P equations are usually high-dimensional and defined on an unbounded domain, which limits the application of traditional grid-based numerical methods. With the Knothe-Rosenblatt rearrangement, our newly proposed flow-based generative model, called KRnet, provides a family of probability density functions to serve as effective solution candidates for the Fokker-Planck equations, which has a weaker dependence on dimensionality than traditional computational approaches and can efficiently estimate general high-dimensional density functions. To obtain effective stochastic collocation points for the approximation of the F-P equation, we develop an adaptive sampling procedure, where samples are generated iteratively using the approximate density function at each iteration. We present a general framework of ADDA-KR, validate its accuracy and demonstrate its efficiency with numerical experiments.

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MS20

Numerical Solver for the Boltzmann Equation with Self-Adaptive Collision Operators

In the numerical solver of the Boltzmann equation, the collision term is the most expensive part due to its binary integral form. To reduce the computational cost, we build a sequence of modeling collision operators that separate the distribution function into a low-frequency part and a high-frequency part and treat the high-frequency part only linearly as our simplification. The idea of such simplification can be considered as extensions of classical BGK and Shakhov models, and it requires a parameter controlling the ratio of the low-frequency part and the high-frequency part. In our work, this parameter is selected adaptively on every grid cell at every time step. This self-adaptation is based on an error indicator describing the difference between the model collision term and the original binary collision term. The indicator is derived by controlling the quadratic terms in the modeling error with linear operators. Our numerical experiments show that such an error indicator is effective and computationally affordable.

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MS20

Neural-Network Based Collision Operators for the Boltzmann Equation

Kinetic gas dynamics in rarefied and moderate-density regimes have complex behavior associated with collisional processes. These processes are generally defined by convolution integrals over a high-dimensional space (as in the Boltzmann operator), or require evaluating complex auxiliary variables (as in Rosenbluth potentials in Fokker-Planck operators) that are challenging to implement and computationally expensive to evaluate. In this work, we develop a data-driven neural network model that augments a simple and inexpensive BGK collision operator with a machine-learned correction term, which improves the fidelity of the simple operator with a small overhead to overall runtime.The composite collision operator has a tunable fidelity and, in this work, is trained using and tested against a direct-simulation Monte-Carlo (DSMC) collision operator.

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MS20

Data-Driven, Structure-Preserving Approximations to Entropy-Based Moment Closures for Kinetic Equations

Moment models approximate the kinetic equations by tracking the evolution of a small number moments of the kinetic distribution. The behavior of these models depends heavily on the moment closure, which prescribes the kinetic information that is lost in the moment approach. Entropy-based moment closures inherit many structural features of kinetic equations, while their use is limited by several implementation challenges. In this talk, I will present a data-driven approach to construct entropy-based closures. The proposed closure learns the entropy function by fitting the map between the moments and the entropy of the moment system, and thus does not depend on the space-time discretization of the moment system and specific problem configurations such as initial and boundary conditions. With convex and approximations, this data-driven closure inherits several structural properties from entropy-based closures, such as entropy dissipation, hyperbolicity, and H-Theorem. We illustrate this approach for a simple linear transport equation in slab geometry. For two-moment models, a convex fit can be constructed with splines. For larger systems, convex splines are not available, so we resort to a fit that uses a neural network. We test the approximation on two- and three- moment systems and find that the resulting systems provide a cheaper alternative to standard entropy-based closures.

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MS20

Hyperbolic Quadrature Method of Moments for Kinetic-Based Flow Models

For applications such as rarefied gas dynamics or disperse multiphase flows, there is an interest in developing moment methods from a kinetic description of the gas or the disperse particle phase since such methods can be computationally efficient. The HyQMOM closure is defined based on the properties of the monic orthogonal polynomials Qn that are uniquely defined by the velocity moments up to order 2n - 1. Thus, HyQMOM is strictly a moment closure and does not rely on the reconstruction of a velocity distribution function with the same moments. Moreover, one can show the hyperbolicity of the corresponding system, and the good behavior of the eigenvalues when the moment vector tends to the boundary of the moment space, a property that can be important for applications such as multiphase flows. An efficient algorithm for computing the moment of order 2n + 1 from the moments up to order 2n is developed, based on the Chebyshev algorithm. The analytical solution to a 1-D Riemann problem is used to demonstrate convergence of the HyQMOM closure with increasing n. As time allows the extension to 2-D and 3-D kinetic equations will be discussed.

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MS21

Computing Committors in Collective Variables via Mahalanobis Diffusion Maps

Many interesting problems concerned with rare event quantification arise in chemical physics. A typical problem is that of finding reaction channels and transition rates for conformal changes in a biomolecule. To reduce the dimensionality and make the description of transition processes more comprehensible, often a set of physically motivated collective variables (dihedral angles, distances between particular pairs of key atoms, etc.) is introduced by means of mapping atomic coordinates to a low-dimensional space and averaging. The dynamics in collective variables remain time-reversible but acquire an anisotropic and position-dependent diffusion tensor. In this talk, I will discuss how one can adapt the diffusion map algorithm with the Mahalanobis kernel to approximate the generator of this diffusion process and use it to compute the committor function, the reactive current, and the transition rate. Applications to alanine-dipeptide and Lennard-Jones-7 in 2D will be presented.

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MS21

Prediction of Error Bars for Energy Barriers in Fusion Materials

Fusion materials are exposed to harsh conditions due to direct contact with the plasma, suffering degradation and limitation of its lifetime. The trapping of plasma components on the surface is one of the major problems faced, and yet its mechanism is still unknown. Elucidation of those can give key clues for the development of new more resilient materials. Molecular dynamics is a powerful method to study such phenomena, but there is a current lack of potentials to describe these specific interactions. Moreover, the models have to correctly capture the kinetics for those events. It is then important to have the ability to establish confidence on those predictions when considering model candidates. Because trapping and detrapping are rare events that typically involve crossing an energy barrier, a first feedback would be to give error bars for energy barrier predictions. In this work we present a method to predict error barriers for energy barriers where the errors on energy per atom is modeled as a Gaussian process. Preliminary results are presented using the spectral neighbor analysis potential (SNAP) over published data sets. This work is part of an effort to develop new potentials that correctly predicts log time scale properties for fusion materials.

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MS21

Twisted State Transitions in Noise Driven Infinite Dimensional Kuramoto Systems

In the noise free setting, Kuramoto systems are known to possess exact, twisted state, solutions, with stability properties depending on the coupling and range of interaction. By introducing noise, the stable twisted states can become metastable. In this work, the metastability of such states in the infinite dimensional continuum limit will be explored. This includes: results on the convergence of a numerical method for the time dependent problem; numerical experiments revealing transitions between twisted states; and the application of transition path and saddle point search methods to obtain the observed transitions directly. Novel challenges in the analysis are also highlighted.

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MS22

Panel: Open Discussion About LGBTQ Inclusion in the Applied Mathematics Community

This time slot is devoted to an open forum attended by the minisymposium speakers to discuss the intersection of LGBTQ identity and applied mathematics.

To Be Announced
To be announced
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MS22

Pursuit-Evasion Games on Graphs

In pursuit-evasion games, a set of pursuers attempts to locate, eliminate, or contain an evader in a network. The rules, specified from the outset, greatly determine the difficulty of the questions posed above. For example, the evader may be visible, but the pursuers may have limited movement speed, only moving to nearby vertices adjacent to them. Central to pursuit-evasion games is the idea of optimizing certain parameters, whether they are the search number, burning number, or localization number, for example. We report on progress in several pursuit-evasion games on graphs and conjectures arising from their analysis. Finding the values, bounds, and algorithms to compute these graph parameters leads to topics intersecting graph theory, the probabilistic method, and geometry.

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MS22

Neuromechanical Wave Resonance in Fluid Transport

Recent studies have found that there are important biomechanical constraints that arise from the timescales associated with neuromuscular activation and the elastic response of flexible appendages or bodies. In jellyfish, the neuromuscular response is governed by the interaction of pacemakers with the underlying motor nerve net that communicates with the musculature. This set of equally-spaced pacemakers, located at the bell rim, alter their firing frequency in response to environmental cues, allowing for different swimming modes to be activated when sets of pacemakers fire in concert. In this work, we explore the control of neuromuscular activation with a model jellyfish bell immersed in a viscous fluid and use numerical simulations to describe the interplay between active muscle contraction, passive body elasticity, and fluid forces. The fully-coupled fluid structure interaction problem is solved using an adaptive and parallelized version of the immersed boundary method (IBAMR). We then further explore the role of neuromechanical wave resonance in the performance of other fluid transport systems.

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MS23

A Hybrid-Mixed Finite Element Method for Single-Phase Darcy Flow in Fractured Porous Media

We present a hybrid-mixed finite element method for a hybrid-dimensional model of single-phase Darcy flow in a fractured porous media with both conductive and blocking fractures. The conductive fractures are treated using the classical hybrid-dimensional approach of the interface model where pressure is assumed to be continuous across the fracture interfaces, while the blocking fractures are treated using the recent Dirac-δ function approach where normal component of Darcy velocity is assumed to be continuous across the interface. The numerical scheme produces locally conservative velocity approximations and leads to a symmetric positive definite linear system involving pressure degrees of freedom on the mesh skeleton only. As an application, we extend the idea to a simple transport model. The performance of the proposed method is demonstrated by various benchmark test cases in both two- and three-dimensions.

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MS23

Numerical Simulation of Coupled Flow and Geomechanical Process in Fractured Karst Carbonate Reservoirs

In this study, we proposed a coupled flow and geomechanics

model for fractured vuggy carbonate reservoirs. For fluid flow, the multiphase multicomponent model is adopted to handle the complex phase behaviors in fractured vuggy carbonate reservoirs. The multiphase Darcys law is used to describe fluid flow in matrix and fractures, and the multiphase free flow in vugs is reasonably simplified with the assumption of instantaneous gravity segregation. For deformation, the stress equation of fractured vuggy reservoirs is derived by considering the elastic deformation of matrix, nonlinear fracture closure and shear dilation effect, and vug deformation. Then we developed three kinds of gridding techniques to discretize the fractured vuggy porous media with complex geometries to meet the demands of different research problems. The flow and mechanical equations are discretized by using finite volume method and finite element method, respectively. Then the fixed-stress splitting method is used to iteratively solve the coupled flow and geomechanics problem. The hydro-mechanical coupled numerical simulator for fractured vuggy reservoirs is developed, which is verified by a series of examples. Finally, application studies are conducted based on the developed hydro-mechanical coupled simulator.

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MS23

A Reinterpreted Discrete Fracture Model for Fracture and Barrier Networks on Non-Conforming Meshes

In this talk, we introduce the reinterpreted discrete fracture model for the flow simulation of fractured porous media containing both highly conductive fractures and low blocking barriers on non-conforming meshes. The methodology of the approach is to modify the traditional Darcy's law into the hybrid-dimensional Darcy's law where fractures and barriers are represented as Dirac-delta functions contained in the permeability tensor and resistance tensor, respectively. As a natural extension of the classic discrete fracture model for highly conductive fractures, this model is able to account for the influence of both highly conductive fractures and blocking barriers accurately on non-conforming meshes. The local discontinuous Galerkin (LDG) method is employed to accommodate the form of the hybrid-dimensional Darcy's law and the nature of the pressure/flux discontinuity. The good performance of the model is demonstrated by many numerical tests.

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MS23

Second Order in Time Bound-Preserving Implicit Pressure Explicit Concentration Methods for Contaminant Transportation in Porous Media

In this talk, we apply the implicit pressure and explicit concentration (IMPEC) methods for compressible miscible displacements in porous media. The method can yield a much larger time step size compared with the fully explicit method. However, most IMPEC methods are only of first order in time. In this talk, we will discuss how to construct a second order in time IMPEC method. The basic idea is to add the correction stage after each time step. Moreover, we will also construct the bound-preserving technique to preserve the upper and lower bounds of the concentration. Numerical experiments will be given to demonstrate the good performance of the proposed method.

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MS24

Pseudo-Spectral Methods for Peridynamic Models of Diffusion, Fracture, and Corrosion

The most convenient way of finding approximate solutions to peridynamic (PD) models of damage and fracture, for example, is by using the meshfree method in which the integral is approximated by one-point Gaussian quadrature, modified to account for the mismatch between a uniform grid and the circular/spherical shape of the nonlocal (horizon) region integrated over. This numerical method is relatively costly, especially when a large number of nodes is used inside the horizon region, which is often required to achieve high definition for crack/damage patterns. We have recently introduced an alternative numerical method that scales as O(NlogN), where N is the total number of nodes used in the simulation, and has significantly lower memory requirements compared with the meshfree method. This allows us to solve large problems (with tens or hundreds of millions of degrees of freedom) efficiently. In this talk I will present solutions to PD problems in diffusion, fracture, and corrosion damage using this method, which is named the Fast Convolution-Based Method (FCBM) for PD models. I will discuss in detail the use of this method for bond-based, state-based, and correspondence PD models in dynamic brittle fracture in 3D.

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MS24

A Fracture Multiscale Model for Peridynamic Enrichment Within the Partition of Unity Method: Part I

Partition of unity methods are of domain decomposition type and provide the opportunity for multiscale and multiphysics numerical modeling. Different physical models can exist within a partition of unity method scheme for handling problems with zones of linear elasticity and zones where fractures occur. Here, the peridynamic model is used in regions of fracture and smooth partition of unity methods is used in the surrounding linear elastic media. Our method is novel in that we evolve the crack path using peridynamics and apply the partition of unity method to compute the elastic fields in the neighborhood of the crack tip. Earlier work uses the peridynamic fields, e.g.

displacement, at the crack tip to approximate enrichment functions for the partition of unity methods. The method is a so-called global-local enrichment strategy. The elastic fields of the undamaged media provide appropriate boundary data for the localized peridynamic simulations. The geometry of the crack path in the damaged media is transferred to partition of unity method. Here, Heaviside and Westergaard functions are used to model the crack. We do not transfer information of the peridynamic fields to the partition of unity method, solely the crack geometry. The first steps for a combined peridynamic and partition of unity method simulator are presented. We show that the local peridynamic approximation can be utilized to enrich the global partition of unity method approximation to capture the true material response with high accuracy efficiently. Test problems are provided demonstrating the validity and potential of this numerical approach.

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MS24

Peridynamic Modeling of Multilayer Graphene

Graphene sheets can be modeled with an ordinary state-based peridynamic material model that captures the most important mechanical properties of the material. These properties include exceptionally high elastic modulus and strength, negative Poisson ratio, and nonlinear response under large tensile strain. Graphene sheets interact with each other through van der Waals forces that are much weaker than the covalent chemical bonds that are present within each sheet. These weaker forces can be modeled with peridynamic bonds that extend between the sheets. The bending response of films composed of one or more layers can be treated through nonlocal interactions without using a plate or shell theory. All the parameters in the peridynamic material model can be calibrated by the coarse graining of molecular dynamics simulations, resulting in a practical multiscale technique for upscaling the mechanics of multilayer graphene.

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MS24

An Asymptotically Compatible Probabilistic Collocation Method for Randomly Heterogeneous Nonlocal Problems

In this talk, we consider nonlocal problems in heterogeneous media with coefficients depending on finitely many parameters. The parameters are realizations of random variables which could come from a truncated Karhunen-Loeve decomposition of a random field. The analyticity of the parameter to solution map is shown for a class of nonlocal elliptic equations. Spatial discretization of the nonlocal problem is done with an asymptotically compatible meshfree method while a probabilistic collocation method is used for discretization in the random parameter space. We present rigorous analysis for the proposed scheme and demonstrate convergence for a number of benchmark problems, showing the spatial asymptotic compatibility of the scheme and an algebraic or sub-exponential convergence rate in the random coefficients space as the number of collocation points grows. Finally, we validate the applicability of this approach to fracture problems with two theoretical and experimental heterogeneous material damage benchmark problems.

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MS25

Annual Emissions Impact from a 100% Electric Vehicle Adoption

The automotive sector is responsible for 14% of direct and indirect CO2 emissions worldwide. A shift to Electric Vehicles (EVs) is occurring due to their independence from fossil fuels and zero tailpipe emissions at the vehicle level. However, accounting for other sources of emissions resulting from EVs and their use to determine their accurate environmental footprint is lacking. This paper outlines a mathematical model that provides a framework to calculate the wholistic emissions impact in grams (g) of CO2 of a shift from status quo to 100% EVs providing better information on the impacts of EVs across their lifecycle. The model analyzes two aspects; firstly, the paper looks at the average total CO2 emissions resulting from a shift to 100% EVs adoption and divides it by the number of years it takes. This average includes emissions from required infrastructure, internal combustion engine (ICE) car waste, and current gas station infrastructure dismantling. Secondly, the paper determines the average yearly emissions from running EVs over a year. These aspects are combined to give a quantitative value to model the impact on CO2 emissions, including the backlog emissions required to facilitate a 100% EV shift. As facts change, the model seamlessly adjusts for technological innovation, recycling rates, and energy generation sources to provide accurate and informed data. Faculty Advisors: Asia Mathews, Quest University Canada

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MS25

Learning to Sparsify Coarse Grid Operators in Multigrid Methods

In this talk, we propose a machine learning framework for sparsifying coarse grid operators of multigrid methods in order to improve the parallel scalability of multigrid methods. Two neural networks are constructed to learn the sparsity pattern and the corresponding values, respectively. The learned sparser operator has the same interpolation accuracy on algebraic smooth basis. Numerical results on challenging anisotropic rotated Laplacian problems, variable coefficient diffusion problems and linear elasticity problems demonstrate the superior performance of the proposed framework over classical hand-crafted methods. Faculty Advisors: Yuanzhe Xi, Emory University, yuanzhe.xi@emory.edu

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MS25

Optimization of Intermodal Mobility Network Operations: Integrating Public Transit with Mobility-on-Demand and Micromobility

Mobility-on-demand transit is a feasible method of connecting highly integrated urban areas with non-urban regions that are far less networked. Micromobility, or last-mile smaller vehicle solutions such as rentable scooters and bicycles, are good options for linking residential areas with those non-urban regions that mobility-on-demand solutions can service. The integration of mobility-on-demand and micromobility has been interrogated and explored, but little has been done to design an all-encompassing mobility solution that takes into account and joins the three options of micromobility, mobility-on-demand, and public transit in order to form a seamless, efficient, and cost-effective transportation experience from front doorstep to urban center and back. This paper expands on prior research done in the formulation of a profit-maximizing cost function that incorporates mobility-on-demand and micromobility as a stochastic model using poisson processes by integrating public transit networks into the function. I have also created a program that can accept various data that describes a given region and optimize the cost function model for this region. Faculty Advisors: Vijay Gupta, Electrical Engineering Professor, vgupta2@nd.edu

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MS25

Characterizing Material Micro- and Nano- Structure using Machine Learning

Scanning Transmission Electron Microscopy (STEM) is used to analyze different materials or defects within a sample. However, STEM microscopy is a time-consuming process due to material scientists having to visually inspect STEM micrographs while hand labeling specific features and pixels to conduct further analysis such as material structures and molecular properties. Chipping is the process of dividing a STEM micrograph into multiple smaller images to be analyzed and clustered. With the help of machine learning such as Neural Networks and Few-Shot Learning, it may provide new methods of automatically segmenting and analyzing pixels to determine what materials exist within a sample. Creating this new algorithm will help analyze, segment and cluster STEM micrographs pixels at a more efficient rate. We want to combine certain pieces of Convolutional Neural Network and Few-shot learnings architecture to train a model that will be able to cluster and classify pixels based on a small support class. Faculty Advisors: Mihhail Berezovski, Embry-Riddle Aeronautical University, berezovm@erau.edu

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MS25

Fingerprinting Gerrymandering

: Gerrymandering refers to the process of drawing electoral districts to favor a particular political party. As computer technology has improved, access to software for drawing unrepresentative districts with high precision has commensurately grown. In the past 6-10 years particularly, mathematicians have produced computational tools to quantify how badly gerrymandered a district map is, and those are computationally feasible on modern hardware. In our research, we have managed to use North Carolina election data in 2020 to generate 100,000 district maps under the rule to create the baseline using the MGGG groups GerryChain software. For each precinct, we gather which district it was for each map, and call it misplaced in the gerrymandered map if that map puts it in a different district. We are able to compute and assign misplacement scores to individual districts to produce the misplacement score map for North Carolina in 2020. In order to determine whether the map has been diluted, we combine the misplacement score with the efficiency gap which is a standard for measuring partisan gerrymandering. Faculty Advisors: Parker Edwards, Department of Applied and Computational Mathematics and Statistics, University of Notre Dame, pedward2@nd.edu

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MS26

Limit Cycles in Three Species Mass-Action Systems

Rank-two bimolecular reaction networks do not admit limit cycles. In this talk we present a couple of simple examples that do admit limit cycles: we start with rank-two trimolecular networks and then turn to rank-three bimolecular networks.

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MS26

Minimal Invariant Regions and Minimal Globally Attracting Regions for Variable-K Reaction Systems

Constructing minimal invariant and minimal globally attracting regions is crucial for proving properties related to permanence and global stability of reaction systems. We give a construction of the minimal invariant and minimal globally attracting regions for two reversible reactions involving two species, where the rate constants of the reactions are permitted to take values in a compact interval. As a consequence, we obtain invariant regions and globally attracting regions for such systems where the rate constants are fixed to certain values.

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MS26

Graph-Theoretic Models of Detecting Broken Detailed Balance in Molecular Information Processing

The linear framework models biochemical reaction networks under timescale separation using finite directed graphs with labeled edges. Recently, the linear framework has provided a deterministic approach to understanding the thermodynamic properties of biological information processing systems. Detecting broken detailed balance in such contexts poses both an experimental and theoretical challenge. To address this difficulty, several mathematical signatures of broken detailed balance have been suggested. While these signatures can identify nonequilibrium steady states (NESSs), little is known about how they relate to underlying thermodynamic forces. Here we use the linear framework to probe the relationship between thermodynamic force and the Steinberg signature, which detects nonequilibrium activity through the inequality of forward and reverse higher-order autocorrelation functions. We have developed software to calculate the Steinberg signature from arbitrary graphs. We find that when a linear framework graph is perturbed progressively from equilibrium and its force increases from zero, the Steinberg signature reaches its maximum at an intermediate value of force before decaying asymptotically, potentially to zero. This non-monotonic relationship shows the Steinberg signatures limitations as a tool for detecting NESSs. Characterizing the mathematical behavior of such signatures may elucidate how biological systems transition from equilibrium to nonequilibrium steady states.

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MS26

Homeostasis in Mass Action Systems

Homeostasis occurs in a system where the chosen output variable is approximately constant despite changes in an input variable. We build the connection between homeostasis and complex balanced reaction network models. In particular, we show when a reaction network can exhibit homeostasis and complex balanced. Moreover, we find the relation between the perfect homeostasis and ACR in some models. We also provide examples of reaction networks that exhibit homeostasis by analyzing their core networks.

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MS27

Representation of the Total Variation as a Gamma-Limit of BMO-Type Seminorms

I will talk about the proof of a conjecture raised by Ambrosio, Bourgain, Brezis, and Figalli, on the Γ-limit approximation of the total variation by BMO-type seminorms. In this vein, I will also discuss a novel Rellich-type compactness result that stems from the boundedness of these BMO-type seminorms.

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MS27

Gamma-Convergence and Homogenisation of Singularly-Perturbed Elliptic Functionals

In this talk we introduce a general class of singularly-perturbed elliptic functionals and we study their asymptotic behaviour as the perturbation paramter e ¿ 0 vanishes. Namely, we consider functionals of the form

$$F_\epsilon(u,v) := \int_D v^2 f_\epsilon(x,\nabla u)\,dx + \frac{1}{\epsilon}\int_D g_\epsilon(x,v,\epsilon\nabla v)\,dx,$$

??where u is a vector-valued Sobolev function and $v \in [0,1]$ is a phase-field variable. Under mild regularity assumptions on f_ϵ and g_ϵ and suitable super-linear growth conditions, which in particular allow us to bound F_ϵ by the Ambrosio-Tortorelli functionals, we show that the functionals F_ϵ Γ-converge (up to subsequences) to a free-discontinuity functional of brittle type. Moreover, we provide asymptotic formulas for the limiting volume and surface integrands, which show that the volume and surface contributions of F_ϵ decouple in the limit. This decoupling finally allows us to apply the abstract Γ-convergence result to the setting of homogenisation.

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MS27

Large Data Limit of the MBO Scheme for Data Clustering

The MBO scheme is a highly performant algorithm for data clustering. Each iteration of the scheme consists of two simple operations: linear diffusion and pointwise thresholding. The combination of these two operations corresponds to one step of implicit gradient descent for the thresholding energy on the similarity graph of the given dataset. When studying large data sets, it is natural to compare this discrete problem to a continuum problem. In this talk, I will present the first convergence proof of the scheme in the large data limit.

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MS27

Efficient and Exact Multimarginal Optimal Transport with Pairwise Costs

Optimal transport has profound and wide applications since its introduction in 1781 by Monge. Thanks to the Benamou-Brenier formulation, it provides a meaningful functional in the image science like image and shape registrations. However, exact computation through LP or PDE is in general not practical in large scale, while the popular entropy-regularized method introduces additional diffusion noise, deteriorating shapes and boundaries. Until the recent work [Jacobs and Leger, A Fast Approach to Optimal Transport: the back-and-forth method, Numerische Mathematik, 2020], solving OT in a both accurate and fast fashion finally becomes possible. Multiple marginal optimal transport is a natural extension from OT but has its own interest and is in general more computationally expensive. The entropy method suffers from both diffusion noise and high dimensional computational issues. In this work, we extend from two marginals to multiple marginals, on a wide class of cost functions when those marginals have a graph structure. This new method is fast and does not blur images. As a result, the new proposed method can be used in many fields those require sharp boundaries. For example, given a temporal sequence of images on sea ices with partial information, we can recover the underlying dynamics. We will illustrate by examples the faithful joint recover via MMOT of images with sharp boundaries.

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MS28

A Bayesian Machine Learning Advanced Forecast Ensemble Method for Complex Turbulent Systems with Partial Observations

Ensemble forecast based on physics-informed models is one of the most widely used forecast algorithms for complex turbulent systems. A major difficulty in such a method is the model error that is ubiquitous in practice. Data-driven machine learning (ML) forecasts can reduce the model error but they often suffer from the partial and noisy observations. In this talk, a simple but effective Bayesian machine learning advanced forecast ensemble (BAMCAFE) method is developed, which combines an available imperfect physics-informed model with data assimilation (DA) to facilitate the ML ensemble forecast. In the BAMCAFE framework, a Bayesian ensemble DA is applied to create the training data of the ML model, which reduces the intrinsic error in the imperfect physics-informed model simulations and provides the training data of the unobserved variables. Then a generalized DA is employed for the initialization of the ML ensemble forecast. In addition to forecasting the optimal point-wise value, the BAMCAFE also provides an effective approach of quantifying the forecast uncertainty utilizing a non-Gaussian probability density function that characterizes the intermittency and extreme events. It is shown using a two-layer Lorenz 96 model that the BAMCAFE method can significantly improve the forecasting skill compared to the typical reduced-order imperfect models with bare truncation or stochastic parameterization for both the observed and unobserved large-scale variables.

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MS28

Learning Closures of Dynamical Systems Using Quantum Mechanics

We present a data-driven scheme for learning closures of dynamical systems based on the mathematical framework of quantum mechanics and Koopman operator theory. Given a system in which some components of the state are unknown, this method models the unresolved degrees of freedom as being in a time-dependent quantum-state, which determines their influence on the resolved variables. The quantum state is an operator on a space of observables and evolves over time under the action of the Koopman operator. The quantum state representing the unresolved degrees of freedom is updated at each timestep by the values oft he resolved variables according to a quantum Bayes law. Moreover, kernel functions are utilized to allow the quantum Bayes law to be implemented numerically. We present applications of this methodology to the Lorenz 63 and multiscale Lorenz 96 systems, and show how this approach preserves important statistical and qualitative properties of the underlying chaotic systems.

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MS28

Discovering State Variables Hidden in Experimental Data

Physical laws are described as relationships between state variables that give a complete and non-redundant description of the relevant system dynamics. However, despite the prevalence of computing power and AI, the process of identifying the hidden state variables themselves has resisted automation. Most data-driven methods for modeling physical phenomena still assume that observed data streams already correspond to relevant state variables. A key challenge is to identify the possible sets of state variables from scratch, given only high-dimensional observational data. We propose a new principle for determining how many state variables an observed system is likely to have, and what these variables might be, directly from video streams. We also demonstrate the effectiveness of this approach using video recordings of a variety of physical dynamical systems, ranging from elastic double pendulums to fire flames. Without any prior knowledge of the underlying physics, our algorithm discovers the intrinsic dimension of the observed dynamics and identifies candidate sets of state variables. We suggest that this approach could help catalyze the understanding, prediction and control of increasingly complex systems.

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MS28

Stochastic Sub-Grid Flux Parametrization for Finite-Volume Discretization of PDEs Using Generative Adversarial Networks

We present a machine learning approach for developing stochastic parametrizations of subgrid fluxes in finite-volume discretizations of PDEs expressed in flux form. In particular, we utilize Generative Adversarial Networks (GANs) to parametrize subgrid fluxes in equations for coarse variables defined via spatial filtering. We discuss how to construct and train the network and demonstrate that our approach reproduces statistical properties of coarse variables in fully resolved simulations. Moreover, we also demonstrate that GANs are robust and can utilized without re-training in new regimes (e.g. changes in forcing). We use Burgers and Shallow-Water equations to illustrate our approach.

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MS29

Synergistic Energy Absorption of Liquid Crystal Elastomer Meta-Structures by Coupling Nonlinear Deformation with Viscoelastic Properties

I will present a unique rate-dependent energy absorption behavior of liquid crystal elastomer (LCE)-based architected materials. The architected materials consist of repeating unit cells of bistable tilted LCE beams sandwiched between stiff supports. The viscoelastic behavior of the LCE causes the energy absorption to increase with strain rate according to a power-law relationship, which can be modulated by changing the degree of mesogen alignment and the loading direction relative to the director. For a strain rate of $600\ \mathrm{s}^{-1}$, the unit cell exhibits up to a $5\ \mathrm{MJ/m}^3$ energy absorption density, which is two orders of magnitude higher than the same structure fabricated from poly(dimethylsiloxane) elastomer and is comparable to the dissipation from irreversible plastic deformation exhibited by denser metals. For a multilayered structure of unit cells, nonuniform buckling of the different layers produces additional viscoelastic dissipation. This synergistic interaction between viscoelastic dissipation and snap-through buckling causes the energy absorption density to increase with the number of layers. The sequence of cell collapse can be controlled by grading the beam thickness to further promote viscous dissipation and enhance the energy absorption density. It is envisioned that our study can contribute to the development of lightweight extreme energy-absorbing metamaterials.

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MS29

Vitrimers and Vitrimer Nanocomposites: Thermochemical and Self-Healing Properties

Vitrimers, an emerging class of materials, are cross-linked by dynamic covalent bonds that change their topology at elevated temperatures. In addition to a traditional glass transition temperature (T_g), vitrimers have a second topology freezing temperature (T_v) above which dynamic covalent bonds allow for rapid stress relaxation, self-healing, and shape reprogramming. Herein, we demonstrate the self-healing, shape memory, and shape reconfigurability properties of this unique material aiming towards recyclability and increased part lifetime. Different nanofillers (e.g., gold nanoparticles coated graphene, graphene, clay) are introduced to make vitrimer nanocomposites. We demonstrate an increase in the T_v as a function of nanofiller concentration, while nanofiller composition produces a negligible change in T_v. Furthermore, we establish the addition of nanofillers into the vitrimer matrix increases the mechanical properties but does not hinder the recyclability of these composites as explored via thermomechanical testing. In addition, the photo-thermal self-healing response of hybrid thin-film materials is demonstrated by exposing them to a 532 nm laser on a damaged site, which illustrates a healing efficiency of $\sim 70\%$ with less than 100 ms of laser exposure. These photothermally activated composites allow for shape memory and shape reconfigurable applications, promising for many aerospace, automobile, and electronics applications.

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MS29

Statistical Mechanics of An Electro-Active Polymer Chain in the Force Ensemble

Constitutive modeling of dielectric elastomers has been of long standing interest in mechanics. Over the last two decades rigorous constitutive models have been developed that couple the electrical response of these polymers with large deformations characteristic of soft solids. A drawback of these models is that unlike classic models of rubber elas-

ticity they do not consider the coupled electromechanical response of single polymer chains which must be treated using statistical mechanics. The objective of this talk is to compute the stretch and polarization of single polymer chains subject to a fixed force and fixed electric field using statistical mechanics. We assume that the dipoles induced by the electric field at each link do not interact with each other and compute the partition function using standard techniques. We then calculate the stretch and polarization by taking appropriate derivatives of the partition function and obtain analytical results in various limits. We also perform Markov chain Monte Carlo simulations using the Metropolis and umbrella sampling methods, as well as develop a new sampling method which improves convergence by exploiting a symmetry inherent in dielectric polymer chains. The analytical expressions are shown to agree with the Monte Carlo results over a range of forces and electric fields. Our results complement recent work on the statistical mechanics of electro-responsive chains which obtains analytical expressions in a different ensemble.

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MS29

Programming Shape Transformation in Ordered Polymers and Living Materials

Stimuli-responsive polymers respond to their environment without requiring motors, sensors, or power supplies. These materials can replace the functions of traditional machines in conditions or at scales, such as in the human body, where traditional actuators, electronics, and batteries are difficult to employ. Here, two orthogonal strategies, one non-living and one living, to create materials that respond in a complex manner to specific environmental conditions will be discussed. First, we will discuss controlling molecular orientation and, therefore, the stimulus-response in liquid crystal elastomers. The entanglement of many liquid crystal elastomer ribbons will be harnessed to create 3D objects that self-assemble and then disperse on command. We will also discuss fabricating living Bakers yeast hydrogel composites capable of undergoing programmed shape change through biological growth. As the cells are higher modulus ($\sim 100\times$) than the gel, cell proliferation results in a macroscopic increase in volume of up to 600%. These morphing materials may enable new strategies for medical devices like artificial muscles or green manufacturing techniques where engineering materials are grown.

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MS30

Finite Element Approximation of Steady Flows with Nonlinear Constitutive Relations

The classical constitutive relations for incompressible Stokesian fluids are explicit expressions (e.g., linear for the NavierStokes equations) for the Cauchy stress in terms of the symmetric part of the velocity gradient. However, many fluids cannot be described by such relations, for instance steady isochoric flows of colloidal suspension. In this work, we consider a model where the symmetric velocity gradient is a monotone nonlinear function of the deviatoric part of the Cauchy stress tensor. We show the existence of a weak solution to the nonlinear system of partial differential equations and, under appropriate assumptions on the input data, the uniqueness. We then introduce and analyze numerical methods based on both conforming and nonconforming finite element spaces. Finally, we propose two iterative algorithms (a LionsMercier type iterative method and a fixed-point iteration) for solving the nonlinear system and we present numerical experiments to illustrate their practical performances.

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MS30

Adaptive Finite Element Approximation of Steady Flows of Incompressible Fluids with Implicit Power-Law-Like Rheology

We present a convergence analysis for an adaptive finite element method for implicit power-law-like models for viscous incompressible fluids. In the considered class of models, the Cauchy stress and the symmetric part of the velocity gradient are related by a, possibly multi-valued, maximal monotone r-graph, with $\frac{2d}{d+1} < r < \infty$. We establish upper and lower bounds on the finite element residual, as well as an estimator for an approximation of the maximal monotone graph. We then present an adaptive strategy and show, under suitable assumptions, the weak convergence of the adaptive algorithm. The argument is based on a variety of weak compactness techniques, including Chacons biting lemma and a finite element counterpart of the AcerbiFusco Lipschitz truncation of Sobolev functions, introduced by L. Diening, C. Kreuzer, and E. Sli [Finite element approximation of steady flows of incompressible fluids with implicit power-law-like rheology, SIAM J. Numer. Anal., 51(2), 9841015].

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MS30

Mixed Finite Element Methods for Large-Strain

Poroelasticity Coupled with Chemotaxis

In this talk we propose a novel coupled poroelasticity-diffusion model for the formation of extracellular oedema and infectious myocarditis valid in large deformations, manifested as an interaction between interstitial flow and the immune-driven dynamics between leukocytes and pathogens. The governing partial differential equations are formulated in terms of skeleton displacement, fluid pressure, Lagrangian porosity, and the concentrations of pathogens and leukocytes. A similar model with applications in morphogenesis is also discussed. A five-field mixed-primal finite element scheme is proposed for the numerical approximation of the problem, and we provide the stability analysis for a simplified system emanating from linearisation. We also discuss the construction of an adequate, Schur complement based, nested preconditioner. Numerical tests exemplify the properties of the new model and of the mixed schemes.

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MS30

Graph Approximation for the Numerical Approximation of Implicitly Constituted Fluids

For the numerical approximation of implicitly constituted fluids one has to regularise the constitutive law. This can be done by means of graph approximation of the maximal monotone graph that represents the constitutive relation. In this talk we present a particular graph approximation. This has some beneficial properties regarding the numerical analysis of finite element schemes: For the admissible range of growth exponents it allows to prove convergence taking the graph approximation and the discretisation limit simultaneously. Furthermore, for sufficiently smooth solutions error estimates in both approximation parameters can be obtained. We demonstrate this for the examples of Bingham and HerschelBulkley fluids.

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MS31

Debonding of Gel Membranes from Rigid Substrates

We consider the problem of debonding of a thin gel domain from a rigid substrate. We start with a variational approach involving the total energy of a gel, as the sum of the bulk elastic energy and the Flory-Huggins energy of mixing of the polymer chains and the solvent fluid. We assume that the gel is partially debonded, formulate the boundary value problem of swelling in two-space dimensions and perform an asymptotic analysis with respect to the thickness aspect ratio. We study the energy release rate due to debonding and obtain the critical membrane thickness for which detaching from the substrate initiates. In the last part of the talk, we discuss the sliding of the gel sheet when adhered to a moving substrate. We present numerical examples showing that sliding occurs by competition between the bending, shearing and adhesion energies of the membrane.

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MS31

Mutable Plasmonic Meta-Surfaces

The approach of the DMREF team uses tunable building blocks, called meta-atoms, that affect light at many different frequencies (or colors). One color of light controls the properties of meta-atoms, which then change properties and in turn control the flow of light of another color. The concept is realized through arrays of nanoscopic metallic particles, separated from a metallic substrate by a thin liquid crystal film. The thickness of the film is controlled through isomerization induced by laser light at a control frequency. This provides the opportunity for light controlled polarization meta-surfaces. Scattered light at different frequencies is polarized differently through plasmon resonances that change with film thickness. With an eye towards design, a rigorous reduced order model is sought that will enable one to sample a sufficiently rich universe of designs enabling optimization. In this talk we present such a model using a combination of matched asymptotic expansions and corrector theory of homogenization. We illustrate the method presenting examples of designs.

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MS31

Elastomers Filled with Liquid Inclusions: Theory, Numerical Implementation, and Some Basic Results

Experimental results of late have pointed to elastomers filled with various types of liquid inclusions as a promising new class of materials. Motivated by these findings, we formulate the homogenization problem that describes the macroscopic mechanical response of elastomers filled with liquid inclusions under finite quasistatic deformations. The focus is on the non-dissipative case when the elastomer is a hyperelastic solid, the liquid making up the inclusions is a hyperelastic fluid, and the interfaces separating the solid elastomer from the liquid inclusions feature their own hyperelastic behavior (which includes surface tension as a special case). We show that the macroscopic behavior of such filled elastomers turns out to be that of a hyperelastic solid, albeit one that depends directly on the size of the inclusions and the constitutive behavior of the interfaces. Strikingly, in spite of the fact that there are local residual stresses within the inclusions (due to the presence of initial interfacial forces), the resulting macroscopic behavior is free of residual stresses. What is more, in spite of the fact that the local moduli of elasticity in the bulk and the interfaces in the small-deformation limit do not possess minor symmetries (due to the presence of residual stresses and initial interfacial forces), the resulting effective modulus of elasticity does possess the standard minor symmetries of an elastic solid.

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MS31

Studying Grain Boundary Regions in Polycrystalline Materials Using Spherical Nano-Indentation

and Electron Backscatter Diffraction

In this presentation we report on the application of our spherical nanoindentation data analysis protocols to study the mechanical response of grain boundary regions in as-cast and 30% deformed polycrystalline Fe-3%Si steel. In particular, we demonstrate that it is possible to investigate the role of grain boundaries in the mechanical deformation of polycrystalline samples by systematically studying the changes in the indentation stress-strain curves as a function of the distance from the grain boundary. Such datasets, when combined with the local crystal lattice orientation information obtained using electron backscatter diffraction, open new avenues for characterizing the mechanical behavior of grain boundaries based on their misorientation angle, dislocation density content near the boundary, and their propensity for dislocation source/sink behavior. Additionally we will demonstrate the capabilities of this technique to probe nanoscale surface modifications in solid materials and quantify the resulting changes in its mechanical response. Using ion irradiation in tungsten as a specific example we will discuss the capabilities of spherical nanoindentation stress-strain curves, extracted from the measured load-displacement dataset, in characterizing the elastic response, elasto-plastic transition, and onset of plasticity in ion-irradiated tungsten under indentation, and compare their relative mechanical behavior to the unirradiated state.

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MS32

Galerkin Neural Network Approximation of Multiscale Problems

We consider the neural network approximation of systems of partial differential equations exhibiting multiscale features. Specifically, we consider the approximation of the Reissner-Mindlin plate model which poses significant challenges due to the presence of boundary layers and numerical phenomena such as locking. This work builds on the basic Galerkin Neural Network approach established in previous work for symmetric, positive-definite problems. The key contributions of this work are (1) the analysis and comparison of several new least squares-type variational formulations for the Reissner-Mindlin plate, and (2) their numerical approximation using the Galerkin Neural Network approach. Numerical examples are presented which demonstrate the ability of the approach to resolve multiscale phenomena such for the Reissner-Mindlin plate model for which we develop a new family of benchmark solutions which exhibit boundary layers.

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MS32

Multifidelity Deep Operator Networks

This talk will discuss an approach to multifidelity machine learning with multifidelity Deep Operator Networks (DeepONets.) In scientific applications there is a need for fast and accurate models using only limited high-fidelity data. We show that DeepONets have the ability to train operators using low-fidelity noisy or low-resolution data and a small amount of high-fidelity data by learning the linear and non-linear correlations between the high- and low-fidelity data. For example, the DeepONet can be trained with data from several low-resolution and low-order simulations and a few high-fidelity experimental measurements or data taken from higher-resolution or higher-order simulations. Our approach allows for accurate models when training with data alone is infeasible.

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MS32

Learning Operators with Coupled Attention

Supervised operator learning is an emerging machine learning paradigm with applications to modeling the evolution of spatio-temporal dynamical systems and approximating general black-box relationships between functional data. We propose a novel operator learning method, LOCA (Learning Operators with Coupled Attention), motivated from the recent success of the attention mechanism. In our architecture, the input functions are mapped to a finite set of features which are then averaged with attention weights that depend on the output query locations. By coupling these attention weights together with an integral transform, LOCA is able to explicitly learn correlations in the target output functions, enabling us to approximate nonlinear operators even when the number of output function measurements in the training set is very small. Our formulation is accompanied by rigorous approximation theoretic guarantees on the universal expressiveness of the proposed model. Empirically, we evaluate the performance of LOCA on several operator learning scenarios involving systems governed by ordinary and partial differential equations, as well as a black-box climate prediction problem. Through these scenarios we demonstrate state of the art accuracy, robustness with respect to noisy input data, and a consistently small spread of errors over testing data sets, even for out-of-distribution prediction tasks.

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MS33

Investigation of Wave Propagation of a One-Dimensional Bi-Material System

In this talk, we explore the theory and implementation of wave propagation in a one-dimensional bi-material system using the local-to-local and nonlocal-to-nonlocal models, respectively. The local description is based on a coupling of two local continuum mechanics and the nonlocal description is based on a coupling of two nonlocal peridynamics with different constants. To study the physical reflection coefficients and diminish the artificial reflection rising from the simulation, one need to maintain the conservation laws across the material interface on a discrete level. We study the conservation laws of linear momentum and total energy

for both local and nonlocal models in a continuous setting and then develop the numerical discretization accordingly to preserve those quantities. This work provides practitioners a tool to achieve robust computations of systems involving interface wave reflections and to ensure preservation of continuum properties on a discrete level.

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MS33

Peridynamics Computations at the Exascale

Peridynamics is a nonlocal reformulation of classical continuum mechanics suitable for material failure and damage simulation, which has been successfully demonstrated as an effective tool for the simulation of complex fracture phenomena in many applications. However, the nonlocal nature of peridynamics makes it highly computationally expensive, compared to classical continuum mechanics, which often hinders large-scale fracture simulations. In this talk, we will present ongoing efforts to develop a GPU-enabled, performance portable, and exascale-capable peridynamics code designed to run on U.S. Department of Energy supercomputers, in particular Summit (currently ranked #2 in the TOP500 list) and Frontier (to be deployed later this year), both at Oak Ridge National Laboratory.

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MS34

Model-Free Portfolio Theory: A Rough Path Approach

Based on a rough path foundation, we develop a model-free approach to stochastic portfolio theory (SPT). Our approach allows to handle significantly more general portfolios compared to previous model-free approaches based on Föllmer integration. Without the assumption of any underlying probabilistic model, we prove a pathwise formula for the relative wealth process which reduces in the special case of functionally generated portfolios to a pathwise version of the so-called master formula of classical SPT. We show that the appropriately scaled asymptotic growth rate of a far reaching generalization of Cover's universal portfolio based on controlled paths coincides with that of the best retrospectively chosen portfolio within this class. We provide several novel results concerning rough integration, and highlight the advantages of the rough path approach by considering (non-functionally generated) log-optimal portfolios in an ergodic Itô diffusion setting.

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MS34

Convex PCA and the Capital Distribution Curve in Stochastic Portfolio Theory

Convex PCA (CPCA), which was originally proposed in [Bigot et al. 2017] to formulate a Wasserstein geodesic PCA on the real line, is an extension of standard PCA to data constrained to lie in a convex set of a Hilbert space. We give an in-depth treatment of CPCA in finite dimensions and provide an efficient implementation when the convex set is polyhedral. We then apply this methodology to study the ranked capital distribution curve of the US equity market using the Aitchison geometry, and show that market diversity, a fundamental concept in stochastic portfolio theory, corresponds closely to the first principal component.

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MS34

Market-to-Book Ratio in Stochastic Portfolio Theory

We present market-to-book ratios of stocks in the context of Stochastic Portfolio Theory. Functionally generated portfolios that depend on market-to-book ratios are developed in two ways, with their relative returns with respect to the market. This enables us to identify the value factor (i.e., market-to-book ratio) in returns of such generated portfolios. Examples of portfolios, as well as their empirical results, are given, with the evidence that the value factor, as well as the size, does affect the performance of the portfolio.

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MS34

Stochastic Portfolio Theory: An Overview

This talk will serve as an introduction to the minisymposium by reviewing some of the key concepts in Stochastic Portfolio Theory. I aim to discuss some empirical features of large equity markets, in particular the capital distribution curve, as well as rank-based models, functionally generated portfolios, and relative arbitrage.

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MS35

Higher Rank Signatures and Filtrations

Filtration is an abstract and important notion that appears naturally in stochastic analysis, which models the infor-

mation flow generated by underlying stochastic processes. However, many well-known statistical methods cannot detect filtrations as they are based on weak topology, and consequently they may lead to significant errors for those circumstances where the evolution of information plays a crucial role. In this talk we will introduce a new methodology based on the signature kernel learning approach developed by Terry Lyons which can be used for giving a precise description of filtrations hidden behind observed signals. We will then illustrate that this method provides a feasible statistical tool for lots of filtration–sensitive cases; in particular, it allows to reduce highly non–linear path-and-filtration dependent functionals (e.g. the pricing of American option) to a linear regression problem, which reveals an interesting combination of (Hopf) algebra and kernel learning.

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MS35

Evaluating Forecasts on Pathspace

Often one is interested in not just forecasting a scalar- or vector-valued quantity but instead, the future evolution of a quantity. Formally, this means that a forecaster provides us with a probability measure on the space of paths. A natural question is how one can compare and rank such forecasts. To address this question, we revisit the classic scoring rule framework which allows deriving natural notions of entropy, divergence, and mutual information that are robust under time-discretization and take the Non-Euclidean structure of path space into account. (Joint work with Patric Bonnier).

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MS35

Sig-Splines: Universal Approximation and Convex Calibration of Time Series Generative Models

We propose a new algorithm for approximating discrete-time time series generative models. Our algorithm is inspired from neural splines and rough path signatures. The combination of both leads to a time series calibration algorithm which is universal and allows for the models parameters to be calibrated using convex optimization methods.

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MS36

Quantum Pixel Representations and Compression for N-Dimensional Images

We introduce a novel and uniform framework for quantum pixel representations that overarches many of the most popular representations proposed in the recent literature, such as (I)FRQI, (I)NEQR, MCRQI, and (I)NCQI. The proposed QPIXL framework results in more efficient circuit implementations and significantly reduces the gate complexity for all considered quantum pixel representations. Our method only requires a linear number of gates in terms of the number of pixels and does not use ancilla qubits. Furthermore, the circuits only consist of RY- gates and CNOT gates making them practical in the NISQ era. Additionally, we propose a circuit and image compression algorithm that is shown to be highly effective, being able to reduce the necessary gates to prepare an FRQI state for example scientific images by up to 90% without sacrificing image quality. Our algorithms are made publicly available as part of QPIXL++, a Quantum Image Pixel Library.

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MS36

Uncertainty Quantification in Ensemble Deep Learning

Neural networks are an emerging topic in the computer science industry due to their high versatility and efficiency with large datasets. Funded by the National Science Foundation, Embry-Riddle Aeronautical University is partnered with the Nevada National Security Site on the project, Ensemble Deep Learning, through the Research Experience for Undergraduates 2022 summer program. The Nevada National Security Site is seeking for deep learning techniques to analyze radiographic images of small-scale nuclear explosions in order to ensure that the United States nuclear stockpile remains safe, reliable and secure. In building a deep learning model, multiple convolutional neural network architectures are developed in parallel and combined to create an ensemble neural network. Neural

networks are often referred to as a black box algorithm due to the uncertainty in the weights and biases applied to the model. This algorithm poses the uncertainty quantification, which is the question of how to correctly measure accuracy in a regressive convolutional neural network. The projects objective is to determine the comparative differences between the efficiency of the ensemble neural network versus each individual convolutional neural network through the uncertainty quantification. As model precision is a key aspect of machine learning, emphasis is placed on the efficiency of ensemble neural networks to produce an error bar alongside the predictions.

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MS36

Information Measures and Random Projection

The Mutual Information (MI) between two random variables measures the reduction in uncertainty of one random quantity due to information obtained from the other. It is an important information-theoretic concept, closely related to Entropy, that plays a role in many applications, including decision trees in machine learning, independent component analysis (ICA), gene detection and expression, link prediction, topic discovery, image registration, feature selection and transformations, and channel capacity. A persistent challenge is the accurate numerical estimation of mutual information from high-dimensional data, a problem arising in image classification, microarray data analysis, and machine learning. For example, in machine learning the mutual information is used to regularize Generative Adversarial Networks (GANs) in order to produce samples of high-dimensional data with greater diversity. In this talk, I will propose a new method which tackles the high-dimensional data. Random projection is applied in order to reduce the dimension of the data.

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MS36

Well-Balanced Scheme for the Shallow Water MHD Equations with a New Divergence-Free Treatment of the Magnetic Field

PDEs constrained by a divergence-free magnetic field or velocity provide mathematical models to many complex physical systems of fundamental interest and are used in a wide range of applications arising in astrophysics, geophysics, and engineering. A close examination of the nature of such PDEs typically reveals their deep mathematical structure, and thus, typically require a very fine mesh resulting in a computationally expensive simulation. To ensure these structures are preserved exactly in numerical approximations on a less computationally expensive mesh, a careful algorithmic construction is required. In this talk, we restrict our attention to an important subclass of divergence-free constrained systems the shallow water magnetohydrodynamic equations, keeping in mind that the developed structure-preserving methods can be extended to other models constrained by zero-divergence. We present a new method that exactly preserves both the divergence-free constraint and equilibrium states of the shallow water magnetohydrodynamic system. The design scheme is successfully tested on a number of examples.

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MS36

Two Blood Flow Models in Arteries

In this talk, two blood flow models in arteries with curvature will be presented. The first model is an unidimensional model where the cross-sections are circumferences, while the second one is a bidimensional model with general cross-sections (it can be elipses, stars, or any other planar geometry). One of the principal aims of the bidimensional model is to study damaged arterial walls with occlusions or bulgings at focalized zones, while the unidimensional model assumes the damaged arterial walls is for all angles. We will show quasilinear properties of both models, as a well-defined central upwind scheme that preserves positivity. The last property is neccesary in the study of arteries. The talk will conclude with the mention of numerical examples of idealized human arteries with damaged arterial walls.

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MS37

Tipsy Cop and Tipsy Robber on Vertex and Edge Symmetric Graphs

We analyze the expected length of a variation to the Cops and Robbers game in graph theory where the cop and robber (rebranded as a zombie and survivor) have probabilities p and q to move to a random adjacent node. A solution is provided on complete graphs, the Petersen graph, n-cycle graphs, and the hypercube graphs (the last is still a work

in progress). Solutions for each are derived using recursive techniques and Markov Chain properties. Faculty Advisors: Gabriel Sosa Castillo, gsosacastillo@colgate.edu

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MS37

Removing Hanging Faces from Tree-Based Adaptive Meshes

Scalable adaptive mesh refinement (AMR) has a successful history in reducing the number of degrees-of-freedom and hence the runtime and memory usage of PDE solvers. The well-known space-filling curve (SFC) techniques for quadrilaterals have been proven to scale to millions of parallel processes and trillions of elements. However, quadrilateral AMR results in non-conforming meshes with hanging nodes and faces in regions where elements of different refinement levels are neighbored. This requires the numerical solvers to introduce interpolation methods at these hanging interfaces. In our work, we develop an extension of quadrilateral SFCs that post-processes adaptive meshes and removes their hanging faces by introducing triangular transition cells into the mesh. The result is a conformal hybrid mesh that has all the benefits of an adaptive SFC mesh. Necessary developments include for example extending the SFC index, identifying parents, children and neighbor elements and interpolating values between regular cells and transition cells. We implement the new method in the t8code library for scalable hybrid tree-based AMR and demonstrate its applicability in the context of a finite volume solver for the advection equation. Faculty Advisors: Gregor Gassner, Department for Numerical Simulation at University of Cologne, ggassner@math.uni-koeln.de; Johannes Holke, Department for High Performance Computing at German Aerospace Center, Johannes.Holke@dlr.de

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MS37

Nonlocal Variational Problems

This talk will explore the intersection of the calculus of variations and nonlocal modeling. The calculus of variations is a very old and beautiful theory investigating optimization problems in infinite-dimensional function spaces. The field played a crucial role in the historical development of mechanics, and has been applied to optimal control theory, boundary value problems in PDEs, and many other fields. The other central topic, nonlocal modeling, has received a huge amount of attention in recent years following Silling's reformulation of elastic theory in terms of nonlocal operators. Unlike classical derivatives, nonlocal operators can handle discontinuities and capture long-range interactions, making them ideal tools for fields like fracture dynamics and diffusion problems. In this talk, I will introduce a class of nonlocal operators and show how it compares to the classical derivative. Then I establish the existence and uniqueness of minimizers for variational problems involving this operator using a version of the classical Direct Method. Finally, I discuss some numerical experiments involving these problems that suggest further results connecting these new problems to classical theory. Faculty Advisors: Mikil Foss, University of Nebraska-Lincoln, mikil.foss@unl.edu

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MS37

Photon-Counting CT Reconstruction with a Learned Forward Operator

Photon-Counting CT is an emerging imaging technology that promises higher spatial resolution and possibility for material decomposition in the reconstruction. A major difficulty is to construct a physics model for cross-talk between detectors that is both accurate and fast to evaluate. In this work, we accelerate image reconstruction tasks for photon-counting CT by training a deep convolutional neural network that adds cross-talk on top of a simplified physics model. The main theoretical result relates to proving convergence when using such a learned cross-talk model together with second-order optimisation methods for spectral CT. The main empirical result is that CT reconstructions generated using the learned physics model agree well with the full model, and are ten times faster to generate. The talk will begin with a brief historical overview of CT reconstruction methods to build intuition for the problem. Then we present the theoretical results. These give rise to two key ideas that carry valuable insights for the field of scientific machine learning. First is the Adjoint correction, in which the adjoint of the derivative of the model is corrected in a similar manner to the model itself. Second is recursive training, in which the partially learned physics model is used to generate new training data. Lastly, we present empirical results. Faculty Advisors: Ozan ktem, KTH, ozan@kth.se; Mats Persson, KTH, mats.persson@mi.physics.kth.se

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MS37

Quantifying Uncertainty with Ensemble Neural Networks for Metal Oxide Spectrograms

Optical absorption spectroscopy is an important characterization of materials for applications such as solar energy generation. The purpose of the study is to build an ensemble neural network for predicting metal oxide spectrograms from images of metal oxide that have been scanned. With an ensemble network, several models are trained to produce a variety of predictions. By averaging these predictions, an even more accurate prediction can be made. Furthermore, uncertainty quantification will be applied by measuring the variance between the predictions, allowing more useful statistical analysis to be done such as producing confidence intervals to determine how accurate the results are. The study was done through a quantitative empirical research method and has found that an ensemble neural network performed better on average then a base single model. Through uncertainty quantification it was also found that neural networks using this approach had a very small variance between models. Faculty Advisors: Mihhail Berezovski, Embry Riddle Aeronautical Univer-

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MS38

Clustering Market Regimes Using the Wasserstein Distance

The problem of rapid and automated detection of distinct market regimes is a topic of great interest to financial mathematicians and practitioners alike. In this paper, we outline an unsupervised learning algorithm for clustering financial time-series into a suitable number of temporal segments (market regimes). As a special case of the above, we develop a robust algorithm that automates the process of classifying market regimes. The method is robust in the sense that it does not depend on modelling assumptions of the underlying time series as our experiments with real datasets show. This method – dubbed the Wasserstein k-means algorithm – frames such a problem as one on the space of probability measures with finite pth moment, in terms of the p-Wasserstein distance between (empirical) distributions. We compare our WK-means approach with a more traditional clustering algorithms by studying the so-called maximum mean discrepancy scores between, and within clusters. In both cases it is shown that the WK-means algorithm vastly outperforms all considered competitor approaches. We demonstrate the performance of all approaches both in a controlled environment on synthetic data, and on real data. This is joint work with Zacharia Issa, Aitor Muguruza

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MS38

Two-Step PCA Anomaly Detection on Financial Time Series

We consider univariate time series representing a wide variety of risk factors in the context of financial risk management. A major issue of these data is the presence of anomalies that induce a miscalibration of the models used to quantify and manage risk, whence potentially erroneous risk measures on their basis. Therefore, the detection of anomalies is of utmost importance in financial risk management. We propose an approach that aims at improving anomaly detection on financial time series, overcoming most of inherent difficulties of anomaly detection. One first concern is to deal with the scarcity of anomalies in the available datasets. To this end, we used time domain data augmentation techniques, which have proved to be efficient tools to enhance the quality and the size of the data. Then, we concentrate on the computation of the anomaly score assigned to each observation, through a forward and backward application of principal component analysis. The contribution of the approach is twofold. On the one hand, with this method the threshold is not a hand-set parameter, instead it is calibrated throughout the learning. On the other hand, besides detecting the anomaly the proposed approach suggests an imputation value at no additional cost. The efficiency of the proposed model over several well-know anomaly detection algorithms is demonstrated by its application on real-world datasets.

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MS38

Synthetic Data Generation via Generative Adversial Networks for Financial Markets with a Focus on Tail Properties

In 2014, Ian Goodfellow et al. presented a new two-step Deep Learning architecture called Generative Adversarial Network (GAN). This network is actually made of two subnetworks: a generator and a discriminator that compete against each other. GANs have shown great success in generating realistic pictures of human beings and other areas. Despite great progress in using them for financial time-series and finance applications, many challenges remain. A real zoo of GANs has evolved and we give a short overview of their properties and which ones could be used for financial applications. Furthermore, we analyze a variation of a conditional GAN that directly incorporates some of the key distributional properties that are needed for a realistic simulation of financial markets. Our GAN is based on an additional subnetwork which is used to directly model some relevant characteristics. For numerical illustrations, we implement this model on liquid futures in a high-frequency intraday setting, and conduct a thorough statistical performance analysis, with a particular focus on the tail properties of those time-series. An outlook on potential applications as well as open research questions is given. This is joint work with Prof. Ali Hirsa and Weilong Fu from Columbia University as well as Dr. Branka Hadji Misheva from Zurich University of Applied Sciences.

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MS38

Model Based vs Model Free Synthetic Data Generators

The aim of this talk is to overview neural SDEs, which combine neural networks with risk models based on classical stochastic differential equations (SDEs). These models can be applied to find robust bounds for prices of derivatives and the corresponding hedging strategies or to simulate market scenarios needed for assessing risk profiles or training machine learning models. Importantly using the stochastic control perspective, it is possible to establish convergence guarantees for neural SDEs in certain settings.

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MS39

What Makes a Reaction Network Chemical?

Reaction networks can be represented as graphs (e.g. as

hypergraphs or complex-reaction graphs). However, not all such graphs admit a chemical interpretation because they may contradict fundamental principles of physics. "Futile cycles" which have no net mass conversion (a trivial net reaction) may violate conservation of energy, and subnetworks that allow a net generation/destruction of mass definitely violate conservation of mass and atom types. The absence of irreversible futile cycles and the existence of a positive left kernel vector for the stoichiometric matrix are well known sufficient conditions (for the soundness of a network). We show that these conditions are also necessary. Moreover, they are also necessary and sufficient for the existence of sum formula representations (of a given network) that preserve atom types and even for the existence of structural formula representations (corresponding to Lewis formulas). In the latter representation, all chemical reactions in the network have an interpretation as rearrangements of bonds/electron pairs. The main motivation and application of our results is the generation of "random" chemical reaction networks. Our main mathematical tools are "theorems of the alternative" from polyhedral geometry/oriented matroids.

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MS39

The Shape of the Parameter Region of Multistationarity

Despite recent developments, describing the set of parameters that enable multistationarity in a chemical reaction network is a challenging problem. In this talk, I will present a new algorithm that permits insights into the shape of the parameter region of multistationarity, in particular on its connectivity. The method is based on the observation that, under some assumptions on the network, one can decide the connectivity of the parameter region of multistationarity, based on the connectivity of the preimage of the negative real line under a multivariate signomial function. The later problem can be addressed by considering the geometry of the Newton Polytope of the signomial function. I will give several examples of reaction networks where our algorithm can be applied. In particular, we show that the parameter region of multistationarity of the sequential and distributive phosphorylation cycle with two or three sites is connected.

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MS39

Multistationarity of Mass-Action Networks with One-Dimensional Stoichiometric Subspace

Our work is inspired by recent results that explain how multistationarity survives over a network expansion and by studies of small networks, which can be viewed as building blocks of multistationary behavior in larger biochemical systems. We devote our attention to networks with one dimensional stoichiometric subspace under mass-action kinetics, and show that their capacity for multiple steady states and multiple non-degenerate steady states can be determined from the structure of the network alone. We give a complete characterization of multistationarity and non-degenerate multistationarity for this class of networks, thus answering a standing question proposed by Joshi and Shiu.

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MS40

A Self-Exciting Point Process with a State-Dependent Intensity to Model the COVID-19 Epidemics

The recent pandemic has shown that when the reproduction number is high and there is no proper measurement taken, the number of infected people can increase dramatically in a short time, producing overdispersion. In this talk I will explore the possibility of using a self-exciting point process with a state-dependent baseline intensity to model the total number of people that have contracted the virus. In particular, and to allow for quick predictions, a closed formula for the joint moments of the number of currently infected and recovered individuals will be presented along with different cases and future research opportunities.

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MS40

Maximum Likelihood Estimation for Multivariate Hawkes Processes with Inhibition and Exponential Kernel Functions. Application to Neurosciences

The Hawkes process is a past-dependant point process used to model the relationship of event occurrences between different phenomena. Since its appearance, it has been widely used in various fields such as finance, criminology and neuroscience. The Hawkes process was originally introduced to describe excitation interactions, which means that one event increases the chances of another occurring. However there has been a growing interest in the opposite effect, known as inhibition. In this talk we propose a Maximum Likelihood estimation method for multivariate Hawkes processes with exponential kernel that can handle both exciting and inhibiting interactions. Parametric estimation methods in the literature are mostly adapted to non-negative interactions and most methods proposed for the inhibiting case are restricted to non-parametric frameworks. We show that the proposed estimator performs better for synthetic data than alternative methods. We also illustrate its application to a neuronal activation dataset.

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MS40

A Macroeconomic SIR Model for COVID-19

There is a close and delicate relationship between a country's public health and its economic health which has been made obvious in recent years. We have developed a macroeconomic SIR pandemic model which explicitly considers herd immunity arrival, behavior-dependent trans-

mission rates, remote workers, and inter-group interactions while also attempting to quantify the economic impacts of disease spread, preventative measures, and associated externalities. As an example, we investigate optimal pandemic management strategies for the beginning of the COVID-19 pandemic in 2020. The model is formulated as an exit time control problem where lockdown ends when the population achieves herd immunity, either naturally or via a vaccine with stochastic arrival time. We also split the adult population into two separate subgroups by age. The mode is able to consider situations where herd immunity could be achieved before vaccine arrival and if this occurs, lockdowns for high-risk populations could be markedly shortened. In addition, we found that modeling a behavior-dependent transmission rate, which reflects increased personal caution in response to increased infection levels, provided further potential for decreasing both output loss and total mortality.

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MS40

Measuring Epidemic Reproduction Numbers at the Beginning of an Outbreak Using Stochastic Point Processes

Dynamic estimation of the reproduction number of diseases is important for assessing the impact of public health measures on virus transmission. State and local decisions about whether to relax or strengthen mitigation measures are being made in part based on whether the reproduction number, Rt, falls below the self-sustaining value of 1. Employing branching point process models and COVID-19 data from Indiana as a case study, we show that estimates of the current value of Rt, and whether it is above or below 1, depend critically on choices about data selection and model specification and estimation.

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MS41

Homogenization and Phase Separation in the Non-insothermal Regime

A vectorial variational model for phase separation within a periodically heterogeneous material is studied. The material is nonisothermal and thus the preferred phases are allowed to change with position. A gamma convergence expansion is proved using techniques of two-scale convergence along with novel improvements in the theory of nonisothermal Modica-Mortola functionals.

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MS41

Higher Codimension Area-Minimizers: Understanding Branch Points Via the Frequency Function

Integral currents are a weak generalization of smooth oriented surfaces and provide a natural setting in which to study the Plateau problem: what are the surfaces of least m-dimensional area that span a given (m-1)-dimensional boundary?. Unfortunately, the weak nature of currents permit the formation of singularities. The problem of determining the size and structure of the singular set of an area-minimizer in this setting has been studied by many since the 1960s, with early ground-breaking contributions from Almgren, Bombieri, De Giorgi, Federer, Giusti, Simon, Simons, White and many others. When the codimension of the surface is higher than 1, due to the presence of singular points with flat tangent cones, little progress has been made since the celebrated (m-2)-Hausdorff dimension bound on the singular set due to Almgren, the proof of which has since been simplified by De Lellis and Spadaro. In this talk I will survey old and new results on this problem and discuss joint work in progress with Camillo De Lellis (IAS) towards getting a more refined characterization of the behaviour of the surface at singular points with flat tangent cones, allowing us to make significant progress towards proving rectifiability for such singularities.

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MS41

A Gradient Flow Perspective for the Mullins-Sekerka Equation

The purpose of this talk is to develop a gradient flow perspective for the Mullins-Sekerka equation, intrinsic to the evolving surface, at the level of a weak solution theory. The solution concept is motivated by the De Giorgi framework for curves of maximal slope and consideration of Gamma-convergence for gradient flows in the spirit of Sandier and Serfaty. Solutions must satisfy an optimal energy dissipation relation, where both the time derivative and metric slope are considered with respect to formal tangent spaces, arising from the mass preserving normal velocities. We

prove that such solutions exist, may be recast in a PDE sense, and subsume the solution concept introduced by Le in the study of Gamma-convergence for the Cahn-Hilliard equation.

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MS42

Approximation Theory for Deep Learning in Time Series Analysis

In this talk, we present some recent results on the approximation theory of deep learning architectures for time series analysis. In particular, we formulate a basic mathematical framework, under which different popular architectures such as recurrent neural networks, dilated convolutional networks (e.g. WaveNet), encoder-decoder structures can be rigorously compared. These analyses reveal some interesting connections between approximation, memory, sparsity and low rank phenomena that may guide the practical selection and design of these network architectures.

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MS42

Robust PDE Identification from a Noisy Data Set

Partial differential equation (PDE) is an important tool to describe physical laws in many disciplines. Usually PDEs are derived from empirical observations. As the advances of technology, large amounts of data are easy to collect and store, which provides new opportunities for data-driven identification of PDE. This presentation addresses our recent work on identifying parametric and nonlocal PDEs. In PDE identification, many existing methods cannot deal with data with heavy noise. We propose a successively denoised differentiation strategy to denoise the data and compute partial derivatives with improved accuracy. We propose two methods to identify parametric PDEs. Our methods are based on the subspace pursuit algorithm, cross validation error and multi-shooting time evolution error, and can efficiently identify the underlying PDE from data with large noise. For nonlocal PDEs, we propose a model and a split Bregman algorithm to identify the underlying potential of the aggregation equation from a noisy data set. We also extend our algorithm to identify time-varying potentials, as well as to identify the interaction kernel in an agent-based system.

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MS42

Auto-Differentiable Ensemble Kalman Filters

Data assimilation is concerned with sequentially estimating a temporally-evolving state. This task, which arises in a wide range of scientific and engineering applications, is particularly challenging when the state is high-dimensional and the state-space dynamics are unknown. This talk will introduce a machine learning framework for learning dynamical systems in data assimilation. Our auto-differentiable ensemble Kalman filters (AD-EnKFs) blend ensemble Kalman filters for state recovery with machine learning tools for learning the dynamics. In doing so, AD-EnKFs leverage the ability of ensemble Kalman filters to scale to high-dimensional states and the power of automatic differentiation to train high-dimensional surrogate models for the dynamics. Numerical results using the Lorenz-96 model show that AD-EnKFs outperform existing methods that use expectation-maximization or particle filters to merge data assimilation and machine learning. In addition, AD-EnKFs are easy to implement and require minimal tuning. This is joint work with Yuming Chen and Rebecca Willett.

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MS42

A Limitation of Deep Learning in Solving PDE with High Frequency or Weak Solution

We demonstrate an implicit bias of deep learning in Fourier domain, that is, a very universal frequency principle that deep neural networks learn low frequency faster. We utilize the frequency principle to understand why deep neural networks (DNNs) work well in low-frequency problem but not high-frequency problem. We also design a multi-scale DNN (MscaleDNN) for solving PDEs, which overcomes the slow convergence of high frequency. In addition, we also show that due to the frequency principle, the DNN method can converge to wrong solutions for the PDE problem with only weak solutions.

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MS43

A Stable Matrix Form of Some Fast Transformations

In this talk, we present a fast stable matrix-version method

for evaluating the discretized transforms in one dimension, such as Gaussian transform, Hilbert transform. With the help of exponential expansions and diagonal form of translation, the kernel matrices from these transforms can be quickly low-rank approximated into structured matrices called sequentially semiseparable (SSS) matrices. Further, we can transfer SSS matrix representation to hierarchical semiseparable (HSS) matrix representation, which would be a more stable form for matrix-vector multiplication. Stability analysis and numerical experiments of two matrix representations will be compared and demonstrated.

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MS43

Low Rank Everywhere (Almost)

Tile low rank and hierarchical low rank matrices can exploit data sparsity discoverable all across computational science: integral equations, differential equations (Schur complements), spatial statistics (covariances), optimization (Hessians), data compression, RBF-based meshing, non-Fickian diffusion, seismic redatuming, acoustic scattering, adaptive optics, and more, and can improve performance dramatically by living higher in the memory hierarchy than their dense counterparts. We illustrate in large-scale applications and hybridize with similarly motivated mixed precision representations.

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MS43

A Black Box O(N) Compression Algorithm for Rank Structured Matrices

The talk describes a randomized algorithm for computing a data sparse representation of a "hierarchically block separable" (aka HSS) matrix. The algorithm is black box in the sense that it interacts with the matrix to be compressed only through its action on vectors, making it ideal for tasks such as forming Schur complements or matrix matrix multiplication. In situations where the operator to be compressed (and its transpose) can be applied in O(N) operations, the compression as a whole has linear complexity.

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MS44

Soft Elasticity via Domain Formation in Magnetoactive Laminates

Reinforced elastomeric composites with periodic microstructures can undergo both microscopic and macroscopic instabilities. This talk is concerned with the post-bifurcation response of magneto-active elastomeric laminates after the possible development of a macroscopic instability. Building on earlier work in the purely mechanical context, it is shown that the response after the onset of a macroscopic instability corresponds to domain formation and is associated with soft modes of deformation that can be controlled by an externally applied magnetic field. Thus, making use of generalized notions of quasiconvexification and rank-1 convexification in the magnetoelastic context, we obtain estimates for the relaxation of the magneto-active composites and find long wavelength instabilities and soft modes of deformation under appropriate loading conditions. While the relaxation can only be computed exactly for certain loading conditions, upper and lower bounds based on the rank-1 convexification and polyconvexity, respectively, remain rather tight so long as the alignment of the magnetic field with the layers is not too close. One important finding is that strict global rank-one convexity of the principal solution is generally lost prior to strong ellipticity. In fact, only under pure shear loading with the magnetic field parallel and perpendicular to the layers are strong ellipticity and strict rank-one convexity lost simultaneously.

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MS44

An Energy Conserving Mechanism in Space-Time Metamaterials

Changing the microstructure properties of a space-time metamaterial while a wave is propagating through it, in general requires addition or removal of energy, which can be of exponential form depending on the type of modulation. This limits the realization and application of space-time metamaterials. We resolve this issue by introducing a novel mechanism of conserving energy in non-linear space-time media. The idea is first demonstrated by considering a wave-packet propagating in a discrete medium of 1-d chain of springs and masses, where using our energy conserving mechanism we show that the spring stiffness can be incremented at several time interfaces and the energy will still be conserved. We then consider an interesting application of time-reversed imaging in 1-d and 2-d spring-mass systems with a wave packet traveling in the homogenized limit. Our numerical simulations show that, in 1-d, when the wave packet hits the time-interface two sets of waves are generated, one traveling forward in time and the other traveling backward. The time-reversed waves re-converge at the location of the source and we observe its regeneration. In 2-d, we use more complicated initial shapes and even then, we observe regeneration of the original image

or source. Thus, we achieve time-reversed imaging with conservation of energy in a non-linear regime. The energy conserving mechanism can be easily extended to continuum media.

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MS44

Origami Structures that Produce, and Interact Constructively with, Twisted and Whorled Light

After a brief introduction to our work on "objective structures", we focus on Maxwells equations. We find solutions of Maxwells equations that are the precise analog of plane waves, but in the case that the translation group is replaced by the (largest) Abelian helical group. These waves display constructive/destructive interference with helical atomic structures, in the same way that plane waves interact with crystals. We show how the resulting far-field pattern can be used for structure determination, and we test the idea theoretically on the Pf1 virus from the Protein Data Bank. We finish with remarks on the generalization of these results to conformal groups, leading to "whorled light".

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MS44

Dispersion in a Coiled Bar-Based Phononic Crystal as a Function of Joint Angle

In the last few years, there has been a great interest in developing spacing-saving acoustic metamaterials (AMM) by coiling acoustic ducts. Two main classes have been studied, where in one case ducts are coiled in a serpentine pattern, while in another ducts are flat wound, coiling about the wave transmission direction. The duct path length can be used to tune a Fabry-Perot type resonance, which has enabled multiple types of acoustic filters to be designed. Recently, elastic versions of coiled phononic crystals (PnC) have been realized by attaching spring-mass systems to a track. In this talk, the dispersion process of PnC composed of rigid masses linked by flexible bars are studied as a function of the coiling angle, which is swept between 0 (the extended case) and 90 (the completely coiled case) degrees. Interestingly, when the PnC is completely coiled, the dispersion characteristics of the extended case are recovered, when proper boundary conditions are imposed. Additionally, it is shown that the discontinuity created at the joint in the frame (i.e. the coiling point node) itself acts as a scatterer and causes phononic bandgaps, in contrast to the coiled AMM designs.

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MS45

A Statistics-Informed Neural Network for Learning Stochastic Dynamics

In this talk, we present a machine-learning framework named statistics-informed neural network (SINN) for learning stochastic dynamics from data. This new architecture was theoretically inspired by a universal approximation theorem for stochastic systems introduced in this paper and the projection-operator formalism for stochastic modeling. We devise mechanisms for training the neural network model to reproduce the correct *statistical* behavior of a target stochastic process. Numerical simulation results demonstrate that a well-trained SINN can reliably approximate both Markovian and non-Markovian stochastic dynamics. We demonstrate the applicability of SINN to model transition dynamics. Furthermore, we show that the obtained reduced-order model can be trained on temporally coarse-grained data and hence is well suited for rare-event simulations.

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MS45

A Deep Learning Method for Distributions in Stochastic Dynamical Systems

The time evolution of the probability distribution of a stochastic differential equation follows the Fokker-Planck equation, which usually has an unbounded, high-dimensional domain. We propose a deep learning method, which represents the solution function as an artificial neural network. The presence of the differential operator in the loss function improves the accuracy of the neural network representation and reduces the demand of data in the training process. The method demonstrates effectiveness on high dimensional numerical examples.

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MS45

Generalized Second Fluctuation-Dissipation Theorem and Far-from-Equilibrium Transport

In this talk, we will introduce a generalized second fluctuation-dissipation theorem (FDT) for stochastic dynamical systems in the nonequilibrium steady state. The established theory is built upon the Mori-type generalized Langevin equation for stochastic dynamical systems using only the properties of the associated Kolmogorov operator. In particular, we show that for nonequilibrium states such as heat transport between two thermostats with different temperatures, the classical second FDT is valid even when the exact form of the steady-state distribution is unknown.

The obtained theoretical results enable us to construct a data-driven nanoscale fluctuating heat conduction model based on the new FDT. We numerically verify that the new model of heat transfer yields better predictions than the Green-Kubo formula for systems far from equilibrium.

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MS46

A DPG Space-Time Vlasov-Poisson Discretization with Adaptive Mesh Refinement

Efficient solution of the Vlasov equation, which can be up to six-dimensional, is key to the simulation of many difficult problems in plasma physics. The discontinuous Petrov-Galerkin (DPG) finite element methodology provides a framework for the development of stable (in the sense of LBB conditions) finite element formulations, with built-in mechanisms for adaptivity. We are developing space-time DPG formulations for Vlasov solvers, with the goal to solve problems in up to the full seven-dimensional setting. For this purpose, we employ tensor-product data representations supported by recent additions to the Intrepid2 package within Trilinos, as well as corresponding developments within Camellia, a finite element library designed to facilitate rapid development of computationally efficient, hp-adaptive finite element solvers, starting with support for DPG. In this talk, we discuss our progress to date, as well as efforts to combat the curse of dimensionality, with some initial adaptive mesh refinement results from space-time Vlasov problems.

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MS46

Asymptotic Preserving Discontinuous Galerkin Methods for a Linear Boltzmann Semiconductor Model

A key property of the linear Boltzmann semiconductor model is that as the collision frequency tends to infinity, the phase space density f = f(x,v,t) converges to an isotropic function M(v)?(x,t), called the drift-diffusion limit, where M is a Maxwellian and the physical density ? satisfies a second-order parabolic PDE known as the drift-diffusion equation. Numerical approximations that mirror this property are said to be asymptotic preserving. In this talk we build two discontinuous Galerkin methods to the semiconductor model: one with the standard upwinding flux and the other with a e-scaled Lax-Friedrichs flux, where 1/e is the scale of the collision frequency. We show that these schemes are uniformly stable in e and are asymptotic preserving. In particular, we discuss what properties the discrete Maxwellian must satisfy in order for convergence in e to an accurate h-approximation of the drift diffusion limit. Discrete versions of the drift-diffusion equations and error estimates in several norms with respect to e and the spacial resolution are also included.

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MS46

Low-Memory, Discrete Ordinates, Discontinuous Galerkin Methods for Radiative Transport

The discrete ordinates discontinuous Galerkin (S_N-DG) method is a well-established and practical approach for solving the radiative transport equation. In this talk, we present a low-memory variation of the upwind S_N-DG method. The proposed method uses a smaller finite element space that is constructed by coupling spatial unknowns across collocation angles, thereby yielding an approximation with fewer degrees of freedom than the standard method. Like the original S_N-DG method, the low-memory variation still preserves the asymptotic diffusion limit and maintains the characteristic structure needed for mesh sweeping algorithms. While we observe second-order convergence in scattering dominated, diffusive regime, the low-memory method is in general only first-order accurate. To address this issue, we use upwind reconstruction to recover second-order accuracy. For both methods, numerical procedures based on upwind sweeps are proposed to reduce the system dimension in the underlying Krylov solver strategy.

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MS47

Enhanced Sampling Methods for the Calculation of Nonequilibrium Steady-States

We present an asymptotic error analysis of stratified MCMC algorithms designed for non-equilibrium systems. The injection measure method, which is also a form of non-equilibrium umbrella sampling (NEUS), can be viewed in the asymptotic limit as an algebraic multi-grid method, or as an iterative aggregation-disaggregation (IAD) method. Accordingly, we apply an analysis inspired by the theory of IAD algorithms to estimate the asymptotic rate of convergence of the stratified sampling method. We derive bounds on the limiting rate and conditions for it to be fast compared to non-stratified MCMC method. We also give examples of how the theory applies to sampling non-equilibrium stochastic systems and numerical evidence of sharpness of the bounds.

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MS47

Steady-State Solutions for Nonequilibrium Langevin Dynamics

Nonequilibrium molecular dynamics (NEMD) techniques are used to study molecular fluids under steady, inhomogeneous flow. We prove that nonequilibrium Langevin dynamics (NELD) applied to planar flows converges exponentially fast to a steady-state limit cycle. We use the automorphism remapping periodic boundary conditions (PBCs) techniques such as Lees and Edwards PBCs and Kraynik and Reinelt PBCs to treat respectively shear flow and planar elongational flow. After reformulating the NELD in the Lagrangian domain, the convergence is shown using a technique similar to [R. Joubaud, G. A. Pavliotis, and G. Stoltz,2014].

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MS47

Tensor-Valued Atomic Cluster Expansion for Inference of Dynamical Systems

Complex physical systems are commonly parametrized by tensor-valued coefficients that are functions of the current state of the system. For example, rigorous derivation of the dynamics via the Mori-Zwanzig projection formalism of coarse-grained atomistic systems typically results in a (generalized) Langevin equation with configuration-dependent friction and diffusion coefficients. Learning the dynamics of such systems from data and simulating the inferred model requires efficient parametric representations of such tensor-valued functions. More specifically, such representations should allow for computationally efficient evaluation and data-efficient estimation of their parametrization from data. The framework of the recently proposed Atomic Cluster Expansion (ACE) [R. Drautz, Atomic cluster expansion for accurate and transferable interatomic potentials", 2018] has been successfully used for inference of potential energy surfaces and force fields of atomistic systems from data. In this talk, I will present some recent work that was performed in collaboration with C. Ortner which extends the framework of the Atomic Cluster Expansion to equivariant tensor-valued functions. I will discuss the derivation of the resulting basis expansions for matrix-valued and vector-valued functions. Moreover, I will present the results obtained by applying our approach to atomistic trajectory data.

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MS47

Mobility Estimation for Langevin Dynamics Using Control Variates

The scaling of the mobility of two-dimensional Langevin dynamics in a periodic potential as the friction vanishes is not well understood for non-separable potentials. Theoretical results are lacking, and numerical calculation of the mobility in the underdamped regime is challenging because the computational cost of standard Monte Carlo methods is inversely proportional to the friction coefficient, while deterministic methods are ill-conditioned. In this talk, we present a new variance-reduction method based on control variates for efficiently estimating the mobility of Langevin-type dynamics. We provide bounds on the bias and variance of the proposed estimator, and illustrate its efficacy through numerical experiments, first in simple one-dimensional settings and then for two-dimensional Langevin dynamics. Our results corroborate previous numerical evidence that the mobility scales as $\gamma^{-\sigma}$, with $0 < \sigma \leq 1$, in the low friction regime for a simple non-separable potential.

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MS48

Communication Bounds for Convolutional Neural Networks

Convolutional neural networks (CNNs) are important in a wide variety of machine learning tasks and applications, so optimizing their performance is essential. Moving words of data between levels of a memory hierarchy or between processors on a network is much more expensive than the cost of arithmetic, so minimizing communication is critical to optimizing performance. In this paper, we present new precise lower bounds on data movement for convolutions in both single-processor and parallel distributed memory models, as well as algorithms that outperform current implementations such as Im2Col. We obtain performance figures using GEMMINI, a machine learning accelerator, where our tiling provides improvements between 13% and 150% over a vendor supplied algorithm.

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MS48

Spectral Instabilities of Periodic Water Waves

Spectral instabilities of small-amplitude, periodic water waves are investigated using a newly developed perturbation method. These instabilities include the classic Benjamin-Feir instability as well as instabilities appearing away from the origin in the complex spectral plane. Explicit estimates of instability growth rates and coherent structures are obtained and compared with numerical results, to excellent agreement.

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MS48

Transmission of Quantum States in Spin Networks

Quantum algorithms are known to solve problems exponentially faster than classical counterparts, such as integer factorizations and the black box problem. For this reason, quantum computing has gained considerable attention in recent years. However, in order to construct a quantum computer, one needs to accomplish the accurate transmission of quantum states from one location in the quantum computer to another, as well as generating entanglements between quantum states. In this talk, we discuss the various types of quantum transport phenomena (such as periodicity, perfect state transfer, and fractional revival), and provide necessary and sufficient conditions for them to occur.

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MS49

A New Higher Order Displacement Discontinuity Method Based on the Joint Element for Analysis of Close-Spacing Planar Fractures

The 2D displacement discontinuity method (DDM) has been widely used to characterize the hydraulic fracture geometry and the induced in-situ stresses in the oil and gas industry owing to its simplicity and accuracy. As smaller fracture spacing is used by multistage fracturing, the constant DDM (CDDM) loses its accuracy in predicting the fracture behaviors, especially for the inner fractures in a stage where they are subjected to the strong stress shadowing effect. In this work, the 2D higher order DDM (HDDM) based on the joint elements was developed to overcome this limitation. The higher order displacement discontinuity intensively increases the accuracy of CDDM but maintains the same amount of computation time by using patched-element pattern. The joint elements are introduced to simultaneously determine the opening, shearing, and closing of each fracture element based on the stress boundary condition, which can avoid the negative width of the inner fractures given by CDDM which are mechanically closed under the strong stress shadowing effect. The developed 2D joint element HDDM (JE-HDDM) gives the same results with the CDDM when the fracture spacing is relatively large, but shows its outperformance in both efficiency and accuracy over the CDDM in predicting the displacement discontinuities and induced in-situ stresses in close fracture-spacing case.

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MS49

Through-Wall Detection of the Moving Paths and Vital Signs of Human Beings

Through-wall detection of the moving paths and vital signs of human beings Abstract: Detection of human activities in complex environments such as through wall by ultrawideband radar has many important applications in security, vital rescue, and so on. It is much more difficult to detect vital signs of moving human beings than static ones. In this letter, we build a model for moving targets and apply the time domain finite element method to simulate single-input multiple-outputs (SIMO) radar data. Human respiration is modeled by changing body size and physical parameters. The background removal is performed for radar data. Then, we use the back projection to reconstruct the consecutive target locations, which constitute the moving path, leading to a curve carrying vital signs in the radar image. Since SIMO radar data are multivariate, we use multivariate empirical mode decomposition (MEMD) and fast Fourier transform to separate and extract the respiratory characteristic frequencies. The reconstructed frequency coincides with that in the original model. The result shows that the combination of SIMO radar and MEMD can effectively identify the moving path of the human being behind the wall and extract vital signs.

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MS49

Application of Discrete Element Numerical Simulation in Fold and Thrust Belts

The discrete element method (DEM) is a particle-based numerical approach that employs iterative calculation of particle displacement and force to solve Newtonian mechanics motion " [Cundall and Strack, A Discrete Numerical Mode For Granular Assemblies: Gotechnique,1979] ". One of the attractions of DEM is that discrete particles under the contact mechanism can localize strain and yield emergent behaviors in the system. We can use different material properties to simulate discontinuities and heterogeneities and apply the stress field of extrusion or tension. The technique resembles a numerical sandbox but can offer added information by monitoring mechanical states correlated with deformation behavior and structure throughout the simulation and directly output the stress-strain characteristics of the deformation process. Our implementation of DEM adopted Hertz-Mindlin contact mechanics model " [Morgan and Julia, Effects of cohesion on the structural and mechanical evolution of fold and thrust belts and contractional wedges: Discrete element simulations, 2015], [Li, Calibration of the discrete element method and modelling of shortening experiments, 2021] ". Based on the numerical experimental results, We can gain insight into the geometric characteristics and tectonic evolutions in the fold and thrust belts deformation of the northwestern Sichuan Basin and eastern Sichuan Basin.

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MS49

Integrating Fractional Flow Theory with Fully Compositional Wellbore Models and Reservoir Simulations

Multi-phase compositional wellbore flow is important in determining the flow and pressure drop in oil, gas and geothermal wells. These effects become increasingly important in long laterals with multiple locations for fluid influx. Complex hydrocarbon phase behavior such as change in the number of phases, phase flipping, gas slippage can happen in the wellbore flow because of changes in pressure,

temperature and inflow fluid rate and composition along the wellbore. This paper introduces a new wellbore model which integrates fully compositional fluid flow with an energy balance and pipe fractional-flow theory with multiple points of fluid entry along the wellbore. Four sets of governing equations: component mass conservation, momentum conservation, phase behavior and temperature are solved fully implicitly along the wellbore. This is then fully coupled with the flow and energy balance equations in the reservoir and fracture domains. The primary unknowns along the wellbore (total flow rate, fluid composition, fluid saturations, pressure, and temperature) can then be obtained. Flash calculation is done to calculate the phase saturation, density, viscosity, etc. and the flow rate of each phase is obtained from the fractional flow theory given the local flow rate and saturations.

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MS50

Machine-Learning of Nonlocal Models for Anomalous Subsurface Transport from Breakthrough Curves

Anomalous behavior is ubiquitous in subsurface solute transport due to the presence of high degrees of heterogeneity at different scales in the media. We propose the use of nonlocal models characterized by integrable kernels and finite interaction length as a computationally feasible alternative to other descriptions, such as fractional models. Due to the difficulty in choosing appropriate nonlocal kernel functions, we introduce a data-driven framework for the discovery of optimal kernels on the basis of very small and sparse data sets. Using spatially sparse breakthrough curves, we learn the best coarse-scale nonlocal model using a nonlocal operator learning technique. Predictions of the breakthrough curves obtained using the optimal nonlocal model show good agreement with fine-scale simulation results even at locations and time intervals different from the ones used to train the kernel, confirming the excellent generalization properties of the proposed algorithm. A comparison with trained classical models and with black-box deep neural networks confirms the superiority of the predictive capability of the proposed model.

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MS50

A Spectral Approach for Time-Dependent PDEs Using Machine-Learned Basis Functions

A major obstacle in the deployment of spectral methods is the choice of appropriate bases for trial and test spaces. If chosen suitably, these basis functions lead invariably to well-posed discretized problems and well-conditioned linear systems, while the resulting approximate solutions are provably high-order accurate. However, barring domain decomposition approaches, devising such functions for arbitrary geometries from scratch is a hugely challenging task. Fortunately, the recently developed DeepONet approach is a highly promising device for generating machine-learned basis functions. In this talk, we propose a Galerkin approach for time-dependent PDEs that is powered by basis functions gleaned from the DeepONet architecture. We shall outline our procedure for obtaining these basis functions and detail their many favourable properties. Next, we shall present the results of numerical tests for various problems, including advection, advection-diffusion, KortewegDe Vries, viscous Burgers equations, as well as some highly intriguing preliminary results from the low-viscosity regime. Finally, we will identify potential obstacles in the course of generalization to higher dimensions and suggest possible remedies.

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MS50

Learning Deep Integral Neural Operators for Heterogeneous Material Modeling

Constitutive modeling based on the continuum mechanics theory has been a classical approach for modeling the mechanical responses of materials. However, when constitutive laws are unknown or when defects and/or high degrees of heterogeneity present, these classical models may become inaccurate. In this work, we propose to use data-driven modeling which directly utilizes high-fidelity simulation and/or experimental measurements on displacement fields, to predict a material's response without the necessity of using conventional constitutive models. Specifically, the material response is modeled by learning maps between loading conditions and its resultant displacement fields, so that the network is a surrogate for a solution operator. To model the complex material responses, we develop a novel deep neural operator architecture based on the Fourier Neural Operator (FNO) method, which we coin DeepFNO. In DeepFNO, we model the increment between layers as an integral operator, to capture long-range dependencies in the feature space and allow for accelerated learning techniques for deep networks. We demonstrate the performance of our method for a number of examples, including hyperelastic, anisotropic and brittle fracture materials. As an application, we employ the proposed approach to learn material models directly from digital image correlation (DIC) tracking measurements, and show that the learnt solution operators substantially outperform conventional constitutive models.

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MS51

Open Markets and Rank Jacobi Processes

We study growth optimization in large equity markets over long time horizons in the context of Stochastic Portfolio Theory. In such settings investors are often confined to trading in an "open market" setup consisting of only the assets with high capitalizations. We relax the notion of an open market and develop a tractable framework to study them under mild structural conditions on the market. Within this framework we introduce a large parametric class of processes, which we call *rank Jacobi models*. These models (i) produce stable capital distribution curves, (ii) exhibit explicit expressions for growth-optimal portfolios, (iii) serve as worst-case models for a robust asymptotic growth problem under model ambiguity and (iv) have capital distribution curves, optimal portfolios and growth rates which are stable with respect to the dimension of the market.

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MS51

Ergodic Robust Maximization of Asymptotic Growth

In this talk, we revisit "Robust Asymptotic Growth" (Kardaras, Robertson 2012) where an investor seeks to maximize the growth rate of her portfolio when there is uncertainty in the drift of asset dynamics. Our goal is to extend analysis to where asset dynamics are stable in that a limiting measure exists. Such stability naturally arises in stochastic portfolio theory, where optimal policies are governed by the ranked relative market capitalizations. We provide simple conditions upon the domain, covariance matrix and limiting measure under which robust growth optimal portfolios exist. After presenting results for the case when asset dynamics do not exhibit local time behavior on the boundary of the state space, the case containing local times will be considered, as this is the natural setting for ranked based diffusions, which our primary example of interest. This is joint work with Kostas Kardaras, of the London School of Economics.

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MS51

Modeling Transaction Costs in Stochastic Portfolio Theory

An important open problem in stochastic portfolio theory is to incorporate transaction cost and turnover in the construction of portfolios. In this talk, we examine empirically the factors which influence the performance of a functionally generated portfolio, under transaction costs, as the rebalancing frequency changes. Then we propose some rebalancing strategies and study their performance.

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MS51

Learning Relative Arbitrage Opportunities in N-Agent and Mean Field Regimes

We shall discuss the multi-agent optimization of relative arbitrage problems. The objective is characterized by the smallest non-negative continuous solution of the Cauchy problem for the associated partial differential equation. However, solving this presents many challenges due to the non-uniqueness and the curse of dimensionality. In this paper, we provide a deep learning approach to tackle minimal solutions in high-dimensional PDEs by studying the associated obstacle problem based on the Deep Galerkin Method. We show that the minimal deep learning based solution is a good approximation in the volatility-stabilized models when compared to the grid-based numerical solution.

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MS52

An Impossibility Theorem for Two-Player Two-Dimensional Vector Addition Game

Consider a constant-sum two-player game where players A and B are taking turns adding 2-dimensional, positive, integer vectors to some vector v, the game will end when the sum of v's components reaches a certain threshold. Then A and B will receive utility such that if v's x component is larger, A will receive more utility, otherwise B receives more utility. We will show that it is impossible for an agent to win by a certain value in this setting.

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MS52

Robust Simulations of Turbulent Mixing due to Richtmyer-Meshkov Instability of an Air/SF_6 Interface Using Front Tracking

Turbulent mixing due to hydrodynamic instabilities occurs in a broad spectrum of engineering, astrophysical and geophysical applications. Theory, experiment, and numerical simulation help us to understand the dynamics of hydro-dynamically unstable interfaces between fluids. In this talk, an increasingly accurate and robust front tracking method for the numerical simulations of Richtmyer-Meshkov Instability (RMI) is used to simulate the growth rate is presented. Front tracking is an adaptive computational method where the front (interface) between fluids is explicitly followed. Front tracking represents interfaces as lower dimensional meshes moving through a rectangular grid. All the states (pressure, density, and velocity) on the center of each grid cell are updated using the classical fifth order weighted essentially non-oscillatory (WENO) scheme of Jiang and Shu along with Yang's artificial compression. The strength of this method is shown through simulation

of the single mode Mach 1.11 and Mach 1.2 shock tube experiments of an air/SF_6 interface by Collins and Jacobs (2002). We observe a very good agreement of early time amplitude and displacement of the Mach 1.11 experiment and 4% discrepancy on our fine grid computation compared to the Mach 1.2 experiment.

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MS52

Finding Patterns in the Inertia of the Distance Squared Matrix of Unicyclic Graphs

We analyze the spectrum of the distance squared matrix of a tree and give a relation between the inertia of the distance squared matrix and the structure of the tree. We take the result one step further and consider the addition of exactly one cycle in the tree. We obtain an expression for the inertia of the distance squared matrix of a cycle graph. We obtain a bound on the inertia of the distance squared matrix of an arbitrary unicyclic graph.

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MS52

Nash Equilibria in Certain Two-Choice Multi-Player Games Played on the Ladder Graph

In this research, we compute analytically the number of Nash Equilibria (NE) for a two-choice game played on a ladder graph and a circular ladder with 2n players, identified by the vertices of the graph. We do not fix the payoff parameters of the underlying two-player game, except for the requirement that a NE occurs if the players choose opposite strategies (anti-coordination game). The results show that for both, the ladder and circular ladder, the number of NE grows exponentially with (half) the number of players as $NE(2n)\ C(\phi)^n$, where $\phi = 1.618.$ is the golden ratio and C is a constant. In addition, the value of the scaling factor C_{ladder} depends on the value of the payoff parameters. However, that is no longer true for the circular ladder (3-degree graph), that is C_{circ} is constant, which might suggest that the topology of the graph indeed plays an important role for setting the number of NE.

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MS53

Equilibria of Charged Hyperelastic Solids

We investigate equilibria of charged deformable materials via the minimization of an electroelastic energy. This features the coupling of elastic response and electrostatics by means of a capacitary term, which is naturally defined in Eulerian coordinates. The ensuing electroelastic energy is then of mixed Lagrangian-Eulerian type. We prove that minimizers exist by investigating the continuity properties of the capacitary terms under convergence of the deformations.

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MS53

Bilevel Learning for Variational Nonlocal Image Denoising Models

We propose a bilevel learning approach for the estimation of parameters in variational nonlocal image denoising models. The considered parameters are both the scale-dependent fidelity weight and the weights within the kernel of the nonlocal operator. For nonlocal means type models, we investigate the differentiability of the solution operator in function spaces and derive optimality systems that characterize local minima. For the case of nonlocal TV type models, nonsmooth properties of the variational models are investigated and a reformulation of the problems as Mathematical Programs with Complementarity Constraints (MPCC) is proposed. For the numerical solution of the problems, we propose a second-order trust-region algorithm and introduce a computational strategy for the solution of the resulting dense linear systems. Several experiments illustrate the applicability and effectiveness of our approach.

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MS53

Regularization of Inverse Problems meets Calculus of Variations

Variational regularization theory of ill-posed inverse problems with known forward models has a long tradition spanning all the way back to the seminal contributions of Tikhonov in the 1940s. It studies questions like consistency as the regularization parameter and noise level converge to zero simultaneously, generally from a functional-analytic point of view. Often, and in particular when dealing with imaging applications like deblurring or Radon transform inversion for tomography, the regularization energies used in such approaches contain spatial derivatives. As such, they also have rich analytical backgrounds in terms of properties of minimizers. In this talk, I will present some recent work bridging these two areas together. Within the regime of vanishing noise and regularization parameter, we obtain results of convergence in Hausdorff distance of level sets of minimizers (which can be interpreted as objects to be recovered in an imaging context) and uniform L^∞ bounds. These hold not only with total variation regularization, but also when penalizing fractional Sobolev seminorms.

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MS53

The Robustness of ENZ Materials

ENZ materials represent a class of electromagnetic materials whose dielectric permittivity is very small at isolated frequencies; they have found applications in the design of entirely new classes of waveguides and in the so-called photonic doping. We study the robustness of ENZ materials in the sense of variation due to the presence of material losses. We also study resonances in such ENZ systems.

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MS54

Fast Boundary Integral Methods for Confined Suspension Flows

Particulate flows are ubiquitous in the study of self-assembly of biological structures and the design of soft materials. In many examples across application fields, it has become apparent that resolving confinement, short term forces (e.g. contact) and long-term forces (e.g. hydrodynamics) is crucial to capture key features of these phenomena. This talk will focus on the current state-of-the-art on the BIE-based methods for fluid suspensions simulation, as well as ongoing challenges in this area. I will discuss some of our recent work applying this boundary integral framework to simulate Janus particle systems, that is, of particles whose surfaces exhibit two distinct physical properties.

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MS54

A Fast Direct Solver for Surface PDEs

We introduce a fast direct solver for variable-coefficient elliptic partial differential equations on surfaces based on the hierarchical PoincarSteklov method. The method takes as input a high-order quadrilateral mesh of a surface and discretizes surface differential operators on each element using a high-order spectral collocation scheme. Elemental solution operators and Dirichlet-to-Neumann maps tangent to the surface are precomputed and merged in a pairwise fashion to yield a hierarchy of solution operators that may be applied in $\mathcal{O}(N \log N)$ operations for a mesh with N elements. The resulting fast direct solver may be used to accelerate implicit time-stepping schemes, as the precomputed operators can be reused for fast elliptic solves on surfaces. We apply the method to a range of problems on both smooth surfaces and surfaces with sharp corners and edges, including the static LaplaceBeltrami problem, the Hodge decomposition of a tangential vector field, and some time-dependent reactiondiffusion systems.

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MS54

A New Class of Hierarchical Matrices for Elliptic Problems in Higher Dimensions

Hierarchical matrices, such as HODLR, HSS, H, H2, etc, are used in solving rank structured linear systems arising out of a wide range of applications including PDEs, machine learning, etc. The talk will focus on a new class of hierarchical matrices that offer an attractive way of representing dense matrices arising out of the discretization of elliptic PDEs in higher dimensions. We will further substantiate the rank structuredness of this new hierarchical structure and demonstrate its applicability and scalability by solving elliptic PDEs using this new rank structured hierarchical matrix.

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MS54

Hierarchical Skeletonization for Integral Equations in Multiply-Connected Domains

This talk presents a general method for applying hierarchical matrix skeletonization factorizations to the numerical solution of boundary integral equations with possibly rank-deficient integral operators. Rank-deficient operators arise in boundary integral approaches to elliptic partial differential equations with multiple boundary components, such as in the case of multiple vesicles in a viscous fluid flow. Our generalized skeletonization factorization retains the locality property afforded by the "proxy point method," and allows for a parallelized implementation where different processors work on different parts of the boundary simultaneously. Further, when the boundary undergoes local geometric perturbations (such as movement of an interior hole), the factorization can be recomputed efficiently with respect to the number of modified discretization nodes.

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MS55

Unsupervised Learning of Observation Functions in State-Space Models by Nonparametric Moment Methods

With advances in technology, unlabeled data can be collected constantly with little cost. However, data labeling is still costly and inaccurate. Therefore, it is desirable to learn the observation map and the hidden dynamics from unlabeled data. We investigate the unsupervised learning of non-invertible observation functions in nonlinear state-space models. Given abundant data of the observation process and the distribution of the state process, we estimate the observation function via constrained nonparametric regression. The major challenge is posed by the non-invertibility of the observation function. We also address the fundamental issue of identifiability. We show that the function space of identifiability is a certain reproducing kernel Hilbert space (RKHS) that is model-intrinsic and data-adaptive. We demonstrate using synthetic data that the first two moments and temporal correlations can identify functions (ranging from piecewise polynomials to smooth functions) in this RKHS. This work is joint with Fei Lu.

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MS55

Graph-Laplacian for Bayesian Elliptic Inverse Problems on Manifolds

I will discuss recent efforts in solving Bayesian inverse problems involving elliptic PDEs on unknown domains, identified with point clouds data that lie on a Riemannian compact embedded manifold. To solve the inverse problems, we devise graph-Laplacian-based methods for constructing Matern type priors and solving mesh-free PDE solvers. When the manifolds have Dirichlet boundary conditions, we represent the prior as linear superpositions of Dirichlet Laplacian eigenfunctions and solutions of harmonic functions with appropriate boundary conditions. Computationally, we will realize these with a graph-Laplacian formulation that is provably consistent with the homogeneous Dirichlet Laplace-Beltrami operator and the Ghost-Point Diffusion Maps algorithm for solving elliptic PDEs with classical boundary conditions.

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MS55

Nonparametric Estimation of Nonlinear Operators Between Function Spaces by Deep Neural Networks

Learning operators between infinitely dimensional spaces is an important learning task arising in wide applications in machine learning, imaging science, mathematical modeling and simulations, etc. This talk is about nonparametric estimation of Lipschitz operators between Hilbert spaces using deep neural networks. I will present a non-asymptotic upper bound for the generalization error of the empirical risk minimizer over a properly chosen network class. Under the assumption that the target operator exhibits a low dimensional structure, our error bounds decay as the training sample size increases, with an attractive fast rate depending on the intrinsic dimension in our estimation. Our assumptions cover most scenarios in real applications and our results give rise to fast rates by exploiting low dimensional structures of data in operator estimation.

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MS55

Adaptive Group Lasso Neural Network Models for Function of Few Variables and Time-Dependent Data

In this paper, we propose an adaptive group Lasso deep neural network for high-dimensional function approximation where input data are generated from a dynamical system and the target function depends on a few active variables or a few linear combinations of variables. We approximate the target function by a deep neural network and enforce an adaptive group Lasso constraint to the weights of a suitable hidden layer in order to represent the constraint on the target function. We utilize the proximal algorithm to optimize the penalized loss function. Using the non-negative property of the Bregman distance, we prove that the proposed optimization procedure achieves loss decay. Our empirical studies show that the proposed method outperforms recent state-of-the-art methods including the sparse dictionary matrix method, neural networks with or without group Lasso penalty.

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MS56

Liquid Metal Networks in Rubber for Highly Elastic Dielectrics and Conductors

Enhancing the electrical permittivity and conductivity of elastomers represents a grand challenge in the field of soft materials engineering. Dielectric and conductive elastomers have a central role in the performance of a wide range of emerging soft-matter technologies, from stretchable electronics to electrostatically-controlled actuators, sensors, and energy harvesting transducers. One approach to tailoring the electrical properties of elastomers is to add metal filler. However, the addition of rigid filler can re-

duce the mechanical compliance and elasticity of the host elastomer. To avoid this trade-off, I introduce an alternative approach in which the rigid filler is replaced with a dispersion of droplets of liquid-phase metal alloy. Using eutectic gallium-indium (EGaIn) as the liquid metal, I show that it is possible to engineer soft conductors and high permittivity dielectrics that preserve the mechanical properties of the host elastomer. In this talk, I will examine the underlying principles of engineering these EGaIn-filled elastomer composites and present theoretical models based on effective medium approximations and computational techniques. In particular, I will use these theories to examine the influence of EGaIn microstructure on dielectric constant, thermal conductivity, and electromechanical coupling and show how they lead to predictions that are in reasonable agreement with experimental measurements.

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MS56

Magneto-Deformations and Instability-Induced Microstructure Transformation in Soft Magnetoactive Materials

We study the behavior of magnetoactive elastomers (MAE) subjected to an external magnetic field. We analyze the role of the microstructures in the overall performance and stability of the soft active composites. We examine the coupled behavior of the active composites with (i) periodically and (ii) randomly distributed active particles embedded in a soft matrix, and (iii) periodic laminate composites and anisotropically structured composites with chain-like structures. We identify the key parameters governing the magneto-mechanical couplings. Moreover, we find advantageous microstructures that give rise to significant enhancement of the coupling and actuation of the active materials. Furthermore, we show that even very similar microstructures, such as periodic composites with hexagonal and rectangular representative volume elements, exhibit very different behavior in terms of their actuation and effective properties. Next, we investigate the coupled magneto-elastic instabilities MAE. These instabilities may occur at different length scales, and, potentially, they may be exploited to achieve new functionalities such as tunable band-gaps. We explore the role of external magnetic fields, microstructure parameters, and consentient properties on the multiscale instabilities.

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MS57

Numerical Method for Surface Quasi-Geostrophic Flows

We consider the surface quasi-geostrophic (SQG) flow system modeling the dynamic of the buoyancy at the poles. The Eckman pumping as well as the relation between the buoyancy and vorticity are expressed using fractional operators resulting to a system defined over a two-dimensional periodic domain. Continuous linear finite elements for the space discretizations and three stages Runge-Kutta method for the time discretizations are analyzed. The positive and negative fractional powers of elliptic operators are represented using DunfordTaylor integrals [Bonito and Pasciak 2015] and thus only require the solution to standard reaction-diffusion problems for their approximations. To cope with the hyperbolic nature of the system, the algorithm takes advantage of a flux corrected transport limiting algorithm coupling a low order maximum principle preserving scheme with a higher order scheme [Guermond and Popov 2017]. In the inviscible case, the resulting numerical method satisfies a maximum principle under a typical CFL condition. It is formally third order in time and second order in space.We briefly describe the analysis of the algorithm and illustrate its performances on different benchmarks. We also discuss a numerical study of freely decaying turbulence to exhibit the intricate nature of the SQG system.

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MS57

Multigrid Methods for Computing Glacier Geometry

Multigrid methods have been applied to the Stokes [Isaac et al 2015] and hydrostatic [Brown et al 2013; Tumarino et al 2016] momentum conservation models for glacier velocity, namely to PDEs for nonlinear viscous flow, but they have not been applied to the coupled problem which determines glacier geometry from flow and climate inputs. Here we consider the steady and implicit-step glacier geometry problems. For land-based glaciers these are nonlinear complementarity problems, or variational inequalities, which combine the surface kinematical equation with the constraint that the ice surface is above the bed. Global solution regularity of these free-boundary problems is low. Multilevel methods must maintain admissibility while not introducing high frequencies at the free boundary during grid transfers. We describe a strategy for these problems based on the multilevel constraint decomposition method [Tai, 2003], in which coarse-grid corrections come from convex sets. The strategy has novel aspects, especially a full-approximation-scheme implementation and asymmetric cycle structure. The strategy is agnostic with respect to the choice of (coupled) velocity equations, but this talk will demonstrate a successful implementation in the shallow ice approximation case.

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MS57

Advances in Initialization of Ice Sheet Models

The study of ice sheet dynamics is essential to estimate sea level rise. At the ice sheet scale, ice behaves like a very viscous shear-thinning fluid and can be modeled with highly nonlinear Stokes equations. The nonlinearities of the model, the large extension and complexity of the geometries, the free boundary nature of the problem and the uncertainties in the data and the model make the problem very challenging from a mathematical and computational point of view. In this talk we focus on the problem of estimating the ice sheet initial state so that it is consistent with the observations and present-day climate forcing (e.g. amount of precipitation). We initialize the ice sheet using a large-scale PDE-constrained optimization approach where the constraint is a simplification of the Stokes equations coupled to a temperature model. We discuss some of the computational challenges we face and provide results for Greenland and Antarctic ice sheets.

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MS58

Microstructure by Design: Thin Film Grain Growth Experiments

A grand challenge problem in engineering of polycrystals is to develop prescriptive process technologies capable of producing an arrangement of grains that provides for a desired set of materials properties. One method by which the grain structure is engineered is through grain growth or coarsening of a starting structure. Grain growth can be viewed as the evolution of a large metastable network, and can be mathematically modeled by a set of deterministic local evolution laws for the growth of an individual grain combined with stochastic models to describe the interaction between grains. Thus, to develop a predictive theory, investigation of a broad range of statistical measures of microstructure are needed. This talk will address not only the challenges of generating the thin film polycrystalline samples that are used as the test bed for in-situ and ex-situ experiments, but also the challenges of extracting the relevant microstructural metrics from the bright-field transmission electron images and the crystal orientation maps. The issues in machine learning approaches to automated grain boundary detection as well in integrating experiments with simulations and mathematical models and theory will also be discussed. The very significant contributions of students and collaborators to the research effort will be highlighted.

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MS58

Recent Advances in Modeling, Analysis and Simulation of Grain Growth in Polycrystalline Materials

Many technologically useful materials are polycrystals composed of small monocrystalline grains that are separated by grain boundaries of crystallites with different lattice orientations. A central problem in materials science is to develop technologies capable of producing an arrangement of grains that provides for a desired set of material properties. The evolution of grain boundaries and associated grain growth (coarsening) is a very complex multiscale process. It involves, for example, dynamics of grain boundaries, triple junctions, and the dynamics of lattice misorientations/grains rotations. It is observed that during grain growth, 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, simulation and analysis of the evolution of the grain boundary network in polycrystalline materials.

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MS58

Mathematics and Physics of Moire Flat Bands

Placing a two-dimensional lattice on another with a small rotation gives rise to periodic moire patterns on a superlattice scale much larger than the original lattice. This effective large-scale fundamental domain allows phenomena such as the fractal Hofstadter butterfly in the spectrum of Harpers equation to be observed in real crystals. Experimentalists have more recently observed new correlated phases at the magic twist angles predicted by theorists. We will give mathematical and computational models to predict and gain insight into new physical phenomena at the moir scale including our recent mathematical results for twisted trilayer graphene.

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MS58

New Perspectives on Grain Boundary Migration in Polycrystals

Using high-energy diffraction microscopy, we have measured the velocities of grain boundaries within a Ni polycrystal evolving by normal grain growth under a capillary driving force. Thousands of grain boundaries were tracked and their velocities and curvatures were classified by their crystallographic characteristics. Among the findings, two are noteworthy and will be discussed in this seminar. First, the velocities vary with all five crystallographic grain boundary parameters. Because boundaries are curved, and a single misorientation has a range of boundary plane orientations, one might expect the migration of grain boundaries with a particular misorientation to be independent of grain boundary plane orientation. However, on average, some orientations are faster than others and for a single misorientation, velocities can vary by a factor of three or more. Second, grain boundary velocity is independent of grain boundary mean curvature. Because curvature is an important component of the driving force, velocity and curvature are expected to be correlated positively. However, the evidence for such a correlation is poor. In the remainder of the talk, I will briefly present three possible explanations for these observations that can be discussed as a group: constrained migration of boundaries in connected networks, defect (disconnection) mediated grain boundary migration, and the influence of grain boundary stiffness on migration.

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MS59

Physics-Informed Neural Network for Ultrasound Non-Destructive Quantification of Cracks and Microstructures in Materials

PINNs are neural networks that can combine data and physics in the learning process by adding the residuals of a system of partial differential equations to the loss function. In this talk, we describe the efficacy of PINNs in solving the inverse problems encountered during non-destructive evaluation of materials. First, we introduce an optimized physics-informed neural network (PINN) trained to solve the problem of identifying and characterizing a surface breaking crack in a metal plate made of Aluminum alloy. PINNs are supervised with realistic ultrasonic surface acoustic wave data acquired at a frequency of 5 MHz. The PINN is physically informed by the acoustic wave equation. We use PINNs to compute the spatially varying speed of sound and identify and characterize the crack as the positions where the speed of sound has decreased. Second, we employed PINNs to quantify the microstructural properties of a polycrystalline Nickel by computing the spatial variation of compressibility and rigidity of the material. Here, PINNs are supervised with realistic ultrasonic surface acoustic wavefield data acquired for the polycrystalline Nickel along with the wavefield data generated numerically. The neural network is informed by the in-plane and out-of-plane elastic wave equations to infer spatially varying stiffness tensor of the polycrystalline Nickel. The spatially varying stiffness coefficients obtained from PINNs are in very good agreement with experimental results.

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MS60

Searching for Singularities in Navier-Stokes Flows Using Variational Optimization Methods

This investigation concerns a systematic computational search for potentially singular behavior in 3D Navier-Stokes flows. Enstrophy $\mathcal{E}(t)$ serves as a convenient indicator of the regularity of solutions — as long as this quantity remains finite, the solutions are guaranteed to be smooth and satisfy the equations in the classical sense. Another well-known conditional regularity result are the Ladyzhenskaya-Prodi-Serrin conditions asserting that the quantity $\mathcal{L}_{q,p} := \int_0^T \|\mathbf{u}(t)\|^p_{L^q(\Omega)}\, dt$, where $2/p + 3/q \leq 1$, $q > 3$, must remain bounded if the solution is smooth on the interval $[0, T]$. However, there are no finite a priori bounds available for these quantities and hence the regularity problem for the 3D Navier-Stokes system remains open. To quantify the maximum possible growth of $\mathcal{E}(T)$ and $\mathcal{L}_{q,p}$, we consider families of PDE optimization problems in which initial conditions are sought subject to certain constraints so that these quantities in the resulting Navier-Stokes flows are maximized. These problems are solved computationally using a large-scale adjoint-based gradient approach. By solving these problems for a broad range of parameter values we demonstrate that the maximum growth of $\mathcal{E}(T)$ and $\mathcal{L}_{q,p}$ appears finite. Thus, in the worst-case scenarios the two quantities remain bounded for all times and there is no evidence for singularity formation in finite time.

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MS60

Time Adaptive POD Reduced Order Model for Fluid Flows

A challenge in constructing proper orthogonal decomposition based reduced order model (POD-ROM) is its input dependency. In order to address this issue, we discuss time adaptive concepts. In particular, we propose a variable time step extrapolated second order backward difference method (VS-BDF2) for reduced order model of the Navier-Stokes equations modelling viscous incompressible flows. We prove stability and convergence of the proposed method under the assumption that the ratios of the adjacent time step sizes are bounded from above by a constant. We provide numerical comparison of the considered methods for a flow past airfoil problem.

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MS61

Framing RNN As a Kernel Method: A Neural ODE Approach

Building on the interpretation of a recurrent neural network (RNN) as a continuous-time neural differential equation, we show, under appropriate conditions, that the solution of a RNN can be viewed as a linear function of a specific feature set of the input sequence, known as the signature. This connection allows us to frame a RNN as a kernel method in a suitable reproducing kernel Hilbert space. As a consequence, we obtain theoretical guarantees on generalization and stability for a large class of recurrent networks. Our results are illustrated on simulated datasets.

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MS61

Signatures and Paths of Persistence Diagrams

Persistent homology is a tool from topological data analysis (TDA) which summaries the multi-scale topological structure of a point cloud data set in an object called a persistence diagram. The path signature is a feature map for sequential data which is both universal and characteristic, allowing us to study both functions and measures on the space of paths using linear methods. In this talk, we combine the theory of path signatures with persistent homology to study paths of persistence diagrams, which describe the temporally evolving topology of dynamic point clouds. Such dynamic point clouds naturally arise in the study of multi-agent systems such as swarms. We explore the theoretical and computational aspects of using path signatures to represent paths of persistence diagrams and apply it to a numerical parameter estimation problem for models of collective motion.

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MS61

Kernel Methods for PDEs and PDEs for Kernel Methods

In this talk I will discuss the interplay between kernel methods and PDEs, focusing on the signature kernel and machine learning applications dealing with sequential data. This relationship is mutually beneficial. Kernel-based techniques can be used to enhance the effectiveness of classical PDE solvers. Conversely, the theory of PDEs can help shed light on the theoretical properties of some kernel methods and help design effective learning algorithms.

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MS62

Mixed Classical and Impulse Control: Theory, Applications, Numerics

We consider a stochastic control problem involving both classical and impulse controls. We introduce a new variant of the stochastic Perron's method which allows us to simultaneously (1) characterize the value function as the unique viscosity solution of the associated dynamic programming equation, (2) establish convergence of a certain class of numerical schemes, and (3) characterize the value function as the pointwise minimum in a suitable class of excessive functions. Moreover, we show how these results can be used to construct optimal controls provided that the value function is sufficiently smooth in the no-action region without the need of a smooth fit principle. Finally, we showcase how our results can be applied to optimal investment problems under transaction costs.

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MS62

Nonsmooth Stochastic Analysis and Stochastic Target Problems

I present a new approach that connects nonsmooth analysis and stochastic target type problems. One application is a new well-posedness result for HJB equations related to Markovian and non-Markovian stochastic optimal control problems.

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MS62

On the Analyticity of the Value Function in Optimal Investment and Stochastically Dominant Markets

We study the analyticity of the value function in opti-

mal investment with expected utility from terminal wealth and the relation to stochastically dominant financial models. We identify both a class of utilities and a class of semi-martingale models for which we establish analyticity. Specifically, these utilities have completely monotonic inverse marginals, while the market models have a maximal element in the sense of infinite-order stochastic dominance. We construct two counterexamples, themselves of independent interest, which show that analyticity fails if either the utility or the market model does not belong to the respective special class. We also provide explicit formulas for the derivatives, of all orders, of the value functions as well as their optimizers. Finally, we show that for the set of supermartingale deflators, stochastic dominance of infinite order is equivalent to the apparently stronger dominance of second order. This talk is based on the joint work with Mihai Sirbu and Thaleia Zariphopoulou.

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MS62

Recent Computational Methods for Stochastic Optimal Control

Stochastic optimal control has been an effective tool for many problems in quantitative finance and financial economics. Although, they provide the much needed quantitative modeling for such problems, until recently they have been numerically intractable in high-dimensional settings. However, readily available and computationally highly effective optimization libraries now make regression type of algorithms over hypothesis spaces with large number of parameters computationally feasible. In the context of stochastic optimal control, these exciting advances allow efficient approximations of the feedback controls. An algorithm, proposed by E, Jentzen & Han, uses artificial neural networks to approximate the feedback actions which are then trained by empirical risk minimization. This methodology and hybrid methods combined with dynamic programming have been explored and developed by many authors, including, Bachouch, Becker, Cheridito, Fecamp, Jentzen, Germain, Gonon, Huré, Langrené, Mikael, Pham, Teichmann, Warin, Welti, Wood. An alternative approach based on the dynamic programming equation - called deep Galerkin method - is also proposed by Sirignano & Spiliopoulosis. In this talk, I will outline this highly effective methodology and discuss it through representative examples from finance.

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MS64

Robust Market Generation: from Adapted Distances to Metric Hypertransformers

In this talk, I will first motivate the employment, in market generation, of adapted versions of optimal transport distances, that result from imposing a temporal causality constraint on classical transport problems. I will then introduce a universal class of geometric deep learning models, called metric hypertransformers, capable of approximating any adapted map, and discuss their application for sequential generation and prediction. This talk is based on joint works with A. Kratsios and G. Pammer.

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MS64

Data Driven Risk and Arbitrage Restrictions for Options Markets

Measuring market risk for option portfolios is challenging; it requires modelling joint dynamics of liquid options under the real world measure, simulating realistic trajectories of risk factors, and evaluating option prices efficiently under a large of amount of risk scenarios. Using an arbitrage-free neural-SDE market model for European call options, we explore the capacity of the model as a realistic option market simulator, in particular as a risk simulation engine for option portfolios. Through backtesting analysis, we show that our models are more computationally efficient and accurate for evaluating Value-at-Risk (VaR) of option portfolios, with better coverage performance and less procyclicality than standard filtered historical simulation approaches.

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MS64

Can Synthetic Time Series Help Build Better AI Tools?

We investigate whether the recent advances in generative models for financial time series can improve the performances of learning algorithms that either detect signals or trade autonomously. For the former, we focus on simpler classification tasks — where the goal is to predict the directions of future price movement — via supervised learning algorithms. Labelling financial data is not straightforward: did the price go up because of noise or because of signal? We compare the performances of a simple classifier trained on the naive (and noisy) labels with those of a classifier trained on the labels generated by a denoising autoencoder. Our results show that our denoised labels improve the performances of the learning algorithm, for both small and large datasets. For the latter, we consider Deep Reinforcement Learning (DRL) trading agents. Deploying DRL in financial markets remains a challenging task – model-based techniques often fall short due to epistemic uncertainty, whereas model-free approaches require large amount of data that is often unavailable.We explore the possibility of using synthetic datasets for training DRL agents without direct access to the real financial data. We show that these DRL agents make a profit which is comparable, and often much larger, than that obtained by the agents trained on real data, while guaranteeing similar robustness. Talk based on joint work with Chunli Liu, Yangqin Ma and Maria Polukarov.

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MS65

An Introduction to Sampling with Measure Transport

Probability theory provides a natural language for describ-

ing uncertainty and lies at the heart of uncertainty quantification, machine learning, and decision making. Indeed, probability distributions arise anywhere statistical techniques are used to bridge the gap between mathematical models and reality. Recent years have seen an explosion in computational techniques for representing, and subsequently analyzing, the probability distributions that arise in statistical applications. Parameterized measure transport is one such technique. This tutorial will provide an introduction to parameterized measure transport, which has emerged in both the uncertainty quantification and machine learning communities as a powerful approach for representing complex probability distributions. Measure transport has been used for density estimation and sampling with broad applications including Bayesian inference, image inpainting, and generative modeling. Following an introduction to the mathematical foundations of measure transport, we will provide a brief overview of active research areas. The tutorial will conclude with a hands-on example in the geosciences, with code provided so that attendees can follow along.

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MS65

Introduction to Deep Generative Modeling

Deep generative models (DGM) are neural networks with many hidden layers trained to approximate complicated, high-dimensional probability distributions from a finite number of samples. When trained successfully, we can use the DGMs to estimate the likelihood of each observation and to create new samples from the underlying distribution. Developing DGMs has become one of the most hotly researched fields in artificial intelligence in recent years. The literature on DGMs has become vast and is growing rapidly. Some advances have even reached the public sphere, for example, the recent successes in generating realistic-looking images, voices, or movies; so-called deep fakes. Despite these successes, several mathematical and practical issues limit the broader use of DGMs: given a specific dataset, it remains challenging to design and train a DGM and even more challenging to find out why a particular model is or is not effective. To help bring new perspectives to this field, this two-hour talk provides an introduction to DGMs and provides a concise mathematical framework for modeling the three most popular approaches: normalizing flows (NF), variational autoencoders (VAE), and generative adversarial networks (GAN). We illustrate the advantages and disadvantages of these basic approaches using numerical experiments. Our goal is to enable and motivate participants to contribute to this proliferating research area. Our presentation also emphasizes relations between generative modeling and optimal transport.

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MS67

Parallel Scalability of Fast Direct Solvers Based on Strong Admissibility

Given the discretization matrix of an integral equation that is not highly indefinite, the celebrated fast multipole method (FMM) for applying the matrix to a vector leverages strong admissibility and achieves linear complexity. In addition, the parallel scalability of the FMM has been carefully analyzed, and large-scale numerical simulations have demonstrated the excellent performance of parallel implementations of the FMM. In situations where fast direct solvers (FDSs) are preferred to iterative solvers, these FDSs based on strong admissibility can also achieve linear complexity under mild assumptions motivated by numerical results. This talk discusses the parallel scalability of such strong admissibility-based FDSs for solving linear systems arising from the discretization of PDEs or associated integral equations. We present numerical results showing the parallel performance of these methods on distributed-memory machines.

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MS67

SpaQR, a Fast Sparse Hierarchical Solver for Least-Squares Problems

Sparse least-squares problems appear in various domains. QR factorization is one method for solving such problems. However, the cost of computing the factorization can be high even for sparse matrices due to fill-in appearing during the factorization. We develop a fast, sparse, approximate QR factorization of the matrix by using rank-revealing factorizations to approximate the fill-in blocks. The factorization time is close to linear in the size of the matrix with linear solve time and memory requirements. We show the effectiveness of the proposed technique for solving least-squares problems in PDE constrained optimization and computer graphics. Finally, we discuss the parallel computing aspects of the algorithm and demonstrate the weak and strong scaling behavior.

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MS67

A Block Householder Based QR Decomposition of Hierarchical Matrices

The efficient computation of an accurate QR factorization

of a hierarchical matrix is a challenging task. Several approaches have been proposed in the past, often accompanied by several difficulties such as numerical instability, loss of orthogonality or a (significant) increase of ranks in the resulting factors. Recently, a Householder based block approach has been introduced for HODLR matrices by Kressner and Susnjara [1]. The approach uses a factored form of the orthogonal Q-factor which allows for a block recursion and is hence suitable for structured H-arithmetic. We will generalize this approach to the more general class of hierarchical matrices. The added flexibility with respect to the hierarchical block structures of the matrix A and its factors Q and R require careful algorithmic adjustments such as splitting and re-agglomerating of admissible low-rank blocks whenever possible. More importantly, we discuss strategies to determine admissibility conditions and hence resulting block structures for the factored representation of Q and the upper triangular matrix R. We will conclude with numerical test comparing the proposed approach to some other approaches from the literature.

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MS67

A New Preconditioner for Covariance Kernels and Green's Function in 2D

Dense linear systems involving covariance kernels or Green's function matrices are solved by representing the underlying matrix as a hierarchical matrix and relying on iterative methods with accelerated matvecs or fast direct solvers. In this talk, we combine the traditional domain decomposition with Hierarchical low-rank representation to construct a new hybrid preconditioner for data-sparse matrices from 2D covariance kernels and Green's functions. Here we analyze the influence of the parameters involved in Hierarchical low-rank representations on the efficiency of the hybrid preconditioner. We then provide numerical results of the developed hybrid preconditioner for various 2D problems and compare it with fast direct solvers.

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MS68

Graph Completion from Spatio-Temporal Samples

We present a framework to complete topological information of a graph based on partial observations of trajectories that are governed by a linear dynamical system based on the graph topology, which can be considered as partial information both with respect to space and time domain. We overcome the intrinsic non-linearity of the resulting inverse problem by reformulating it as a matrix completion problem that utilizes a low-rank property of a suitable block Hankel embedding matrix, which is even low-rank if the graph operator is of full rank. We show local quadratic convergence of a suitable Iteratively Reweighted Least Squares algorithm under a random uniform sampling model, which applies already for few such spatio-temporal samples. Furthermore, we show how our analysis informs a suitable adaptive sampling strategy that takes the structure of the dynamics into account to distribute a budget of spatio-temporal samples more efficiently.

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MS68

Convergence and Complexity of Stochastic Block Majorization-Minimization

Stochastic majorization-minimization (SMM) is an online extension of the classical principle of majorization-minimization, which consists of sampling i.i.d. data points from a fixed data distribution and minimizing a recursively defined majorizing surrogate of an objective function. We introduce stochastic block majorization-minimization, where the surrogates can now be only block multi-convex and a single block is optimized at a time within a diminishing radius. Relaxing the standard strong convexity requirements for surrogates in SMM, our framework gives wider applicability including online CANDECOMP/PARAFAC (CP) dictionary learning and yields greater computational efficiency especially when the problem dimension is large. We provide an extensive convergence analysis on the proposed algorithm, which we derive under possibly dependent data streams, relaxing the standard i.i.d. assumption on data samples. We show that the proposed algorithm converges almost surely to the set of stationary points of a nonconvex objective under constraints at a rate $O((\log n)^{1+\epsilon}/n^{1/2})$ for the empirical loss function and $O((\log n)^{1+\epsilon}/n^{1/4})$ for the expected loss function, where n denotes the number of data samples processed. Our results provide first convergence rate bounds for various online matrix and tensor decomposition algorithms under a general Markovian data setting.

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MS68

Matrix Sensing under Structured Deterministic Measurements

The problem of recovering a low rank matrix given few structured measurements arises as sub-problem in many applications. We will show that the problem can be formulated as a matrix sensing problem with respect to a dual basis corresponding to the measurement operator. Two optimization programs are then proposed to recover the underlying matrix. We discuss a Riemannian algorithm to solve the objective and state conditions under which the algorithm obtains the true solution. Finally, we illustrate the utility of our formulation on the Euclidean distance geometry problem.

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MS69

Learning Methods for Nonlinear Dynamics Based on Variational Autoencoders having Manifold Latent Spaces

We develop data-driven methods for learning parsimonious representations of non-linear dynamics motivated by problems in fluid mechanics and other physical systems. We introduce ways to incorporate physical priors and other information through geometric and topological structures introduced into general manifold latent spaces. Our approach builds on Variational Autoencoders (VAEs) to learn nonlinear state space models. We use noise-based regularizations and priors to help ensure continuity in latent encoding and in disentangling latent features. We show how our manifold latent space approaches can be used to obtain low dimensional representations for parameterized PDEs and other dynamical systems. We also demonstrate our methods for learning non-linear dynamics in fluid mechanics and related problems.

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MS69

Learning Dynamical Systems with Invariant Measures

Standard data-driven techniques for learning stochastic dynamical systems struggle when the observational data has been sampled slowly and derivatives cannot be accurately estimated. To address this challenge, we assume that the available measurements reliably describe the asymptotic statistics of the dynamical process in question, and we instead treat invariant measures as inference data. We reformulate the inversion as a PDE-constrained optimization problem by viewing invariant measures as stationary distributional solutions to the Fokker-Planck equation, which is discretized via an upwind finite volume scheme. The velocity is parameterized by fully-connected neural networks, and we use the adjoint state method along with backpropagation to efficiently perform model identification. Numerical results for the Van der Pol Oscillator and Lorenz-63 system are presented to demonstrate the proposed approach's effectiveness. Initial results are also shown for an empirical weather dataset to explore the approach's ability to reliably perform prediction and quantify uncertainty.

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MS69

Structure and Properties of Random Feature Methods for Surrogate Modeling

We present a data-driven method for reduced order modeling using a randomized basis approach. In order to provide guarantees of success, we investigate statistical bounds on the condition number of the associated random feature matrices. In this talk, we will show that if the complexity ratio is sufficiently away from 1, then the random feature matrix is well-conditioned and that associated regression problems have low risk. The risk bounds include the underparameterized setting using the least squares problem and the overparameterized setting where using either the minimum norm interpolation problem or a sparse regression problem. We also show that the approximations remain accurate even in the data scarce regime. Examples include shape modeling and modeling spatio-temporal dynamics.

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MS69

Kernel Methods for Learning Dynamical Systems, Learning/Solving Differential Equations, and System Identification

We cover (possibly data adapted) kernel methods for learning dynamical systems, solving/learning differential equations, and system identification.

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MS70

An Introduction to Sensitive Biophysical Measurements with Field-Effect Transistors

Field-effect transistors (FETs) allow the sensitive and label-free measurements of numerous biomarkers. We will outline the operating principles of FETs as applied to biophysical sensing including the different modes of operation. We will then describe our recent techniques for signal recovery and optimization to maximize the resolution of biologically relevant quantities such as pH, proteins-ligand interactions, and nucleic acid hybridization. This talk will provide the experimental system to validate mathematical modeling and optimization of FET-based sensors described in other presentations in this minisymposium.

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MS70

A Mathematical Model for Simulating BioFET

Biological field effect transistor experiments can be modeled with a diffusion equation nonlinearly coupled to a first-order kinetics equation describing reaction at the sensor surface. There is a discontinuity in one of the boundary conditions owing to the geometry of the device. In this presentation, we introduce an elegant reformulation of this coupled set of partial differential equations allowing us to obviate the discontinuity. The mathematical model will be presented together with a comparison of the model to experimental data.

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MS70

Optimal Bandwidth Selection in Biofet Measurements

The use of stochastic regression to separate signal from noise produced by Bio-FETs will be discussed in this talk. The noise realized by BioFETs interferes with quantitative and qualitative analysis, thus determining optimal bandwidth associated with experimental Bio-FET data measurements is an important task. Presented results suggest consistent across aspect rations and a choice of stochastic regression kernel function and yield what appear to be good results.

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MS70

Gmres and Approximate Preconditioners Performance for Biofet Simulations

Several important preconditioners for saddle point problems yield linear systems for which the GMRES iterative method converges exactly in a few iterations. However, all these preconditioners involve inverses of large submatrices. In practical computations such inverses are approximated, increasing the number of iterations needed for a solution. In this talk, we present perturbation analysis results for GMRES leading to rigorous upper bounds on the number of iterations as a function of the accuracy of the preconditioner to the ideal and spectral properties of the constituent matrices. In addition to summarizing analysis of the spectral properties of these common saddle point preconditioners, we present numerical results associated with solving linear systems arising both simulation and optimal design of Biological Field-Effect Transistor-Based Biosensors (BioFET).

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MS71

Predictable Forward Performance Processes: Infrequent Evaluation and Robo-Advising Applications

We study discrete-time predictable forward processes when trading times do not coincide with performance evaluation times in the binomial tree model for the financial market. The key step in the construction of these processes is to solve a linear functional equation of higher order associated with the inverse problem driving the evolution of the predictable forward process. We provide sufficient conditions for the existence and uniqueness and an explicit construction of the predictable forward process under these conditions. Furthermore, we show that these processes are time-monotone in the evaluation period. Finally, we argue that predictable forward preferences are a viable framework to model preferences for robo-advising applications and determine an optimal interaction schedule between client and robo-advisor that balances a tradeoff between increasing uncertainty about the client's beliefs on the financial market and an interaction cost.

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MS71

Partially Egalitarian Portfolio Selection

It is a well known fact in the portfolio optimization liter-

ature that the naive equal weights (1/N) portfolio is hard to beat. The classical Markowitz mean-variance portfolio optimization, as well as its many descendants and regularizations, often fail to beat the 1/N portfolio out of sample. Inspired by recent developments in machine learning and forecast combinations, we propose a partially egalitarian portfolio selection (PEPS) approach by regularizing the mean-variance portfolio optimization problem to select weights of some of the assets in the portfolio to zero and select and shrink the surviving weights towards equality via LASSO-like regularization terms added to the portfolio optimization formulation. The resulting formulation is non-convex. We apply recent advances in mixed integer optimization to solve the PEPS formulation at scale and empirically demonstrate how PEPS outperforms an array of alternatives, that often fail to outperform the 1/N portfolio, while PEPS is at least as good as the 1/N portfolio out of sample across a range of applications.

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MS71

Proof-of-Work Cryptocurrencies: Does Mining Technology Undermine Decentralization?

Does the proof-of-work protocol serve its intended purpose of supporting decentralized cryptocurrency mining? To address this question, we develop a game-theoretical model where miners first invest in hardware to improve the efficiency of their operations, and then compete for mining rewards in a rent-seeking game. We argue that because of hardware constraints faced by miners, centralization in mining is lower than indicated by both public discourse and recent academic work, and centralization is countercyclical with respect to mining reward. Furthermore, our results highlight that advancements in hardware efficiency do not necessarily lead to larger miners increasing their advantage, but may rather allow smaller miners to expand and new miners to enter. We show that our model predictions are consistent with a detailed empirical analysis of the Bitcoin network.

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MS71

Recover Utility of Rational Inattentive Agent and Applications on Robo-Advising

We consider a rational inattentive agent who acquires costly signal to make decisions. By observing agents actions, we formulate an inverse reinforcement learning problem to recover agents utility. We propose an efficient numeric algorithm and prove its convergence. The framework is applied to robotics-advising problems to recover investors utilities by observing their investment strategies.

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MS72

On-the-fly Reduced-Order Modeling of Turbulence-Chemistry Interactions Using Dynamically Bi-Orthonormal Decomposition

The performance of the dynamically bi-orthogonal (DBO) decomposition for the reduced-order modeling of turbulence-chemistry interactions is assessed. DBO is an *on-the-fly* low-rank approximation technique, in which the instantaneous composition matrix of the reactive flow field is decomposed into a set of orthonormal spatial modes, a set of orthonormal vectors in the composition space, and a factorization of the low-rank correlation matrix. Two factors that distinguish between DBO and the reduced-order models (ROMs) based on the principal component analysis (PCA) are: (i) DBO does not require any offline data generation, and (ii) in DBO the low-rank composition subspace is time-dependent as opposed to static subspaces in PCA. Because of these features, DBO can adapt on the fly to intrinsic and externally excited transient changes in the state of the transport variables. For demonstration, simulations are conducted for a non-premixed CO/H2 flame in a temporally evolving jet. The GRI-Mech 3.0 model with 53 species is used for chemical kinetics modeling. The results are appraised via *a posteriori* comparisons against data generated via full-rank direct numerical simulation (DNS) of the same flame, and the PCA reduction of the DNS data. The DBO also yields excellent predictions of various statistics of the thermo-chemical variables.

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MS72

Efficient Reduced Order Models for Fluid Dynamics: from Linear to Nonlinear Manifold Solution Representation

Traditional linear subspace reduced order models (LS-ROMs) are able to accelerate physical simulations, in which the intrinsic solution space falls into a subspace with a small dimension, i.e., the solution space has a small Kolmogorov n-width. However, for physical phenomena not of this type, such as advection-dominated flow phenomena, which is prevalent for combustion simulations, a low-dimensional linear subspace poorly approximates the solution. To address cases such as these, we have developed an efficient nonlinear manifold ROM (NM-ROM), which can better approximate high-fidelity model solutions with a smaller latent space dimension than the LS-ROMs. Our method takes advantage of the existing numerical methods that are used to solve the corresponding full order models (FOMs). The efficiency is achieved by developing a hyper-reduction technique in the context of the NM-ROM. Numerical results show that neural networks can learn a more efficient latent space representation on advection-dominated data from 2D Burgers equations with a high Reynolds number. A speed-up of up to 11.7 for 2D Burgers equations is achieved with an appropriate treatment of the nonlinear terms through a hyper-reduction technique.

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MS72

Challenges and Progress in Model Reduction for Rocket Combustion

Even with exascale computing capabilities, high-fidelity, full-scale simulations of turbulent combustion in realistic applications like rocket combustion remain computationally expensive and inaccessible for many-query applications. Projection-based model order reduction methods have shown promise in greatly improving computational efficiency. However, classical model order reduction methods that seek reduced solutions in low-dimensional subspaces fail for realistic turbulent combustion problems because reacting flows feature extreme stiffness, sharp gradients and multi scale transport, posing great challenges in deriving low order representations. In this talk, we discuss recent advances in projection-based methods for reduced-order model (ROM) development of turbulent combustion problems. We introduce an adaptive reduced-order modeling technique which updates the low-dimensional space, thus circumventing representation barriers faced by static reduced dimensional spaces. The method leverages model-form preserving least-squares projections with variable transformation (MP-LSVT) for improved robustness of ROM and adapt the low-dimensional subspaces based on the evaluated dynamics during online calculations to greatly enhance predictive capabilities. In addition, we discuss applications of the adaptive ROM method towards modeling systems for which full order models are unaffordable. We propose a component-based modeling framework, which only requires high-fidelity simulations of small components in the full system. These component ROMs are then integrated in a full system ROM.

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MS72

Reduced Operator Inference for Nonlinear PDEs

We present a new *scientific machine learning* method that learns from data a computationally inexpensive surrogate model for predicting the evolution of a system governed by a time-dependent nonlinear partial differential equation (PDE). Our formulation generalizes to the PDE setting the *Operator Inference* method previously developed in [B. Peherstorfer and K. Willcox, *Data-driven operator inference for non-intrusive projection-based model reduction*, Computer Methods in Applied Mechanics and Engineering, 306 (2016)] for systems governed by ordinary differential equations. The method brings together two main elements. First, ideas from projection-based model reduction are used to explicitly parametrize the learned model by low-dimensional polynomial operators which reflect the known form of the governing PDE. Second, supervised machine learning tools are used to infer from data the reduced operators of this physics-informed parametrization. For systems whose governing PDEs contain non-polynomial nonlinearities, the learned model performance can be improved through the use of *lifting* variable transformations, which expose polynomial structure in the PDE. The proposed method is demonstrated on a three-dimensional combustion simulation with over 18 million degrees of freedom, for which the learned reduced models achieve accurate predictions with a dimension reduction of six orders of magnitude and model runtime reduction of 5-6 orders of magnitude.

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MS73

Stability and Multiscale in Deep Learning Algorithms for Modeling Active Ink for 3D Printing

We propose a new concept of ink for 3D printing termed active ink. This ink contains a small fraction of functionalized self-propelled rod-like particles capable of transducing chemical energy into motion. We have shown that properties of active ink such as the ink flow intensity, the shape of particles, and their activity strength may significantly affect distribution of particles in the printed materials. These properties of active ink can be easily controlled, and the distribution of active particles in the printed material determines its physical properties paving the path to novel materials with tunable properties. Our experiments raised an issue of classification of particle distribution which we addressed using deep neural network (DNN) algorithms. There is a pressing need for a mathematical understanding of the behavior of DNNs to improve existing algorithms and develop new ones since there is no rigorous understanding of DNNs performance and, in particular, why and when DNNs may fail. We present our analytical results on stability of DNN training algorithms. We obtained conditions on the data sets and DNN architecture to ensure stability. We discuss a recently introduced multiscale loss function. We anticipate that these results will not only lead to robust algorithms to control active ink properties but will also contribute to the fundamental understanding of DNN algorithm performance. Joint work with P.-E. Jabin, PSU students C. Safsten and R. Creese.

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MS73

DMREF Program Q&A Session with MPS/DMS Program Officers

The NSF Program Officers in attendance will give a brief overview of the DMREF program from the perspective of the Division of Mathematical Sciences, followed by a question and answer period.

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MS73

Design of Materials with Low Magnetic Hysteresis: the Unexpected Role of Magnetostriction Revealed by Computational Mathematics

Owing to the development of a quantitative mathematical theory of hysteresis, phase transforming crystals 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 for phase transformations applicable to magnetic hysteresis? The answer is no, but the way of thinking is promising. Numerous studies in the 1950-1970s based on linear stability analysis of the single domain state on the shoulder of the hysteresis loop show that this method fails to predict the size of the loop, a conclusion referred to as the "coercivity paradox'. Using the combined tools of numerical micromagnetics, analysis of the simulations and ideas from the calculus of variations, we find that the systematic study of large localized disturbances gives surprising predictions of the causes of soft magnetism. The research is partly supported by the NSF-DMREF program, relating to the fact that low hysteresis magnetic materials enable the advancement of induction motors that would then play an important role in green economies. Joint work with Ananya Renuka Balakrishna (USC).

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MS73

Overview of the NSF DMREF Program

The Materials Genome Initiative (MGI) is a multi-agency partnership that seeks to accelerate the progression of materials research across the Materials Development Continuum for the benefit of society. Through use of a computationally led and data-driven approach, MGI promotes the rapid design, discovery, development, and deployment of advanced materials that will ensure sustained American leadership in sectors including clean energy, national security, and human welfare. After a decade of progress, the second MGI Strategic Plan was released in 2021 defining three primary goals for the next five years: 1) Unifying the Materials Innovation Infrastructure, 2) Harnessing the Power of Materials Data, and 3) Educating, Training, and Connecting the Materials Research and Development Workforce. The Designing Materials to Revolutionize and Engineer our Future (DMREF) program at the National Science Foundation (NSF) partners with other federal agencies to promote these objectives. DMREF currently supports about one hundred projects that cover the full spectrum of materials research. Mathematical sciences play a key role in this endeavor. This talk will provide an overview of the DMREF program and provide specific examples of mathematical contributions to this ambitious effort. Results of the 2021 DMREF competition, future priorities, and funding opportunities for the MGI-related research will be discussed.

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MS74

Quantitative Justice: An Introduction

In this talk I will provide an introduction to and some examples from the emerging field of "quantitative justice" (QJ) which we are defining as the intersection(s) of quantitative science and social justice. QJ can be said to encompass all forms of mathematical, computational, and statistical (i.e. quantitative) analysis of problems that are sourced in the real world, often in domains that are considered "social science." The key component that differentiates QJ from typical quantitative analysis of social science phenomena is that either the topic under investigation or the rationale for the analysis have direct connection to social justice.

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MS74

Quantifying Federal Sentence Disparities Through Inferred Sentencing Records

The US public has a constitutional right to access criminal trial proceedings. In practice, it is difficult to exercise this right as well as to quantitatively study federal sentencing disparities. We have assembled a public database of criminal sentence decisions made in federal district courts called JUSTFAIR: Judicial System Transparency through Federal Archive Inferred Records. This large-scale database links information about defendants with information about their federal crimes and sentences, and, crucially, with the identity of the sentencing judge. I will discuss challenges associated with assembling this database as well as work and observations from studying sentencing equity and patterns of federal judges.

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MS74

Emerging Research in Data Science for Social Justice

As quantitative justice is growing as a field, the corresponding subfield engaging mathematical scientists is codifying into a research domain with its own set of cultural practices. One way we can see the emergence of mathematics for social justice or quantitative justice as a field is to look at major mathematical institute workshops charting the courses in a number of areas from gerrymandering to healthcare injustice during COVID. On the heels of numerous one week workshops, the first semester program took place in June-July of 2022 at the Institute for Computational and Experimental Research in Mathematics (ICERM) on Data Science for Social Justice. We use work at ICERM to discuss emerging mathematical research

and its implications, community-empowering practices utilized, and human-centered considerations for undertaking social justice research in mathematics. We also highlight resources for learning more about this research area and offer open avenues for engagement.

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MS75

Speeding Up Nonlinear Iterative Methods with Anderson Acceleration: Asymptotic Convergence Properties

We consider Anderson acceleration (AA) with a moving window of size m, and investigate the linear asymptotic convergence behaviour of AA(m) applied to linear and nonlinear fixed-point methods. Anderson acceleration has been shown empirically to be very effective for accelerating nonlinear iterative methods such as alternating algorithms for tensor decomposition or the ADMM optimization method for machine learning, but there is no theory to explain and quantify the asymptotic convergence improvement that is observed in practice. We first observe numerically that the root-linear convergence factor of sequences generated by AA(m) strongly depends on the initial condition, and that the acceleration coefficients oscillate while the approximation converges to the fixed point. To shed light on this behaviour, we write AA(m) itself as an augmented fixed-point method and investigate the continuity and differentiability of the fixed-point iteration function and the acceleration coefficients. To further investigate AA(m) convergence, we consider the case of accelerating linear fixed-point methods and write AA(m) as a Krylov space method. We obtain polynomial residual update formulas for AA(m) and derive an (m+2)-term recurrence relation for the AA(m) polynomials. This allows us to demonstrate several properties of AA(m). The main question to quantify the asymptotic convergence acceleration provided by AA(m) remains, however, an open problem.

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MS75

Iterative Solution of Marker and Cell Discretization of Darcy-Stokes Equations

In this talk, we focus on multigrid methods for the Darcy-Stokes problem discretized by the marker-and-cell scheme. We propose two types of block-structured multigrid relaxation schemes for the Darcy-Stokes equations: Uzawa relaxation and BSR relaxation. We apply local Fourier analysis for these relaxations, applied to the Stokes equations and Darcy problem separately, to build the choices of relaxation parameters and grid-transfer operators. In these relaxation schemes, the mass matrix obtained from finite element discretization is used to approximate the inverse of discrete Laplacian, and this leads accelerates convergence. We find that the convergence speed of the Darcy-Stokes problem is in line with that for the Stokes and Darcy problems separately.

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MS75

Local Fourier Analysis of Multigrid Methods for the MAC Scheme for the Stokes Equations

In this talk, we propose a local Fourier analysis for multigrid methods with coarsening by a factor of three for the staggered finite-difference method known as marker-and-cell scheme, applied to the Stokes equations. In our recent work, local Fourier analysis has been applied to a mass-based Braess-Sarazin relaxation scheme, a mass-based σ-Uzawa relaxation, and a mass-based distributive relaxation, with standard coarsening on staggered grids for the Stokes equations. Here, we consider the same mass-based multigrid relaxation schemes, but with coarsening by a factor of three. We derive theoretically optimal smoothing factors for this coarsening strategy, which are competitive with those obtained from standard coarsening algorithms. Moreover, coarsening by three generates a nested hierarchy of grids, which simplifies and unifies the construction of grid-transfer operators.

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MS75

Parallel Methods for Large Scale Eigenvalue Problems

This lecture is to present a type of parallel method for solving eigenvalue problems. This method is designed by using the augmented subspace method which can deduce the eigenpair-wise parallel eigensolver. In this way, we can prevent from doing the vector inner products in the high dimensional space which is the bottleneck for scalability. By using the augmented subspace method, the iterative step for eigenvalue problem only includes solving the linear boundary value problems in the high dimensional space and a very low dimensional eigenvalue problems. Actually, the augmented subspace method provides a reasonable way to design the multigrid method for nonlinear problems. The theoretical analysis and numerical examples are also provided to validate the efficiency.

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MS76

A C0 Interior Penalty Method for the Phase Field Crystal Equation

We present a C0 interior penalty finite element method for the sixth-order phase field crystal equation. We demonstrate that the numerical scheme is uniquely solvable, unconditionally energy stable, and convergent and benchmark our method against numerical experiments previously established in the literature.

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MS76

Strategies for Massively Parallel Solvers for Stokes Flow in Mantle Convection

We present a large scale, parallel geometric multigrid method for Stokes flow on adaptively refined meshes. The motivation is the simulation of convection in the Earth's mantle. The governing equations are solved using the Finite Element method on adaptively refined meshes, which allows us to resolve features at high resolution, without intractable computational cost. Nevertheless, linear systems can become quite large (100+ million unknowns), so efficient, parallel solvers are necessary. In this talk we present massively-parallel, matrix-free, geometric Multigrid solvers to solve the Stokes part of the governing equations, show numerical results including parallel scaling, and discuss various challenges that arrise from real world, challenging computations including periodic geometries, null spaces, averaging of coefficients, and more. The solver is implement in the open source mantle convection code ASPECT that is built on the open source deal.II finite element library. We will show benchmark results that confirm far better performance and scalability compared to the algebraic multigrid solvers built on assembled matrices, that were used in ASPECT until now. We can show good scalability to 100,000+ cores and 100s of billions of unknowns.

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MS76

Divergence-Free Finite Element Methods for Incompressible Flow on Domains with Curved Boundaries

In this talk we discuss a CutFEM discretization for the Stokes problem based on the Scott-Vogelius pair on smooth domains. The discrete piecewise polynomial spaces are defined on macro-element triangulations which are not fitted to the smooth physical domain. Boundary conditions are imposed via penalization through the help of a Nitsche-type discretization, whereas stability with respect to small and anisotropic cuts of the bulk elements is ensured by adding local ghost penalty stabilization terms. We show stability of the scheme as well as a divergence–free property of the discrete velocity outside an $O(h)$ neighborhood of the boundary. To mitigate the error caused by the violation of the divergence-free condition, we introduce local grad-div stabilization. The error analysis shows that the grad-div parameter can scale like $O(h^{-1})$, allowing a rather heavy penalty for the violation of mass conservation, while still ensuring optimal order error estimates.

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MS76

Simulating Diffusive Processes in Complex Geometries Without Time Stepping

Several challenges arise when simulating diffusive processes in complex unbounded domains. First, many numerical methods only achieve low-order accuracy in both space and time. Second, far-field boundary conditions are often artificially satisfied. Third, determining long-time behaviors requires taking a large number of expensive time steps. I will describe a numerical method that recasts the time-dependent diffusion equation as a collection of elliptic PDEs by applying the Laplace transform. To achieve high-order accuracy in space, and to satisfy far-field boundary conditions, these elliptic PDEs are solved with an integral equation method. Then, a numerically accurate and stable numerical method is used to apply the inverse Laplace transform. The resulting numerical method returns a high-order accurate solution of the diffusion equation at any point in space and time without the need to time step.

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MS78

Gradient Flows for Unsupervised Learning

This paper develops a gradient flow, governed by a Langevin-type McKean-Vlasov equation, for a general unsupervised learning problem. We show that the gradient flow converges to the underlying (unknown) distribution of a given dataset, which is characterized as the unique invariant measure of the aforementioned McKean-Vlasov equation. Based on our theoretic results, we modify the algorithm of the generative adversarial network (GAN, the state of the art of unsupervised learning), so that the convergence to the underlying data distribution is guaranteed. Such a theoretic guarantee of convergence is new in the literature.

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MS78

Minimal Entropy to Achieve a Pathwise Goal

Given an n-dimensional stochastic process X driven by $\mathbb{P}$-Brownian motions and Poisson random measures, we seek the probability measure $\mathbb{Q}$, with minimal relative entropy to $\mathbb{P}$, such that the $\mathbb{Q}$-expectation of the sum a terminal and running cost is constrained. We derive the explicit form of the measure change and characterize the optimal drift and compensator adjustments under the optimal perturbed measure. We apply our results to a risk manage-

ment setting where a trader seeks to ask the question: what dynamics induces a perturbation of the value-at-risk (VaR) or conditional VaR of the base process?

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MS78

Optimal Capital Structure with Stochastic Variable Costs

We examine the optimal capital structure of a firm with stochastic revenues, stochastic variable costs, and fixed costs. In this two-state variable setting with stochastic operating leverage, we establish an Early Default Premium (EDP) formula for the value of equity and derive an integral equation for the endogenous default boundary, a function of variable costs. The value of debt, the endogenous coupon, the optimal leverage ratio and the credit spread are solved for. The impact of taxes, fixed costs and bankruptcy costs is assessed. [This is joint work with Jerome Detemple and Kristoffer Glover.]

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MS78

Multivariate Dynamic Programming

In several time-inconsistent problems, the time-inconsistency is due to the fact that the underlying problem is multi-variate in some sense. Examples include the mean-risk problem, Nash equilibria in a dynamic game, or dynamic risk measure in a market with frictions. What unifies these examples is that one can formulate these problems with a set-valued value function. In this talk, the Bellman's principle is extended to value functions that are set-valued. It is shown that the problems mentioned above do satisfy this Bellman's principle under reasonable assumptions and are thus actually time-consistent in a set-valued sense. Practical implications and economic interpretations are discussed. Numerical examples are given which lead to a sequence of vector optimization problems solved backwards in time.

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MS79

Research as Education as Research

As applied mathematicians we regularly use mathematical modeling to situate mathematics in real-life contexts. In educational settings, mathematical modeling is growing in popularity and is now part of many secondary (and earlier) mathematics curricula because it is rooted in real-life problem solving; however, finding relevant questions is non-trivial. In this session we will discuss strategies to broaden the impact of your scientific research across a variety of communities and various formats. Well share a collection of resources that you can use to communicate your modeling research to educational audiences, including pathways for obtaining funding for education focused projects and opportunities to engage in pedagogical research. The NSF-funded project M2Studio, an in-development web-based integrated modeling environment, will be highlighted.

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MS79

Conducting Biologically Oriented Research Using Agent-Based Modeling

This tutorial will guide students in how to start and conduct computational science research with applications to biology using an agent-based modeling (ABM) tool. Widely used in such research, ABMs incorporate autonomous, decision-making agents, each one of which has states and behaviors, and can be effective in modeling dynamic, spatially complex situations and visualizing emerging patterns. With minimal programming experience, such research can be successful even if the professor and/or student(s) has limited background in biology and no experience with ABM. The tutorial will show how to get started with a free ABM tool, NetLogo; how to find interesting projects; and demonstrate several ABMs, such as spread of COVID and other diseases, invasion of cane toads, growth of biofilms, food insecurity, antibiotic resistance, invasive species with various predator-prey scenarios, and generation of telemetry data for Hidden Markov Model projects.

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MS80

On Involutions of Finite Fields by Binomials

Permutations of finite fields F_q have many applications ranging from cryptography and combinatorics to the theory of computation. In many of these applications, a permutation and its inverse are stored in memory. A good option to reduce the memory footprint is to generate the permutation with a polynomial at the time of implementation. A better option is to use a permutation polynomial that is its own inverse, called an involution. In applications to cryptography, the number of fixed points is correlated with its cryptographic properties. In 2017, Castro et. al gave explicit formulas for monomial involutions of F_q and their fixed points. The next simplest polynomials to implement would be the binomials. We present explicit formulas for obtaining involutions of the form $x^m(x^{(}(q-1)/2)+a)$ with a prescribed number of fixed points.

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MS80

Self-Reconfigurable Robots: Pivoting via Electromagnetism

Self-reconfigurable robots offer a level of adaptation not found on conventional robots. The adaptability of said robots is further enhanced when parts of the robot are fully untethered since their movement is not constrained by joints or fasteners to other components. One way this is achieved is by building a swarm of individual units, each containing its own array of electronics, but can all come together to create different structures. I will talk about our approach to creating a scalable cuboid that can electromagnetically pivot on each other (even against gravity moments), to achieve self-reconfigurability.

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MS80

Topological Approaches in Computational Cardiology

Accurate and proactive diagnosis of heart conditions significantly improves the quality and quantity of options available to patients. The advent of machine and deep-learning approaches has ushered in many opportunities that contribute to the improvement of the speed and quality of diagnosis via automated solutions that tap readily-available, non-intrusive, and inexpensive sources of data. A common prerequisite to these approaches is a good set of features that is not only effective in training models, but also decreases the dependence on highly specialized skills for feature extraction. In this talk, I will talk about how various mathematical strategies have played a central role in shaping directions in this task. In particular, I will discuss how Topological Data Analysis can contribute to the advancement of this task, and share about some experiences, challenges, and ideas on this approach as well as needs and opportunities that other areas of mathematics could potentially fill.

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MS80

Intermittent Synchronization in Gamma Rhythm

Gamma synchronization plays a significant role in many cognitive functions; abnormal gamma synchronization is often associated with brain diseases. Gamma synchronization level fluctuates over time. Networks with similar synchrony strength may have different temporal patterning of synchrony; these temporal patterns of intermittent synchronization may be functionally important and thus correlated with behavior (S Ahn, LL Rubchinsky. Potential mechanisms and functions of intermittent neural synchronization. Front Comput Neurosci 11: 44, 2017; E. Malaia, S. Ahn, L.L. Rubchinsky. Dysregulation of temporal dynamics of synchronous neural activity in adolescents on autism spectrum. Autism Research 13: 24-31, 2020). Based on results on a small circuit (Q-A Nguyen, LL Rubchinsky. Temporal pattern of synchrony in a pyramidal-interneuron gamma (PING) network. Chaos 31: 043133, 2021), we use a medium-sized conductance-based pyramidal-interneuron network to study neuronal synchrony in gamma frequency band. Our simulation shows that synaptic connections alter synchrony strength as well as the temporal patterns of synchrony. The latter may be altered independent of synchrony strength. Furthermore, we show that circuits with different patterning of synchronization in time may have different sensitivity to synaptic input. Acknowledgement: This work receives support from NSF DMS 1813819

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MS81

On the Polygonal Faber-Krahn Inequality

It has been conjectured by Pólya and Szegő in 1951 that among n-gons with fixed area the regular one minimizes the first eigenvalue of the Dirichlet-Laplace operator. Despite its apparent simplicity, this result has only been proved for triangles and quadrilaterals. In this work we show that the proof of the conjecture can be reduced to finitely many certified numerical computations. Moreover, the local minimality of the regular polygon is reduced to a single validated numerical computation. The steps of the proof strategy include the analytic computation of the Hessian matrix of the first eigenvalue, the stability of the Hessian with respect to vertex perturbations and analytic upper bounds for the diameter of an optimal set. Explicit a priori error estimates are given for the finite element computation of the eigenvalues of the Hessian matrix of the first eigenvalue associated to the regular polygon. Results presented are obtained in collaboration with Dorin Bucur.

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MS81

An Isoperimetric Problem Involving the Competition Between the Perimeter and a Nonlocal Perimeter

In this talk, I will present an isoperimetric problem in which the perimeter is replaced by the difference between the classical perimeter and a nonlocal energy P_ε which converges to a fraction of the perimeter when ε vanishes. This problem is derived from Gamow's liquid drop model for the atomic nucleus in the case where the repulsive potential is sufficiently decaying at infinity and in the large mass regime. I will discuss the existence, and characterization of minimizers for small ε.

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MS81

Crystallization and Coarse Graining for Particles Governed by Pairwise Interactions

In this talk I will briefly introduce the classical problem of crystallization and coarse graining to macroscopic Wulff shapes for systems of particles governed by short range repulsive/long range attractive potentials. Then, I will describe some recent results on systems governed by power law type potentials, focusing on the role played by the tail of the potentials. Finally, I will describe new crystallization problems for oriented particles, with possible applications to collective behavior.

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MS81

An Uncertainty Principle for Zero-Sets and the Wasserstein Distance

The study of zero sets is a classical problem in analysis and differential equations. We show how the study of zero sets is intimately related to the notion of optimal transport through an uncertainty-principle type result: if a (multivariate) function has a small zero set, the Wasserstein distance between its positive and negative parts cannot be arbitrarily small. We apply this fundamental inequality to quantify the zero sets of infinite sums of Laplacian eigenfunctions, establishing a multi-dimensional analog of a classical result of Sturm and Hurwitz. The relation between optimal transport and zero sets can be treated as an optimization problem. This approach leads to sharp inequalities on intervals, curves, and metric star-graphs, and a new minimal surface problem in higher dimensions.

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MS83

Recent Insights for Iterated Brownian Bridge Kernels

Iterated Brownian bridge kernels were introduced by Cavoretto, Fasshauer and McCourt [R. Cavoretto, G. E. Fasshauer, M. J. McCourt, An Introduction to the Hilbert-Schmidt SVD Using Iterated Brownian Bridge Kernels, Numerical Algorithms 68 (2015): 393–422], where they were primarily used to illustrate the Hilbert-Schmidt SVD introduced by the latter two authors in [G. E. Fasshauer, M. J. McCourt, Stable Evaluation of Gaussian Radial Basis Function Interpolants, SIAM J. Sci. Comput. 34, No. 2 (2012): A737–A762]. In this talk we view iterated Brownian bridge kernels as Green's kernels of the fractional Laplacian $(-\nabla)^s$, $s > \frac{d}{2}$, apply them to the solution of fractional Poisson problems and discuss their approximation order. This is joint work with Hamed Mohebalizadeh and Hojatollah Adibi (Amirkabir University of Technology, Tehran).

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MS83

Kernel-Based Methods for Solving Surface PDEs

The convergence analysis technique in [SINUM, 56, pp. 614–633, 2018] is extended to various theoretically proven convergent kernel-based least-squares collocation methods for surface elliptic equation by [SISC, 40, A266–A287, 2018] and projection [SINUM, 58, pp.988–1007, 2020] and recently for surface parabolic equations [arXiv: 2109.0340, 2021]. These PDEs on surfaces closely assemble their Euclidean counterparts, except that the problem domains change from bulk regions with a flat geometry to some manifolds, on which curvatures play an important role in the physical processes. We do not focus on proofs in this talk, but on implementation details instead. First, we present an embedding formulation to solve surface PDEs in a narrow band domain containing the surface. Next, we present another extrinsic projection formulation that works solely on data points on surface. Lastly, we solve surface diffusion problem using kernels and the method of lines.

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MS83

A Partition of Unity Kernel-Based Method for Surface PDEs

In this talk, a new localized kernel-based technique, called "direct RBF partition of unity (D-RBF-PU)" method, is presented for solving surface PDEs on embedded and smooth submanifolds of Euclidean spaces. This method avoids all surface derivatives of PU weights as well as all lower derivatives of local approximants. It is faster and simpler than the standard RBF-PU method and allows the use of discontinuous weights for PU approximation. The later property paves the way for developing a more efficient and less expensive method. Alternatively, the new method is an RBF-generated finite difference (RBF-FD) scheme in a PU setting which is much faster and in some situations more accurate than the original RBF-FD. Theoretical bounds and sufficient number of examples support our assertions.

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MS83

Adaptive Meshfree Solution of Linear PDEs: Analysis of Target-Data Dependent Greedy Kernel Methods

We consider meshless solving of PDEs Lu = f on a bounded domain with suitable boundary conditions via symmetric kernel collocation by using greedy kernel methods. In this way we avoid the need for a mesh generation, which can be challenging for non-standard domains O or manifolds. We introduce and discuss different kind of greedy selection criteria, such as the PDE-P-greedy and the PDE-f-greedy. Subsequently we analyze the convergence rates of these algorithms and provide bounds on the approximation error in terms of the number of greedily selected points. Especially we prove that target-data dependent algorithms

exhibit faster convergence rates. The provided analysis is applicable to PDEs both on domains and manifolds. This and the advantages of target-data dependent algorithms is highlighted by numerical examples

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MS84

Optimal and Near Optimal Krylov Space Approximations to F(A)b

We describe a Lanczos-based or Arnoldi-based algorithm for approximating the product of a rational function of a matrix A with a given vector b. This algorithm is optimal over the Krylov subspace, in a norm induced by the denominator of the rational function, and the approximation can be computed using information from a slightly larger Krylov subspace. It requires storage of just a few additional vectors, proportional to the degree of the denominator of the rational function. It can be used to construct near-optimal approximations for other matrix functions such as the matrix sign function.

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MS84

Computing Spectral Properties of Topological Insulators with Disorder

Topological insulators (TIs) are a class of materials with remarkable electronic properties that can persist even in the presence of material defects and disorder. However, a TIs electronic behavior is governed by an infinite-dimensional Hamiltonian with exotic spectral properties, which has frustrated the development of rigorous computational methods for defective and disordered TIs. We present new methods that rigorously and efficiently calculate conductivities and the generalized eigenstates that mediate interior and interfacial electronic transport. This approach extends a recent framework that uses rational filters to compute spectral measures of infinite-dimensional operators [Colbrook et al., SIAM Rev. 2021].

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MS84

Hutch++ and More: Toward Optimal Spectral Sum Estimation

Spectral Sums are a huge family of important-to-compute statistics about matrices, with examples like the log-determinant of a covariance matrix, or the trace-exponential of the adjacency matrix of a graph. This talk discusses recent progress on both designing faster algorithms for spectral sums, and proving that these algorithms are near-optimal in the canonical *Matrix-Vector Oracle Model*. Concretely, we lightly discuss trace estimation and the Hutch++ algorithm, followed by extensions to trace-polynomial estimation, and conclude with general spectral sum estimation. This work not only shows some fast and practical algorithms, but also more broadly explores some fundamental computational limits of numerical linear algebra.

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MS84

Computation of Functions on Complex Arcs

Analytic functions often have special properties across certain arcs: examples include the Cauchy and Hilbert transforms, the Sokhotski-Plemelj formula, Stone's formula for spectral measures, Riemann-Hilbert problems, and the theory of hyperfunctions. This talk will review some old and new numerical methods in this space involving both scalars and matrices or operators, based on both polynomial and rational approximations.

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MS85

Finite Element Analysis for a Generalized Robin Boundary ValueProblem in a Smooth Domain

We present finite element analysis to a generalized Robin boundary value problem in a smooth domain. It consists in solving an elliptic equation in a bulk domain, which is coupled with another elliptic equation given on the boundary, through the normal directional derivative. Such a bulk-interface coupled PDE appears as a simplified model for fluid-structure interaction problems. Taking into account

the discrepancy of the original domain and its polygonal approximation, we derive an optimal error estimate for the case of linear finite element approximation.

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MS85

Simulating Complex Fluid-Structure Interactions in Living Cells

Many basic processes within living cells, like cell division, are mediated by the cytoskeleton which is a collection of biopolymers, cross-linkers, and motor-proteins. Here I focus on microtubules, a flexible biopolymer which, among other things, comprises the spindle apparatus, the central organelle orchestrating cell division, and which serves as the pliant substrate from which motor-proteins drive circulating flows in large developing cells. I will discuss numerical methods and coarse-graining procedures for simulating assemblies of microtubules in these challenging situations, where the geometries can be exceedingly complex.

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MS85

Modelling Complex Suspensions

We look at the modelling of dense two-phase materials: a solid suspended in a viscous liquid. Ingredients are drawn from theoretical concepts in solid mechanics, from the mathematical study of dilute suspensions, and from particle-based simulations. From these various elements we can create constitutive models which go some way to mimicking the simulations and to explaining experimental observations.

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MS85

The Numerical Methods for the Coupled Fluid Flow under the Leak Interface Condition of the Friction-Type

The friction-type (or called barrier-type) leak interface condition (FLIC) is proposed to modelling the viscous fluid through a perforated membrane with a threshold permeability, where the flow passes through the perforations only when the stress difference on the membrane is above a threshold. In this work, we study three numerical approaches for the Stokes/Stokes coupled fluid flow under the FLIC, including the projection, regularization and domain decomposition methods. For discretization, we apply the finite element method using the $\mathbb{P}_1$-bubble/$\mathbb{P}_1$ element. We prove the convergence of the projection and domain decomposition algorithms. For the regularization method, the convergence of the Picard iteration is investigated. The error analysis of the finite element approximation is established. And the theoretical results are confirmed by the numerical experiments.

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MS86

A Neural Network Method for Solving Conservation Laws and Beyond

This talk is based on a joint work (arXiv:2109.09316) with Haoxiang Huang and Vigor Yang. We introduce neural networks with inputs based on domain of dependence and a converging sequence for solving conservation laws, the 2-Coarse-Grid neural network (2CGNN) and 2-Diffusion-Coefficient neural network (2DCNN). We use a neural network to predict a high-fidelity solution at a space-time grid point. Two solutions of the conservation laws from a converging sequence, computed from a low-cost numerical scheme, and in a local domain of dependence of the space-time grid point, serve as the input. Despite smeared input solutions, the output provides sharp approximations to solutions containing shocks and contact surfaces, and the method is efficient to use, once trained. It works not only for discontinuities, but also for the smooth part of the solution, implying broader applications for other differential equations.

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MS86

Goal-Oriented Parameter Upscaling for PDE's with Uncertain Inputs

In physical systems modeled by partial differential equations with uncertain, spatially varying parameters, the statistical complexity of the parameter space greatly determines the feasibility of many efficient stochastic simulation methods, such as reduced order- or surrogate models. It also limits the accuracy of Bayesian approaches to parameter identification. In this work we propose a goal-oriented algorithm for adaptively upscaling spatially varying uncertain parameters. Local parameter resolution levels are chosen to optimally capture the variation of a related quantity of interest, subject to a limited computational budget. The problem is solved and analyzed within a stochastic optimization framework.

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MS87

A Hybrid High-Order Method for the Incompressible NavierStokes Problem Robust for Large Irrotational Body Forces

In this talk we discuss a novel Hybrid High-Order method for the incompressible NavierStokes problem robust for large irrotational body forces. The key ingredients of the method are discrete versions of the body force and convective contributions in the momentum equation formulated in terms of a globally divergence-free velocity reconstruction. Two key properties are mimicked at the discrete level,

namely the invariance of the velocity with respect to irrotational body forces and the non-dissipativity of the convective term. A full convergence analysis is carried out, showing optimal orders of convergence under a smallness condition involving only the solenoidal part of the body force. The performance of the method is illustrated by a complete panel of numerical tests, including comparisons that highlight the benefits with respect to more standard formulations.

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MS87

Pressure Robust Staggered Discontinuous Galerkin Methods

In this talk, we present a pressure-robust staggered discontinuous Galerkin method for the Navier-Stokes equations and its application to the Boussinesq problem. A carefully chosen discrete pair yields stabilization-free discrete formulation. Here, we use a locally divergence conforming space for the velocity approximation. However, the resulting velocity approximation is globally conforming and also satisfies the exact divergence-free condition. Those properties play essential roles in the convergence analysis. We present pressure error independent velocity error estimates so that the proposed method is indeed a pressure-robust method. We present several numerical experiments to verify the convergence behavior and its pressure-robustness. In the end, we apply this method to the Boussinesq problem.

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MS87

Recent Advances for Pressure-Robust Discretisations of the Incompressible Navier-Stokes Equations

The talk concerns pressure-robust discretisations for incompressible flow problems that compute discrete velocities which are independent of the exact pressure, despite a relaxation of the divergence constraint to ensure inf-sup stability, by avoiding errors that may arise from a false balancing of irrotational forces within the data or the material derivative. Such a misbalance can also occur in classical residual-based a posteriori error control and convection stabilisations and the talk will give an overview over some novel pressure-robust alternatives in these areas. First, guaranteed pressure-robust error estimators via a novel design of equilibrated fluxes based on a mass-conservative mixed stress method are presented. Second, a pressure-robust convection stabilisation based on the residual of the vorticity equation is discussed.

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MS88

A Sample-Wise Back-Propagation Method for Uncertainty Quantification in Deep Learning

We develop a backward stochastic differential equation based probabilistic machine learning method, which formulates a class of stochastic neural networks as a stochastic optimal control problem. An efficient stochastic gradient descent algorithm is introduced with the gradient computed through a backward stochastic differential equation. Convergence analysis for stochastic gradient descent optimization and numerical experiments for applications of stochastic neural networks are carried out to validate our methodology in both theory and performance.

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MS88

Nonparametric Learning of Interaction Kernels in Mean-Field Equations of Particle Systems

Systems of interacting particles/agents arise in multiple disciplines, such as particle systems in physics, flocking birds and swarming cells in biology, and opinion dynamics in social science. We consider the learning of the distance-based interaction kernels between the particles/agents from data. A challenging case is when the system is large with millions of particles, and we can only observe the population density. We present an efficient regression algorithm to estimate the interaction kernel, along with a systematic learning theory addressing identifiability and convergence of the estimators. We demonstrate our algorithm on three typical examples: the opinion dynamics with a piecewise linear kernel, the granular media model with a quadratic kernel, and the aggregation-diffusion with a repulsive-attractive kernel.

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MS88

Topological Artificial Intelligence and Neuroscience

Improving flexibility and adaptability of next generation AI is possible by designing networks that generate abstract spatial representations in the same way that humans do. Complex spatial representation patterns, as recorded by neuroscience data, may be uncovered through the discovery of their underlying manifolds. Such manifolds may be represented by a rich in information simplicial complex. Simplicial complexes form an important class of topological spaces that are frequently employed in various application areas from materials science and chemistry to biology and neuroscience, etc. for addressing supervised and unsupervised learning. In this talk, we will discuss topological aspects of AI (TAI) and precisely simplicial complex representation learning. A simplicial complex arising from neurospiking data is embedded to an artificial neural net with the inverse potential to predict the head direction of a mouse while it moves around a maze. Our method employs a novel geometric message passing scheme, which naturally builds on ideas from graph neural networks.

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MS90

Kernel Mean Embeddings for Stochastic Processes

The idea of embedding probability distributions into a reproducing kernel Hilbert space (RKHS) via kernel mean embeddings (KMEs) has become ubiquitous in many areas of statistics and data science such as hypothesis testing or distribution regression. Despite strong progress in the study of KMEs, most of the examples considered in the literature tend to focus on random variables supported on some finite (possibly high) dimensional euclidean spaces. In this talk I will introduce a family of KMEs for function-valued random variables which allows to solve challenging, real-world optimisation problems in quantitative finance (such as the pricing of American options) via classical kernel-based regression methods.

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MS90

Human Action Recognition with Signatures and Deep Learning

In this talk we will discuss how signatures have been combined with machine learning and deep learning methods in the domain of human action recognition. We will discuss some of the benefits and intuitions behind these approaches and some open questions arising from these works.

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MS91

Optimal Brokerage Contract in Almgren-Chriss Model

The role of the broker is to implement transactions on behalf of an investor, charging him a fee, which usually depends on the performance of the investor, in return for better conditions such as lower price impact. From a rational point of view, the goal of the broker is to set a fee that maximizes her profit while her client invests optimally. Mathematically, optimal brokerage problems can be viewed as stochastic optimal contract problems where the broker is the Principal and the investor is the Agent. In our setting we assume the Almgren-Chriss model with temporary and permanent price impact. Using the recently developed general methods for optimal contract problems, we (i) construct optimal contracts for multiple investors trading with the same broker, (ii) construct an optimal contract in a partial information setting where the investor observes a signal that is unobserved by the broker.

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MS91

Markov Decision Processes with Kusuoka-Type Conditional Risk Mappings

The Kusuoka representation of proper lower semi-continuous law invariant coherent risk measures allows one to cast them in terms of average value-at-risk. Here, we introduce the notion of Kusuoka-type conditional risk-mappings and use it to define a dynamic risk measure. We use such dynamic risk measures to study infinite horizon Markov decision processes with random costs and random actions. Under mild assumptions, we derive a dynamic programming principle and prove the existence of an optimal policy. We also provide a sufficient condition for when deterministic actions are optimal.

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MS91

Risk-Averse Control of Systems with Model Uncertainty

We consider a Markov decision process subject to model uncertainty in a Bayesian framework, where we assume that the state process is observed but its law is unknown to the observer. In addition, while the state process and the controls are observed at time t, the actual cost that may depend on the unknown parameter is not known at time t. The controller optimizes these running costs by using a family of special risk measures, that we call risk filters and that are appropriately defined to take into account the model uncertainty of the controlled system. These key features lead to non-standard and non-trivial risk-averse control problems, for which we derive the Bellman principle of optimality. We illustrate the general theory on several practical examples. This is a joint work with Andrzej Ruszczynski and Tomasz R. Bielecki.

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MS91

A Counterexample in Stochastic Control Theory

We construct a model with a non-differentiable value function for a popular stochastic convex control problem stemming from mathematical finance. The example has two time points and is based on a countable underlying probability space. The presentation will be simple and self-contained. This is joing work with Mete Soner and Gordan Zitkovic.

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MS93

DNA Clusters and Viral Structures

Problems of packaging, organization and condensation of DNA, semiflexible polymers and actin-type biological networks, either in confined domains, capsids, or in free solution, present many mathematical modeling challenges. A key ingredient to our study of organized DNA is the earlier discovery that, under confinement, DNA arranges itself as an hexagonal chromonic liquid crystal. This motivates us to present results stemming from recent experiments on chromonic liquid crystal clustering. Our mechanically based models lead to energy minimization problems and their associated free boundary problems.

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MS93

Dynamics of Grain Boundaries in Polycrystals: Modeling, Analysis, Simulation and Experiments

Most technologically useful materials are polycrystalline microstructures composed of a myriad of small monocrystalline grains delimited by grain boundaries. An understanding of the evolution of grain boundaries and associated grain growth (coarsening) is essential in determining the properties of materials. Grain growth is a very complex multiscale process. It can be viewed as the anisotropic evolution of a large metastable network, and can be mathematically modeled by a set of deterministic local evolution laws for the growth of an individual grain combined with stochastic models to describe the interaction between them. In this talk, we will discuss recent progress on experiments, modeling, simulation and analysis of the evolution of the grain boundary network in polycrystalline materials.

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MS93

The Preasymptotic Model for Prestrained Plates

A prestrained plate is a thin sheet of material that naturally deforms into some target configuration. Prestrained plates can be used to model various physical phenomena, from the closing of a Venus flytrap to the movement of microscopic medical devices. In this talk, we will discuss the preasymptotic model for the large bending of prestrained plates, which assumes a small thickness of the plate and consists of minimizing a bending energy and a stretching energy. After deriving this model, we will discuss an LDG-type discretization of the energy and a discrete gradient flow for minimizing the energy. This discrete gradient flow will be compared to an alternate scheme involving a Nesterov acceleration. Finally, we present some simulations to demonstrate the applications of the model.

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MS94

Exploring the Dynamics, Dysfunction, and Disparities of Ovulation

A normally functioning ovulatory cycle results from a tightly regulated system of crosstalk between the brain and the ovaries. Failure to regulate reproductive hormones may cause ovarian dysfunction and sometimes infertility. Polycystic ovary syndrome (PCOS) is a relatively common cause of such dysfunction, which is often accompanied by irregular glucose metabolism. Racial and ethnic disparities further complicate the manifestation of PCOS and associated health complications. We first use mathematical models to examine mechanisms of disruption and to characterize ovulatory phenotypes. We then use our models and available data to examine how disparities might influence–or be influenced by–model-based phenotypes.

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MS94

Hashtags As Identity Signals: the Case of #AllLivesMatter vs. #BlackLivesMatter

We evaluate the potential for hashtags to serve as identity signals, such that their interpretation might differ greatly depending on the social identity of the audience. We had U.S. participants of varying political orientation view tweets with and without the #BlackLivesMatter and #AllLivesMatter hashtags and queried them on their perceptions of the tweets as racist, offensive, or both. We analyzed the responses to uncover patterns/correlations between demographics, political orientation, hashtag presence, and evaluative responses. We find, above all, that not only is the perception of a tweet's content predicted by the reader's political orientation, but that hashtags carry identity signaling content above and beyond the text in which they are embedded.

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MS94

Mentoring Undergraduate Research in Math Biology

Undergraduate research has become integral in the education of future mathematicians, regardless of career plans. In this talk we will discuss ways of finding appropriate mathematical biology projects for students with their career goals in mind and how to mentor students through the research process. Several examples will be provided and the choices made in each example will be discussed.

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MS94

Fostering IntellectualRisk-Taking in Undergraduate Math Classrooms - Insights from a Game-Theoretical Model

How exactly do math students and instructors contribute to the construction of successful classroom learning communities? In this talk, I will present a collaborative self-study involving three minority mathematics instructors at an urban public research university. A discrete-time replicator dynamics model was developed to explore the impact of instructor teaching style on student mindset and academic achievement. The model reflects several hypotheses including: (i) the classroom is a social environment in which conflicts are negotiated and resolved, (ii) students and instructors are strategic agents who learn the best way to interact to achieve their goals, and (iii) instructors actions shape students behaviors and vice-versa. Preliminary analysis and simulations of the model will be presented.

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MS95

Weak Galerkin Method on Elements of General Geometric Shapes

In this talk, the weak Galerkin finite element method for second order problems on curvilinear polytopal meshes with Lipschitz continuous edges or faces is analyzed. The method is designed to deal with second order problems with complex boundary conditions or complex interfaces. With Lipschitz continuous boundary or interface, the method's optimal convergence rate for H^1 and L^2 error estimates are obtained. Arbitrary high orders can be achieved.

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MS95

Time-Step Adaptivity for Phase-Field Models

One of the known computational challenges that arises even in unconditionally solvable, stable, and convergent numerical schemes for phase field models is that little is known *a priori* about the different time scales that arise in the dynamics of these models. In this talk, we present an adaptive time-stepping strategy and apply it to a sixth order phase field model capturing microemulsions where preliminary findings suggest a strong need for time-step adaptivity.

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MS95

Solving Navier-Stokes Equations with Stationary and Moving Interfaces on Unfitted Meshes

In this talk, we introduce a high-order immersed finite element (IFE) method for solving Navier-Stokes equation with discontinuous viscosity coefficient across fluid interface. Immersed P2-P1 Taylor-Hood finite element space are developed for spatial discretization without requiring mesh to align interfaces. The existence and uniqueness of IFE basis functions are established. In spatial discretization, we use an enhanced partially penalized IFE method with ghost penalties. In temporal discretization, theta-scheme and backward difference differentiation formulas are adopted. Extensive numerical experiments show that the proposed method is optimal-order convergent for both velocity and pressure in both stationary and moving interface cases.

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MS96

Rational-Type Approximations of Prabhakar Function and Its Application to Multi-Term Fractional PDEs

Mittag-Leffler functions is of fundamental role in the theory of fractional calculus. In this talk, we present a rational-type approximation of the Prabhakar function(three-parameters Mittag-Leffler function) on the real negative semi-axis and discuss its applications in the numerical treatment of fractional PDEs.

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MS96

Higher-Order Methods for Time-Fractional Convection-Diffusion-Reaction Equation with Time Varying Drift Term

Exponential integrators, due to their robust stability properties, are considered reliable schemes for time integration of partial differential equations. In this talk we present efficient high-order exponential time differencing schemes for solving time-fractional convection-diffusion-reaction equations with time-dependent drift term. Exponential integrators are traditionally utilized for differential equations with constant coefficients. Thus, due to the time-dependence of the drift function in our problem, some careful manipulation of the problem is carried out to set up the framework of the exponential integrators. In addition to stability concerns, numerical schemes applied to time-fractional problems often suffer loss of accuracy due to the weak singularity exhibited by the continuous solution of the problem. To counter this issue of order reduction, we utilize time-graded mesh to obtain uniform optimal convergence rates.

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MS96

Spectral Methods for Integral Fractional Laplacian

The fractional Laplacian is a promising mathematical tool modeling turbulence intermittency in fractional Navier-Stokes equation. However, efficient computation on bounded domains is challenging, due to the intrinsic singularity and nonlocal nature of the fractional Laplacian. In this talk, we will discuss spectral methods for elliptic equations with integral fractional Laplacian in 1D and 2D.

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MS97

An FMM Accelerated Poisson Solver for Complicated Geometries in the Plane Using Function Extension

We present a potential theory-based adaptive solver for the Poisson equation in complicated geometries in the plane, accelerated with a fast multipole method (FMM). The solution is given explicitly as the sum of a volume potential and a double layer potential. To simplify the evaluation of the volume potential over the complicated domain, we extend the source data to a geometrically simpler domain, which contains the original geometry. It remains only to solve the homogeneous Laplace equation, with modified boundary data, to obtain the full solution. This is done with existing fast and accurate boundary integral methods. The novelty of our solver is the scheme used for creating the extension. The source data is represented on boxes in an adaptive quad-tree. For leaf boxes intersected by the boundary we extend the source data locally to a subset of its colleagues. The extension is created by sampling data from neighboring boxes and using a box-independent precomputed interpolation matrix. The resulting potential induced by the extended source data can then be efficiently computed with existing volume-integral FMMs. We demonstrate speed, robustness and high-order convergence through several examples, including piecewise smooth domains.

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MS97

A Fast Convergent Boundary Integral Framework for Slender Bodies

The dynamics of active and passive filaments in viscous fluids is frequently used as a model for many complex fluids in biological systems such as: microtubules which are involved in intracellular transport and cell division; flagella and cilia which aid in locomotion. The numerical simulation of such systems is generally based on slender-body theory which give asymptotic approximations of the solution. However, these methods are low-order and cannot enforce no-slip boundary conditions to high-accuracy, uniformly over the boundary. Boundary-integral equation methods which completely resolve the fiber surface have so far been impractical due to the prohibitive cost of current layer-potential quadratures for such high aspect-ratio geometries. In this talk, we will present new quadrature schemes which make such computations possible and new integral equation formulations which lead to well-conditioned linear systems upon discretization. We will present numerical results to show the efficiency of our methods.

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MS97

Accelerating Potential Evaluation over Unstructured Meshes in Two Dimensions

In this talk, we first give a brief overview of an algorithm for evaluating and interpolating 2D volume potentials over complicated geometries. Then, we present several novel and complementary techniques for accelerating the evaluation of 2D volume potentials over unstructured meshes. Firstly, we observe that the standard approximation of the near field by a ball or a triangle often leads to an overestimated near field. We rigorously characterize the geometry of the near field, and show that this analysis can be used to reduce the number of near field interaction computations dramatically. Secondly, as the near field can be made arbitrarily small by increasing the order of the far field quadrature rule, the expensive near field interaction computation can be efficiently offloaded onto the FMM-based far field interaction computation, which leverages the computational efficiency of highly optimized parallel FMM libraries. Finally, we observe that the usual arrangement in which the interpolation nodes are placed on the same

mesh over which the potential is integrated results in an artificially large number of near field interaction calculations, since the discretization points tend to cluster near the boundaries of mesh elements. We show that the use of a separate staggered mesh for interpolation effectively reduces the cost of near field and self-interaction computations. We demonstrate the effectiveness of the techniques with several numerical experiments.

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MS97

An Efficient Sparse Direct Solver via Domain Decomposition into Thin Subdomains

This talk concerns 2D sparse direct solvers for scalar wave propagation problems in the time harmonic regime on rectangular domains. A high order discretization based on a multidomain spectral collocation scheme is used to resolve the highly ill-conditioned physics of the problem, and to minimize pollution errors. The scheme decomposes the domain into a sequence of electrically thin slabs. We build sparse direct solvers for each subdomain in parallel, then build a global solution operator by solving a sequence of rank-structured matrix equations. Randomized low-rank compression is used to compress interactions down to the minimal rank dictated by the Nyquist limit of two points per wavelength. The scheme leads to a surprisingly efficient solver that we accelerate on GPUs with batched linear algebra.

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MS98

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MS98

The Kagome Lattice as a Mechanism-Based Metamaterial

Mechanism-based metamaterials are synthetic materials that exhibit microscale buckling in response to mechanical deformation. Our research focuses on a specific example: the kagome metamaterial. This periodically arranged material has many energy-free buckling patterns without loads on boundaries. In this talk, we will discuss the large-scale behavior of the kagome metamaterial as a nonlinear homogenization problem. We will also discuss the adequacy of our macroscopic theory with various numerical experiments. The theory is joint work with Robert Kohn, and the numerical results are joint work with Katia Bertoldi and Bolei Deng.

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MS98

Stochastic Nash Evolution

We introduce a probabilistic formulation for the Nash embedding theorems. This approach uses relaxation as in Nashs work, but replaces his iteration (in low codimension) or continuous flow (in high codimension) with a stochastic flow. The main issue in the derivation of this flow is a principled resolution of a semidefinite program. As in Nashs work, the same fundamental structure applies to several hard constraint systems and nonlinear PDE.

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MS98

Compactness and Regularity for a Generalized Aviles-Giga Functional

The classical Aviles-Giga functional is a well known second order energy functional that has been used to model smectic liquid crystals and thin film blisters. In this talk I will discuss a generalized Aviles-Giga functional in two dimensions, where the zero set of the potential is a strictly convex C^1 manifold instead of $\mathbb{S}^1$. Among other things, we generalize the notion of entropies, and use this tool to establish compactness for sequences with bounded energy and regularity for zero and finite energy states. Our analysis sheds light on what parts of the classical Aviles-Giga theory are contingent on specific algebraic properties of $\mathbb{S}^1$, and what parts are more flexible. This is joint work with Xavier Lamy and Andrew Lorent.

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MS99

Numerical Approximation of a Membrane Model of Liquid Crystal Elastomers

Liquid crystal elastomers are materials where a liquid crystal is coupled with a rubbery material. When actuated with heat or light, the interaction of the liquid crystal with the rubber creates complex shapes. We present a numerical method to minimize the stretching energy developed by Ozenda, Sonnet, and Virga (2020). One significant challenge is the lack of quasi convexity of such energy; in fact we show that the energy is not rank-one convex. To address the lack of quasiconvexity, we regularize with a term that mimics a higher order bending energy. We illustrate the geometric effects of defects via numerical computations as well as approximate special solutions.

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MS99

Optimal Control of the Landau–de Gennes Model of Nematic Liquid Crystals

This talk presents an optimal control framework for the time-dependent, Landau–de Gennes (LdG) model of nematic liquid crystals. Since the LdG energy is non-convex, we develop parabolic, optimal control techniques for controlling the L^2 gradient flow of the LdG energy, which is uniquely solvable. The controls in the problem are the weak anchoring conditions and a body force term. We seek to find optimal controls that drive the LdG Q-tensor variable toward a desired "texture" state. The objective functional we minimize is of tracking type with additional regularization terms for the controls. To the best of our knowledge, this is the first time PDE-based optimal control has been developed for the LdG model. Existence of a minimizer for the control problem is established. Moreover, with various regularity estimates, we prove first order Freche't differentiability results for the control objective, by introducing an adjoint PDE, thus allowing gradient based optimization methods. In the talk, we highlight the analytical issues that arise, especially those due to the gradient flow being a parabolic system. We then describe a finite element discretization of the full control problem and present numerical simulations in two and three dimensions that exhibit point and line defects.

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MS99

A Thermodynamically Consistent Q-Tensor Model of Curved Fluidic Liquid Crystal Films with General Orientational Order

In this talk a novel surface Beris-Edwards model is presented. The film is represented by a stationary surface along which the liquid crystal material may flow. The Q-tensor is assumed to be a general traceless symmetric matrix without any simplifications on how its eigenframe is related to the tangent plane of the surface. Generalized Onsager principle is applied to create a model with an energy structure similar to the Beris-Edwards equation but for curved surfaces. The resulting model contains a non-standard force which is necessary for thermodynamical consistency and for the energy law of the novel model in case of generally oriented Q-tensors fields.

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MS100

Linking Cell Shape to Population Structure in Synthetic Bacterial Collectives: a Theoretical Perspective

The increased complexity of synthetic microbial biocircuits highlights the need for distributed cell functionality due to concomitant increases in metabolic and regulatory burdens imposed on single-strain topologies. Distributed systems, however, introduce additional challenges since spatiotemporal dynamics of constituent strains must be controlled to achieve desired circuit behaviors. In this talk, we discuss how to address these challenges with a modeling-based investigation of emergent spatiotemporal population dynamics using cell-length control in monolayer, two-strain bacterial consortia. We demonstrate that nematic cell alignment in close-packed monolayers can be destabilized by changing cell length. We find that this destabilization confers an emergent, competitive advantage to smaller-length strains with mechanisms that differ depending on initial conditions. We used complementary models to reveal underlying mechanisms: an agent-based model to simulate detailed interactions between competing strains and a stochastic lattice model to represent cell-cell interactions with a single rotational parameter. We show that spatial strain-fraction oscillations can be generated when cell-length control is coupled to quorum-sensing signaling in negative feedback topologies. Our research employs novel methods of population control and points the way to programming strain fraction dynamics in consortial synthetic biology.

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MS100

Clusters and Chimeras: Unfolding Bifurcations in Networks of Coupled Oscillators

The Kuramoto model of coupled oscillators has been used to model synchronization in a variety of biological and physical systems ranging from neuron synapses to firefly flashes. In this talk we explain how both the network topology and distribution of intrinsic frequencies lead to a variety of bifurcations. The structure of these bifurcations provides insights into the formation of complex pattern formation beyond synchronization, such as cluster formation, twisted states, and chimeras. Time permitting, we will also describe how time series data of oscillator phases can be used to solve the inverse problem of reconstructing the

underlying network of interactions.

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MS100

Modeling Provides Insight into Self-Organization in Biological Systems

In this talk we will consider how mathematical modeling, analysis, and simulation can be used to provide new insight into biological phenomena. In particular, we focus on the self-organization of large-scale groups of insects and swimming bacteria. This talk will provide an overview of the relation of modeling in finding new insight into application in biology and medicine. What makes these problems interesting is that individual interactions at the microscale lead to the onset of mesoscale and then macroscale patterns. In addition, when animals exhibit collective behavior one can observe remarkable properties such as enhanced movement speed, pattern formation, and increased mixing. Mathematics provides a deeper understanding of how and why these properties emerge and is fundamental to pressing biological problems.

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MS100

Computational Modeling of Pressure-Driven Cell Motility Under Confinement

Cell migration is critical for many vital processes, such as embryogenesis and tissue repair, as well as harmful processes, such as cancer cell metastasis. In experiments, cells have been shown to exhibit different migration strategies, such as myosin-driven rear contraction or blebs, based on the properties of their external environment. Additionally, recent experiments demonstrate that cells do not need to adhere to the channel walls in order to migrate under confinement, yet it is unclear how traction forces are coordinated in space and time to generate motion. Dynamic 2D computational models of a migrating cell using intracellular pressure gradients generated by (1) rear contraction and (2) blebbing in a narrow channel are presented. The cell model consists of an elastic membrane, poro-(visco)elastic cortex, membrane-cortex adhesion, and the fluid cytoplasm. Evolution equations for the actin density of the cortex are included for modeling bleb retraction. The channel walls are modeled as rigid structures with different shapes. The model is formulated using the method of regularized Stokeslets. Results show that cells can effectively migrate in symmetric and asymmetric straight channel walls only if the cortical turnover is included by modeling the cortex as a poro-viscoelastic structure.

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MS101

Analysis of Discontinuous Galerkin Methods Combined with Splitting Techniques for Incompressible Flow

We combine a discontinuous Galerkin spatial discretization with the pressure correction approach to solve the time dependent NavierStokes equations. Such discretizations are preferable since, at each timestep, the nonlinearity of the velocity is decoupled from the pressure. We theoretically show that our scheme is unconditionally stable. In addition, we establish convergence of the discrete velocities in various norms. Under additional assumptions, we employ duality arguments and show optimal convergence rates in the L^2 norm in time and in space. Further, convergence of the pressure is established by deriving error bounds for the discrete time derivative of the velocity. Numerical results verify the convergence rates.

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MS101

A Sequential Discontinuous Galerkin Method for Three-Phase Flows in Porous Media

In this talk, we first present and analyze a sequential discontinuous Galerkin method for the incompressible three-phase flow problem in porous media. We show existence and uniqueness of a discrete solution and obtain a priori error estimates. Then, we present a novel formulation for the black oil problem which uses as primary unknowns the liquid pressure and the aqueous and liquid saturations. This choice of primary variable produces a well-posed numerical scheme without any stringent restriction on the data, and without the introduction of nonphysical quantities. The equations are solved sequentially using an implicit time stepping scheme. We demonstrate the convergence properties of the method numerically, and present different realistic simulations such as injection problems in highly heterogeneous media.

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MS101

Finite Element Numerical Schemes for a Chemo-Attraction and Consumption Model

During this talk I will introduce and compare several finite element numerical schemes to approximate a chemo-attraction model with consumption effects, which is a nonlinear parabolic system for two variables; the cell density and the concentration of the chemical signal that the cell feel attracted to. I will detail the main properties of each scheme, such as conservation of cells, energy-stability and approximated positivity. Moreover, I will present numerical results to illustrate the efficiency of each of the schemes and to compare them with others classical schemes.

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MS102

Error Estimation for the Time to a Threshold Value in Evolutionary Partial Differential Equations

This talk presents an error analysis for the time of the first occurrence of an event, specifically, the time at which a functional of the solution to a partial differential equation first achieves a threshold value on a given time interval. This novel quantity of interest (QoI) differs from classical QoIs which are modeled as bounded linear (or nonlinear) functionals. The fundamental tools used in this analysis are adjoint solutions, computable residuals and variational analysis. A computable and accurate error estimates is derived for semi-linear parabolic and hyperbolic partial differential equations. The accuracy of the error estimates is demonstrated through numerical solutions of the heat equation and shallow water equations.

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MS102

Krylov Subspace Spectral Methods for Modeling Acoustic Singular Surfaces

Krylov Subspace Spectral (KSS) methods are explicit time-stepping methods for PDEs in which each component of the solution, in some basis, is computed using an approximation of the solution operator of the PDE that is, in some sense, optimized for that component. This individualized approximation, based on techniques due to Golub and Meurant for approximating bilinear forms involving matrix functions, results in stability associated with implicit methods, as well as superior scalability as spatial resolution increases. Within the last few years, it has been seen that KSS methods are particularly well-suited to various problems arising in acoustics. This talk provides an overview of recent and ongoing work in this area. This work includes (1) the use of techniques for approximating bilinear and quadratic forms involving matrix functions to measure the sensitivity of solutions of PDEs, (2) the application of KSS methods to the parabolic equation for acoustic pressure in the ocean, and (3) KSS methods for wave propagation problems featuring heterogeneous media, shock waves, or acceleration waves.

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MS102

Dual-Wind Discontinuous Galerkin Methods for a Parabolic Variational Inequality

In this talk we investigate a symmetric dual-wind discontinuous Galerkin method for solving a parabolic variational inequality. By employing a symmetric dual-wind DG discretization in space and a backward Euler discretization in time, we propose a fully discrete scheme to solve a time-dependent obstacle problem. Under reasonable regularity assumptions on the exact solution, we prove the convergence of numerical solutions with rates in the $L^{\infty}(L^2)$ and $L^2(H^1)$-like energy errors by introducing a new interpolation operator which is a combination of the standard interpolation operator and a positive-preserving interpolation operator. Numerical experiments are provided to demonstrate the effectiveness of the proposed method.

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MS103

Homotopy Sampling with an Application to Particle Filters

We explore a sampling procedure and its generalization to find, via homotopy, the unknown normalization of a target distribution, as well as samples of the target distribution. Derived estimates are a useful in making computational efficiency decisions on how the calculation should proceed, given a computer architecture. Consideration is given to how the procedure can be adapted to Bayesian stationary and non-stationary estimation problems. The connection between homotopy sampling and thermodynamic integration is made. Emphasis is placed on the non-stationary problems, and in particular, on a sequential estimation technique known as particle filtering. It is shown that a modification of the particle filter framework to include the

homotopy process can improve the computational robustness of particle filters.

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MS103

Robust Modeling of Unknown Dynamical Systems via Ensemble Averaged Learning

Recent work has focused on data-driven learning of the evolution of unknown systems via deep neural networks (DNNs), with the goal of conducting long time prediction of the evolution of the unknown system. Training a DNN with low generalization error is a particularly important task in this case as error is accumulated over time. Because of the inherent randomness in DNN training, chiefly in stochastic optimization, there is uncertainty in the resulting prediction, and therefore in the generalization error. Hence, the generalization error can be viewed as a random variable with some probability distribution. Well-trained DNNs, particularly those with many hyperparameters, typically result in probability distributions for generalization error with low bias but high variance. High variance causes variability and unpredictably in the results of a trained DNN. In this talk we present a computational technique which decreases the variance of the generalization error, thereby improving the reliability of the DNN model to generalize consistently. In the proposed ensemble averaging method, multiple models are independently trained, and the average of all the single-step model predictions is used as the initial condition for all models at the next time step. A mathematical foundation for the method is presented, including results regarding the distribution of the local truncation error.

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MS103

An Autoencoder Based Deeponet for Solving Forward and Inverse Problems of Stochastic Partial Differential Equations

A new data-driven method for operator learning of stochastic differential equations is proposed in this paper. The proposed method is built based on the recently proposed Deep operator network(DeepONet). Compared to other neural networks to learn functions, DeepONet aims at the problem of learning nonlinear operators. It can be challenging by using the original DeepONet to learn operators in the form of stochastic differential equations, especially when the dimension of physical space or stochastic operator is relatively high. We propose a new network referred to as MultiAuto-DeepONet which enables to deal with this difficulty using convolutional autoencoder. The encoder part of the network is designed to reduce the dimensionality as well as discover the hidden features of stochastic inputs. The decoder is designed to be two DeepONets with a common Branch Net. The first DeepONet is designed to reconstruct the input function involving randomness and the second one is used to find an approximation of the solution. The two Trunk Nets in our network also enable us to deal with multi-resolution inputs naturally. By adding L_1 regularization to our network, we found the outputs from the Branch Net and two Trunk Nets all have sparse structures. This reduces the number of trainable parameters thus making the model more efficient. Finally, we conduct several numerical experiments to illustrate the effectiveness of our proposed model dealing with uncertainty quantification problem.

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MS103

A Nonlocal Gradient for High-Dimensional Black-Box Optimization in Scientific Machine Learning

We consider the problem of minimizing multi-modal loss functions with a large number of local optima. Since the local gradient points to the direction of the steepest slope in an infinitesimal neighborhood, an optimizer guided by the local gradient is often trapped in a local minimum. To address this issue, we develop a novel nonlocal gradient to skip small local minima by capturing major structures of the loss's landscape in black-box optimization. The nonlocal gradient is defined by a directional Gaussian smoothing (DGS) approach. The key idea of DGS is to conducts 1D long-range exploration with a large smoothing radius along d orthogonal directions in R^d, each of which defines a nonlocal directional derivative as a 1D integral. Such long-range exploration enables the nonlocal gradient to skip small local minima. The d directional derivatives are then assembled to form the nonlocal gradient. We use the Gauss-Hermite quadrature rule to approximate the d 1D integrals to obtain an accurate estimator. The superior performance of our method is demonstrated in three sets of examples, including benchmark functions for global optimization, and two real-world scientific problems.

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MS104

On the Hydrodynamic Stability of Viscoelastic Hele-Shaw Flows

We perform linear stability analysis in a rectilinear Hele-Shaw cell where a viscous Newtonian fluid displaces an Upper Convected Maxwell (UCM) fluid in the moderate to high Deborah number regime. We find that the viscosity contrast still plays a decisive role in determining the stability. Increasing Deborah number, capillary number or flow speed worsens the instability. Elasticity has a variety of effects and can give rise up to three types of sin-

gular behaviors: (i) velocity becomes singular at infinitely many distinct wavenumbers; (ii) stress becomes singular when the wavenumber exceeds a certain value; and (iii) the growth rate increases very rapidly near a certain wavenumber and eventually becomes singular if the displacing fluid becomes inviscid. If both fluids are UCM, many features and conclusions found in Newtonian-UCM setup are still valid. The long wave stability is still determined by the viscosity contrast, however short waves are always unstable. The critical wavenumber beyond which instability occurs depends only on the relaxation time of the displacing fluid and flow speed. The growth rate can still be singular but only happens over a relatively narrow region in the parameter space and may be avoided in multiple ways. The case where one or both fluids are Oldroyd-B is ongoing.

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MS104

Nonmodal Amplification of Disturbances in Channel Flows of Viscoelastic Fluids

Whether and how channel flows of viscoelastic fluids with weak levels of inertia and initially small-amplitude perturbations can transition to elastic turbulence is a fundamental yet unsettled issue in non-Newtonian fluid mechanics. Standard (modal) linear stability analysis typically predicts that these flows are stable in the absence of inertia. However, initially small-amplitude perturbations can undergo considerable transient (nonmodal) amplification due to the non-normal nature of the linearized problem. Such amplification may put the flow into a regime where nonlinear terms are no longer negligible, thereby triggering a transition to elastic turbulence. This talk will provide an overview of the basic ideas of nonmodal amplification, elucidate their relevance to viscoelastic channel flows, and present some recent results showing that polymer-stress fluctuations due to a spatially localized time-periodic disturbance can be amplified by an order of magnitude while there is only negligible amplification of velocity fluctuations. This stress amplification is highly localized in space and may be relevant for understanding recent experimental observations (by P. Arratia and co-workers) of elastic turbulence in microchannel flows of viscoelastic fluids (G. Hariharan, M. R. Jovanovic, and S. Kumar, J. Non-Newtonian Fluid Mech. 291 (2021) 104514).

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MS104

A Fast and Accurate Boundary Integral Method for Superhydrophobic Flow Computations

We present a fast and accurate boundary integral method for the computation of incompressible Stokes flow over surfaces featuring corners, free surfaces, solid boundaries, and mixed boundary conditions. Such surfaces arise in simple models of superhydrophobic (SH) materials. Boundary integral methods have several advantages in SH flow computations, such as a reduction in the dimension of the problem and the ability to deal with complex boundary geometries. However, such problems exhibit flow singularities at boundary transition points and geometric corners, and thus standard quadrature rules for smooth integrals result in a severe loss of accuracy. Adaptive mesh refinement mitigates the issue, however, the size of the discrete problem grows significantly with refinement level, and it can still be difficult to obtain satisfactory accuracy due to the ill-conditioning of the linear system. To resolve these issues, we combine the recently developed Recursively Compressed Inverse Preconditioning (RCIP) method with a scaling technique and the Fast Multipole Method to obtain a fast and accurate numerical scheme for SH flow computations. Several examples are presented to illustrate the performance of the method. This is joint work with Kosuke Sugita and Shidong Jiang (NJIT).

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MS106

Discrete-to-Continuum Modelling of Weakly Interacting Incommensurate Two-Dimensional Lattices

A graphene sheet is a single-atom thick macromolecule of carbon atoms arranged in a honeycomb hexagonal lattice. When observing a graphene sheet suspended over a substrate, moir patterns appear driven by lattice and orientation mismatches. In this talk, we present a formal discrete-to-continuum procedure to derive a continuum variational model for two slightly incommensurate lattices. We show that the continuum model recovers both qualitatively and quantitatively the behavior observed in the corresponding discrete model.

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MS106

Dimensional Reduction for the Ferroelectric SmA-type Phase in BCLC

We analytically derive and numerically simulate a two-dimensional energy functional modeling the effects of a constant electric field on a thin sample of a bent-core liquid crystal in the ferromagnetic SmA-like phase. We start from a three-dimensional domain, and we show that under proper rescaling and in the limit of small thickness the electric self-interactions term gives rise to boundary terms. We compare our results to previously proposed models.

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MS106

A Continuum-Based Model of Lipid Domain Coarsening and Fluidity in Lipid Vesicles

Liposomes that achieve a heterogeneous and spatially organized surface through phase separation have been recognized to be a promising platform for delivery purposes. However, their design and optimization through experimentation can be expensive and time-consuming. To assist with the design and reduce the associated cost, we propose a computational platform for modeling membrane coarsening dynamics based on the principles of continuum mechanics and thermodynamics. This model couples phase separation to lateral flow and accounts for different membrane fluidity within the different phases, which is known to affect the coarsening dynamics on lipid membranes. The simulation results are in agreement with the experimental data in terms of liquid ordered domains area fraction, total domains perimeter over time and total number of domains over time for two different membrane compositions that yield opposite and nearly inverse phase behavior.

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MS107

A Stable Mimetic Finite-Difference Discretization for Convection Dominated Diffusion Equations

Convection-diffusion equations arise in a variety of applications such as particle transport, electromagnetics, and magnetohydrodynamics. Simulation of the convection-dominated case, even with high-fidelity techniques, is particularly challenging due to sharp boundary layers and shocks causing jumps and discontinuities in the solution, and numerical issues such as loss of the maximum principle in the discretization. These complications cause instabilities, admitting large oscillations in the numerical solutions when using traditional methods. Drawing connections to the simplex-averaged finite element method (S. Wu and J. Xu, 2020), we develop a mimetic finite-difference (MFD) discretization using exponentially averaged coefficients to guarantee monotonicity of the scheme and stability of the solution as the diffusion coefficient approaches zero. The finite-element framework allows for transparent analysis of the MFD, such as proving well-posedness and deriving error estimates from the finite-element setting. Numerical tests are presented confirming the stability of the method and verifying the error estimates.

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MS107

Structure-Preserving Machine Learning Moment Closures for the Radiative Transfer Equation

In this talk, we present our work on structure-preserving machine learning (ML) moment closure models for the radiative transfer equation. Most of the existing ML closure models are not able to guarantee the stability, which directly causes blow up in the long-time simulations. In our work, with carefully designed neural network architectures, the ML closure model can guarantee the stability (or hyperbolicity). Moreover, some other mathematical properties, such as physical characteristic speeds, are also discussed. Extensive benchmark tests show the good accuracy, long-time stability, and good generalizability of our ML closure model.

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MS108

Deep Learning Methods for Reduced Order Modeling of Advection-Dominated Problems

The need to simulate coupled, nonlinear, advection-dominated physical systems can be found across the broad engineering and computational science community. There have been several efforts to develop classical and deep learning (DL)-based, data-driven reduced order models (ROMs) that can be used to mitigate the computational burden of simulating these complex systems by identifying low-dimensional coherent structures, and accurately modeling relevant correlations in the system dynamics. However, advection-dominated transport processes still pose significant challenges for the design of reliable ROMs, especially when linear subspace approximations are employed. In this work, a physics-aware, deep learning-based ROM framework is developed for advection-dominated transport processes, and is applied to the problem of predicting hydrodynamics in riverine and near-shore systems. Specifically, a neural network architecture capable of learning the advection-dominated flow features is proposed using deep autoencoders and recurrent neural networks. The performance of the proposed advection-aware autoencoder network is demonstrated using different one and two-

dimensional, parametric benchmark problems.

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MS108

Biot System with Friction and Unilateral Constraints

A fully saturated poroelastic medium is confined by the sides of a cylinder, and the regions below and above the medium are filled with fluid at respective known pressures. The quasi-static Biot system of partial differential equations describes the filtration flow of fluid through the medium and its small deformations. In this talk, we discuss the existence of a solution to an initial-boundary-value problem for this system in which normal fluid flow is sealed and the medium has tangential slip (Tresca friction law) with friction arising from known normal stress on the sides. The medium is in partial contact with the exterior fluid on the top and bottom, and on top, the displacement of the medium is unilaterally constrained by a Signorini-type free boundary condition. The Biot model was initially motivated by consolidation problems in soil mechanics and acoustic problems. It has applications in modeling problems arising from geophysics, petroleum engineering, and, more recently, biomedical sciences, particularly the fluid flow inside cartilages, bones, scaffold-based tissue engineering, and perfusion in the optic nerve head.

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MS108

Modeling and Simulation of Filtrations and Separations Environments

Filtration and separations environments appear in a variety of physical applications. They can be used to prevent materials from entering a production stream, or they can be used to pull materials from a carrying fluid. In particular, this adsorption process is a vital component of biopharmaceutical manufacturing. There are currently over 200 biotherapeutics on the market, with many more in trials or in the pipeline. Many of the recent biotherapeutics are monoclonal antibody therapies, with the treatment for COVID-19 being one of the more famous examples. Monoclonal antibody therapies are quickly becoming the standard of care for various cancers, anti-immune disorders, and chronic inflammatory diseases. This increase in demand requires the development of novel adsorptive chromatography media to ensure high-volume throughput of purified product. These media use multiple modes of interaction with the product to recover it selectively from impurities in the feed solution, leading to mathematically complex models to describe the adsorption process. In this talk, we provide an overview of the development of a computational simulation environments to aid in the design of separations processes with distinct removal mechanisms. In particular, we highlight methods for resolving the temporal nonlinearities and present validation of these strategies.

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MS108

A Second-Order Symplectic Approach for an Advection-Diffusion-Reaction Problem in Bioseparation

We consider an advection-diffusion-reaction problem modeling the chromatography process, with non-homogeneous boundary conditions. We prove stability and error estimates for both linear and nonlinear adsorption, using the midpoint method for time discretization and finite elements for spatial discretization. The numerical tests validate our theoretical results.

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MS109

Approximate Computing of Sparse Matrix Orderings via Neural Acceleration

Determining an ideal ordering for a sparse matrix is difficult. In the case of finding an ordering to minimize fill-in for factorization of a general sparse matrix, the problem is NP-Hard. Meanwhile, the selection of an ordering for an iterative method, such as Conjugate Gradients, that reduces iteration counts and efficiently uses the cache hierarchy is based on observations and rules of thumb. The selection of an ordering is exacerbated in applications that solve a series of sparse matrix problems that change over time, e.g., those found in some circuit simulations. Modern computing systems tend to be heterogeneous containing accelerators, such as a GPU or neural device, that can be co-scheduled with the main CPU. These accelerators are ideal for the computation of complex artificial neural networks. This work uses these accelerators to construct a neural network model that approximates an ordering for a given sparse matrix. This approximation model acts at accelerating the selection of an ordering during the application. Moreover, a trained model can be used iteratively in the case of applications where sparse matrices evolve during execution to determine if a new ordering should be implemented at some point in the computation to speed up the application.

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MS109

Greedy Mesh Coarsening with Spectral Guarantees

Coarsening graphs while preserving particular properties of the original is of significance in many fields such as computational geometry, partitioning, and scientific computing. Two appealing objectives for preservation are the eigenvalues and eigenvectors of the graph Laplacian. This spectrum confers important connectivity and cut information about the graph. We present a method for coarsening arbitrary weighted graphs while closely preserving eigenvalues and eigenvectors of the original. Our algorithm uses the nodal domains of Laplacian eigenvectors to filter potential merge edges before applying a greedy coarsening approach based on the linear-dependence of node adjacencies. We present bounds for the quality of eigenvector preservation and empirically show that this algorithm performs particularly well on meshes.

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MS109

Performance-Portable Graph Coarsening

The multilevel heuristic is an effective strategy for speeding up graph analytics, and graph coarsening is an integral step of multilevel methods. We perform a comprehensive study of multilevel coarsening in this work. We primarily focus on the graphics processing unit (GPU) parallelization of the Heavy Edge Coarsening (HEC) method executed in an iterative setting. We present optimizations for the two phases of coarsening, a fine-to-coarse vertex mapping phase, and a coarse graph construction phase. We also express several other coarsening algorithms using the Kokkos framework and discuss their parallelization. We demonstrate the efficacy of parallelized HEC on an NVIDIA Turing GPU and a 32-core AMD Ryzen processor using multilevel spectral graph partitioning as the primary case study.

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MS109

Direct Graph Ordering Optimization for Cache-Efficient Graph Analysis

Vertex reordering for efficient memory access in graph-based data analysis shows considerable improvement to the cache efficiency and runtimes of widely used graph analytic algorithms. Despite these improvements, modern efficient ordering methods are often complex and tend to optimize towards the improvement of a single analytic operation. This paper conducts an experimental study into vertex ordering optimization and introduces a universal graph partitioning-inspired optimization approach focusing on CPU shared-memory parallelism to the vertex ordering problem through the explicit refinement of low-degree vertices. Refinement focuses on the optimization of the Linear Gap Arrangement and Log Gap Arrangement problems as comprehensive metrics for ordering improvement. We present and evaluate this degree-based refinement method upon a number of algorithm-generated orderings and the natural ordering with timing and cache efficiency results relative to three shared-memory graph analytic algorithms: PageRank, Louvain and the Multistep connectivity algorithm. We further these results through the association of the gap arrangement problem metrics to ordering quality and show non-trivial improvement to analytic algorithm efficiencies with some refinement. These findings demonstrate the feasibility of an optimization approach to vertex ordering for processing networks in main memory at a large scale.

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MS110

Meshless Cubature Using Radial Kernels

In this talk we present in the context of meshless cubature a leave-one-out cross validation (LOOCV) criterion for the optimization of the radial basis function (RBF) shape parameter. Using this approach we are able to select a (near) optimal value of the RBF parameter, which allow us to obtain more precise results for any type of RBF. Some numerical results will be showed to illustrate the performance of the obtained cubature formulas.

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MS110

Kernel Interpolation on Compact Riemannian Manifolds

Starting from existing results on (strictly) positive definite and radial kernels on specific manifolds, like spheres or tori, we generalize the result to non-radial kernels and to general manifolds. The goal of our current research is to unify the existing results as far as possible and to simplify the study of new specific manifolds and kernels. The class of strict positive definite kernels, $K : \mathbb{M}^d \times \mathbb{M}^d \to \mathbb{C}$, allows the unique solution of the scattered data interpolation problem in any distinct point set $\Xi \subset \mathbb{M}^d$. We use the series expansion of the kernel in eigenfunctions of the Laplace-Beltrami Operator on $\mathbb{M}^d$ to characterize (strict) positive definiteness. We study especially the class of kernels that have a convolution from and can be described using a simple series expansion. If applied to two-point homogeneous manifolds our results extend the necessary and sufficient characterization of strict positive definite isotropic basis functions, proven for $(d-1)$-dimensional spheres and for two-point homogeneous manifolds, to a non-radial kernel class. We also describe implications for the case of product manifolds.

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MS110

Kernel Based Techniques for Scattered Data Discontinuity Detection

Accurate interpolation of non-regular two-variate functions from a given set of scattered data is a challenging problem that occurs in many applications going from signal processing to geophysics. By non-regular function we mean that the function or its partial derivatives are discontinuous along some planar curves of the given domain. The choice of the interpolation model plays a crucial role for the quality of the reconstruction. If the basis of the interpolation space does not reflect the properties of the underlying function, artifacts will usually appear in the final reconstruction. In order to get a good approximation, we need to precisely define the locations of such curves. In this talk we discuss a kernel-based adaptive strategy to extract the needed information from the given data.

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MS110

On Stability Properties of the Radial Basis Function Methods for Solving PDEs

In this talk we focus on stability properties of three different radial basis function (RBF) methods for solving PDEs: Kansa's method, Radial basis function generated finite difference (RBF-FD) method and Radial basis function partition of unity method (RBF-PUM). These methods differ in how the interpolating basis functions that the methods generate are localized. In the Kansa's method case the support of the interpolating basis functions is global, while the support of the interpolating basis functions is local in the RBF-FD case and the RBF-PUM case. Another differentiator between the three methods is the regularity property of the interpolating basis functions. We present results in the context of solving a linear time-dependent hyperbolic PDE. Our theoretical and numerical results indicate that the regularity of the interpolating basis functions is one of the crucial factors that decide the stability of the RBF methods when a solution is propagated in time. Another important factor when it comes to stability in time is a residual minimizing framework used in order to set up a system of equations that discretize a PDE. We show the differences between the collocation framework and the least-squares (employing equation oversampling/overtesting) framework. Here the framework with oversampling turns out to be a good approximation of the strong Galerkin's variational form, which leads to better stability properties in time compared with the collocation framework.

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MS111

Three Dimensional Solitons in Nematic Liquid Crystals

We model experimentally observed 3-dimensional solitons that develop in flexoelectric nematic liquid crystals, with negative dielectric and conduction anisotropies, when subject to an applied alternating electric field. The liquid crystal is confined in a thin region between two plates, perpendicular to the applied field. The horizontal, uniformly aligned director field is at equilibrium due to the negative anisotropy of the media. However, such a state is unstable to perturbations that manifest themselves as confined, bullet-like, director distortions traveling up and down the sample at a speed of several hundred microns per second. We develop a variational model that couples the Ericksen-Leslie equation of director field distortion and the Poisson-Nearnst-Planck equations governing the diffusion and transport of electric charge, and the electrostatic potential. The governing equations form a coupled nonlinear parabolic-elliptic system with multiple length scales. The model predicts values of the phase-shift, soliton size and speed consistent with the experimentally measured ones. Reference: Liquid Crystals (2022), 1-16.

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MS111

Young and Young-Laplace Equations for a Static Ridge of Nematic Liquid Crystal, and Transitions Between Equilibrium States

Situations involving interfaces between a nematic liquid crystal (nematic), a solid substrate, and a passive gas that includes nematic-substrate-gas three-phase contact lines are of great interest, both scientifically and technologically. In particular, in recent years, the push to exploit the interfacial, dielectric, and viscoelastic anisotropies of nematics has led to the development of devices used in flow processing, microelectronic production, and adaptive-lens technologies that extend beyond the well-known application of nematics in liquid crystal displays. Understanding many of these emerging technologies, which often involve nematic droplets or films, requires a theoretical description of the wetting and dewetting phenomena of nematics. To further understand wetting and dewetting phenomena for nematics, we analyse a two-dimensional static ridge of nematic resting on a solid substrate in an atmosphere of passive gas. Specifically, we obtain the first complete theoretical description for this system, including nematic Young and Young-Laplace equations. Then, under the assumption that anchoring breaking occurs in regions adjacent to the contact lines, we analyse the nematic Young equations and find a range of anisotropic wetting and dewetting phenomena, including discontinuous transitions between the equilibrium states of the ridge, that do not occur in the classical case of an isotropic liquid.

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MS111

Modeling Bacteria Swimming in a Nematic Liquid Crystal

Models of dilute systems of bacteria swimming in a nematic liquid crystal are considered. The motion and orientation of the bacteria are simulated using ordinary differential equations coupled with the partial differential equations modeling the nematic liquid crystal (Ericksen Leslie equations). The analysis and numerical simulations of this system are shown to predict interesting phenomena observed experimentally.

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MS112

Stable and Unstable Shape-Shifters: Slender Structures of Photo-Active Materials

Photo-active materials change shape when illuminated. Since deformation can be non-local, the deformation can lead to a change in illumination conditions. Thus, the behavior of photo-active materials couples the equations of photo-chemistry, geometric optics and mechanics. The latter is especially interesting in slender structures like rods, plates and shells due to geometry. This unusual coupling can lead to many unusual phenomena like cyclic motion under steady illumination, sudden snap-through instabilities etc. This talk will introduce the subject and describe a series of examples to illustrate the rich phenomenology. This talk is in memory of Mark Warner, a mentor, colleague and friend.

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MS112

From Soft Response to Strong Actuation in LCE Sheets

Research on the mechanics and actuation of Liquid Crystal Elastomer sheets has provided insight into mechanical phenomena that transcend the specifics of the material, and are applicable to a broad range of material systems. These include the soft response due to cooperative evolution of stripe domains, to the strong actuation that can be achieved by converting the large energy associated to non-uniform in-plane stretching into bending, as suggested by Gausss Theorema Egregium. I will review our own results in these two areas, both pioneered by Mark Warner, as a tribute to his achievements and as a testimony of his legacy.

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MS112

Design of Origami Structures with Curved Tiles Between the Creases

An efficient way to introduce elastic energy that can bias an origami structure toward desired shapes is to allow curved sheets between the creases. Isometric bending of the sheets then supplies the energy, and typically the sheets themselves have additional functionality. The h^3 scaling of the energy of thin sheets (h = thickness) spans a broad energy range, that is also consistent with a single origami design. And different tiles can have different values of h. In this lecture we present a theory and systematic design methods for quite general curved origami structures that can be folded from a flat sheet. The tiles are allowed to undergo curved isometric mappings, and the curves representing the creases are also allowed to undergo isometric mappings as curves. These assumptions are consistent with a variety of practical methods for crease design. Following developments for piecewise rigid origami, we develop further the Lagrangian approach and the group orbit method in this context.

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MS112

A Ribbon Model for Nematic Polymer Networks

We present a theory of deformation of ribbons made of nematic polymer networks (NPNs). These materials exhibit properties of rubber and nematic liquid crystals, and can be activated by external stimuli of heat and light. A two-dimensional energy for a sheet of such a material has already been derived from the celebrated neo-classical energy of nematic elastomers in three space dimensions. Here, we use a dimension reduction method to obtain the appropriate energy for a ribbon from the aforementioned sheet energy. We also present an illustrative example of a rectangular NPN ribbon that undergoes in-plane serpentine deformations upon activation under an appropriate set of boundary conditions.This is joint work with H. Singh.

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MS113

A Stable Hierarchical Spectral Solver for Parabolic Equations

A stable and high-order accurate solver for linear and nonlinear parabolic equations is presented. An additive Runge-Kutta method is used for the time-stepping, which integrates the linear stiff terms by an explicit, singly diagonally implicit Runge-Kutta (ESDIRK) method and the nonlinear terms by an explicit Runge-Kutta (ERK) method. In each time step, an implicit solve is computed via the recently developed Hierarchical Poincaré-Steklov (HPS) method. The HPS method is a fast direct solver for elliptic equations that decomposes the space domain into a hierarchical tree of subdomains and builds spectral collocation solvers locally on the subdomains. These ideas are naturally combined together in the presented method because the singly diagonal coefficient in ESDIRK and a fixed time-step ensure that the coefficient matrix in the implicit solve of HPS remains the same for all time stages. Therefore the precomputed inverse can be efficiently reused. The stability of the proposed method is proved for first order in time and higher order in space, and numerical evidence shows the proposed method is stable for a broader class of equations.

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MS113

Broadband Recursive Skeletonization

In recent years there have been many advances in the development of fast direct solvers for the linear systems arising from the discretization of integral equations. In this talk I present a new technique for accelerating the application of a particular class of these solvers to scattering problems where multiple frequencies are of interest. The technique works by accelerating the "compression stage" of direct solvers by precomputing bases that approximately span the column and row spaces of various off-diagonal blocks of all coefficient matrices corresponding to a range of different wavenumbers. The key observation is that the ranks when this is done are often comparable to those in the single frequency case at the highest frequency considered. This is joint work with Per-Gunnar Martinsson at UT Austin.

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MS113

Computing the Square Root of a Low-Rank Perturbation of the Scaled Identity Matrix

We consider the problem of computing the square root of a perturbation of the scaled identity matrix, $A = \alpha I_n + UV^*$, where U and V are $n \times k$ matrices with $k \leq n$. This problem arises in various applications, including computer vision and optimization methods for machine learning. We derive a new formula for the pth root of A that involves a weighted sum of powers of the pth root of the $k \times k$ matrix $\alpha I_k + V^*U$. This formula is particularly attractive for the square root, since the sum has just one term if $p = 2$. We also derive a new class of Newton iterations for computing the square root that exploit the low-rank structure. We test these new methods on random matrices and on positive definite matrices arising in applications. Numerical experiments show that the new approaches can yield much smaller residual than existing alternatives and can be significantly faster when the perturbation UV^* has low rank.

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MS113

Noisy Iterative Methods for Matrix Functions

Iterative Krylov subspace methods for computing matrix functions typically assume access to a subroutine for mul-

tiplying vectors by a target matrix A. In this talk, we will discuss recent work in the harder setting where we instead assume access to an imperfect matrix-vector multiplication oracle, which returns Ax perturbed by a small amount of noise. This model captures several algorithms of interest, including rational function approximation methods based on stochastic iterative solvers. It also captures recent sublinear time algorithms for spectral density estimation, which are based on randomized matrix-vector multiplication. We will show how recent progress on analyzing the stability of the Lanczos method and other Krylov subspace methods allows us to analyze these algorithms, and provide a tool for developing other applications which push beyond the traditional model. Based on work with Aaron Sidford, Cameron Musco, Aditya Krishnan, and Vladimir Braverman.

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MS114

Analysis of a Warm Start Krylov-Schur Method

Sequences of eigenvalue problems arise in a range of applications, among others, in computing the eigenvectors for parameterized PDEs, for example, in acoustics, model reduction, updating an approximate invariant subspace for Krylov subspace recycling, and for data analytics problems. Rather than starting from scratch for each matrix, it may be advantageous to jump-start the Krylov-Schur algorithm with the approximate invariant subspace of a previous matrix. While this may reduce the total number of matrix-vector products required to converge to an invariant subspace, this also brings some complications. The approximate invariant subspace for a previous matrix, even if computed using the Krylov-Schur algorithm, is generally not a Krylov space for the new matrix, and we need to make adaptations to the Krylov-Schur algorithm. We compute the approximate Krylov decomposition with the smallest backward error (residual matrix), following [Stewart 2002], followed by a sequence of Arnoldi iterations with a subsequent Krylov-Schur truncation that takes the residual matrix into account. We analyze how a cycle of Arnoldi/Krylov-Schur reduces the norm of the residual, and how this relates to the convergence to an approximate invariant subspace as for the standard Krylov-Schur algorithm.

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MS114

A Randomized Feast Method

Randomized NLA methods have recently gained popularity because of their easy implementation, computational efficiency, and numerical robustness. We propose a randomized version of a well-established FEAST eigenvalue algorithm that enables computing the eigenvalues of the Hermitian matrix pencil (A,B) located in the given real interval. In this talk, we will present deterministic as well as probabilistic error analysis of the accuracy of approximate eigenpair and subspaces obtained using the randomized FEAST algorithm. First, we derive bounds for the canonical angles between the exact and the approximate eigenspaces corresponding to the eigenvalues contained in the interval of interest. Then, we present bounds for the accuracy of the eigenvalues and the corresponding eigenvectors. This part of the analysis is independent of the particular distribution of an initial subspace, therefore we denote it as deterministic. In the case of the starting guess being a Gaussian random matrix, we provide more informative, probabilistic error bounds. Finally, we will illustrate numerically the effectiveness of all the proposed error bounds.

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MS114

Thick-Restarted Lanczos with Sketched Rayleigh-Ritz for Computing Many Eigenpairs

The accuracy of Krylov-based iterative methods for symmetric eigensystems depends on the level of orthogonality of the Krylov basis. In theory the Lanczos three-term recurrence guarantees full orthogonality, but in practice orthogonality is lost after eigenvector approximations start to appear in the basis. Especially when a large number of eigenvectors is required, the time to orthogonalize these methods becomes a bottleneck. One could avoid orthogonalization by solving a generalized Rayleigh-Ritz problem with the Gram matrix of the basis. However, this has similar complexity and worse numerical behavior. Recently, Nakatsukasa and Tropp proposed a randomized sketching for Rayleigh-Ritz which guarantees no loss of accuracy as long as the condition number of the basis is less than 1/(machine eps). While there is little benefit to this algorithm for finding one or a small number of eigenpairs (as JDQMR or GD+k achieve effectively the same), it has potentially significant benefits to finding a large number of eigenpairs. We present a thick restarted Lanczos with sketched Rayleigh-Ritz that reduces the amount of orthogonalization significantly (albeit not eliminating it). This

allows for larger basis sizes and thus faster convergence with smaller iteration costs.

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MS114

Krylov-Schur and the Departure from Normality of Correction Matrices

Low synchronization Gram-Schmidt algorithms for the Arnoldi expansion of a non-symmetric matrix A were introduced in Swirydowicz et al (2019) for GMRES and Bielich et al (2022) applied these to the Krylov-Schur algorithm. These orthogonalization schemes improve parallel strong scaling by reducing global communication. The loss of orthogonality of the computed Krylov vectors is closely related to Henrici's departure from normality $dep(T_k)$ of the correction matrices $T_k = (I + L_k)^{-1}$, in the projector $P = I - Q_k T_k Q_k$, where $T_k \approx (Q_k^T Q_k)^{-1}$ at iteration k. We examine how the dimension of invariant subspaces computed by the Krylov-Schur algorithm depends on the non-normality of T_k. The modified (MGS) and classical (CGS) Gram-Schmidt algorithms are further revised, based on Ruhe (1983) and truncated series expansions for T_k, in order mitigate $dep(T_k)$ and maximize the dimension of the invariant subspaces. Randomization can be applied using a product form of MGS with sketching matrix B, where $Q_k = BG_k$.

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MS115

A New Method for Grade-Two Fluids

Non-Newtonian fluids arise in many applications, including industrial manufacturing and food production. Here we will discuss the grade-two model of non-Newtonian fluids, which features a stress-strain relationship that involves derivatives of the fluid velocity. While important for modeling, this more complicated relationship in comparison to Newtonian counterparts create challenges for numerical simulation. We will discuss a new algorithm for posing the grade two fluid model which allows for nontrivial inflow boundary conditions. The proposed method is amenable to discretization by the finite element method.

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MS115

Improving Eddy Viscosity Modeling

Direct computation in numerical simulations of turbulent flow are often unfeasible. Large Eddy Simulations (LES) have been shown to provide efficient alternative. We analyze a generalization of the Smagorinsky model that attempts to fix the over dissipation, i.e. the well known drawback of the model. We present finite element analysis and numerical computations based on several benchmark problems.

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MS115

Enabling Fast Convergence of the Iterated Penalty Picard Iteration with $O(1)$ Penalty Parameter for Incompressible Navier-Stokes via Anderson Acceleration

This paper considers an enhancement of the classical iterated penalty Picard (IPP) method for the incompressible Navier-Stokes equations, where we restrict our attention to $O(1)$ penalty parameter, and Anderson acceleration (AA) is used to significantly improve its convergence properties. After showing the fixed point operator associated with the IPP iteration is Lipschitz continuous and Lipschitz continuously (Frechet) differentiable, we apply a recently developed general theory for AA to conclude that IPP enhanced with AA improves its linear convergence rate by the gain factor associated with the underlying AA optimization problem. Results for several challenging numerical tests are given and show that IPP with penalty parameter 1 and enhanced with AA is a very effective solver.

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MS115

An Algebraic Splitting Method for Solving Bingham Problem

In this work, we study an algebraic splitting method for solving the Bingham problem. It breaks the Picard iteration of the Bingham problem into 3 simpler linear finite element systems and thus reduces the linear solve time per iteration. Our analysis and numerical tests show that this method converges linearly with a good initial guess and the

mesh size may lag the convergence speed if it is too small.

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MS116

Pressure-Robust Discrete De Rham and Virtual Element Schemes for the Stokes Problem

The Discrete De Rham (DDR) and Virtual Element Method (VEM) are arbitrary-order numerical methods on generic polytopal mesh that provide discrete versions of the de Rham complex, whose properties are crucial to the well-posedness of certain PDE models. Reproducing these properties at the discrete level ensures stable numerical schemes. We will first present the principles underlying the constructions of DDR and VEM, discussing how each method can be interpreted in the other's framework (leading to different schemes nonetheless). We will then discuss the DDR and VEM discretisations of the Stokes equations in curl-curl form. The exactness of the discrete complexes and discrete Poincar inequalities ensure the inf-sup and well-posedness of the schemes. Primal and adjoint consistency properties provide optimal error estimates. An important feature of schemes for the Stokes equations is pressure-robustness: error estimates that are independent of the pressure magnitude. This is often achieved through discretisations of the source term using H_{div} conforming spaces, which are fully computable only on specific elements (tetrahedra, hexahedra). In the DDR and VEM frameworks, pressure-robust estimates are instead obtained using a commutation property of the interpolator and the continuous/discrete operators, and a well-chosen fully computable discretisation of the source term. Numerical tests confirm the optimal rate of convergence and the pressure-robustness.

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MS116

Preconditioning a Divergence-Free HDG Scheme for the Generalized Stokes Problem

Although hybridizable discontinuous Galerkin (HDG) schemes have been developed and successfully applied to various partial differential equations, the challenge of constructing optimal and robust solvers and preconditioners for the condensed schemes has not been fully addressed. In this report, we propose a block diagonal preconditioner and a multigrid preconditioner for the condensed $H(\mathrm{div})$-conforming HDG schemes for the generalized Stokes problem which are robust with respect to model parameters and mesh size. For the block diagonal preconditioner, an optimal preconditioner on the global velocity space is obtained based on the auxiliary space preconditioning (ASP) technique, and an operator spectrally equivalent to the Schur complement on the element-wise pressure space is also constructed. For the multigrid preconditioner, we propose a natural prolongation operator for the hybrid velocity space on the mesh facets and thus an optimal multigrid preconditioner for the HDG scheme is obtained. Numerical results are presented to verify the robustness of the proposed preconditioners.

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MS116

A Family of Conforming and Divergence-Free Finite Elements for Stokes Problem in Three Dimensions

We present a family of conforming finite elements for the Stokes problem on general tetrahedral meshes. On each element, the pressure space consists of k-1-th order polynomials; the velocity space consists of k-th order polynomials enriched with continuous piecewise polynomial bubbles. The elements satisfy inf-sup condition and converge with order k for both the velocity and pressure. In addition, the divergence of the velocity space is exactly the pressure space, therefore the divergence-free condition holds precisely on the discrete level. Moreover, the elements can fit into a discrete Stokes complex starting with Lagrange finite element space. This leads to a family of gradcurl-conforming elements which can be used to discretize fourth-order curl problems. With an explicit characterization of the kernel spaces in a discrete complex, one may also construct parameter robust preconditioners for solving the Navier-Stokes equations.

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MS117

Stability of Robust Dynamical Low-Rank Approximations for Hyperbolic Problems

There has been significant interest lately in applying dynamical low-rank approximations (DLR) to kinetic equations. Both for problems from plasma physics (e.g. Vlasov-Maxwell) and radiation transport (e.g. Boltzmann-BGK). DLR methods have been found to perform well (even in the fully nonlinear regime) as they are able to resolve filamentation and schemes have been constructed that can capture the associated diffusive and fluid limits. Even though it is well known that certain spatial and temporal discretizations, when combined with the DLRA approach, can result in numerical instability, this phenomenon is poorly understood. Here we present a L^2 stability analysis for the nonlinear equations of motion. This allows us to identify the source of instability in the combined spatial and dynamical low-rank approximation. Whether DLR first then discretize or discretize first and then perform DLR is superior has been the subject of some debate in the community. We observe that performing DLR first results in a stable scheme, while the same is not necessarily true if the discretization is performed first. We also note that the obtained CFL condition can be more restrictive than for

the original problem and that the unconventional integrator is usually more stable than the more commonly used projector splitting integrator.

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MS117

An Adaptive Dynamical Low Rank Method for the Nonlinear Boltzmann Equation

Efficient and accurate numerical approximation of the full Boltzmann equation has been a longstanding challenging problem in kinetic theory. This is mainly due to the high dimensionality of the problem and the complicated collision operator. In this work, we propose a highly efficient adaptive low rank method for the Boltzmann equation, concerning in particular the steady state computation. This method employs the fast Fourier spectral method (for the collision operator) and the dynamical low rank method to obtain computational efficiency. An adaptive strategy is introduced to incorporate the boundary information and control the computational rank in an appropriate way. Using a series of benchmark tests in 1D and 2D, we demonstrate the efficiency and accuracy of the proposed method in comparison to the full tensor grid approach.

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MS117

Efficient, Low-Rank Methods for Radiation Transport Simulations

This talk presents a low-rank method for reducing the computational cost of the discrete ordinates (SN) radiative transfer calculations. The reduced system that evolves on a low-rank manifold is constructed via an unconventional basis update and Galerkin integrator to avoid a substep that is backward in time, which could be unstable for dissipative problems. By applying separate low-rank decompositions in each octant where angular flux has the same sign of the direction cosines, the resulting system preserves the information of angular direction. The transport sweeps and source iteration can efficiently solve this low-rank-SN system. The numerical results in 2-D and 3-D Cartesian geometries demonstrate that the low-rank solution requires less memory and computational time than solving the full rank equations using transport sweeps without losing accuracy. The low-rank solution does not preserve the number of particles. The fix is present by solving a conservative two-moments approximation with closure terms computed by the low-rank method.

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MS117

Rank-Adaptive Integration of Nonlinear Evolution Equations on Tensor Manifolds

We present new adaptive algorithms for temporal integration of high-dimensional PDEs on tensor manifolds. These algorithms are based on functional tensor train (FTT) series expansions, operator splitting time integration and a new adaptive criterion to add or remove tensor modes adaptively from the FTT solution as time integration proceeds. The adaptive criterion is based on thresholding the component of the time derivative of the solution normal to the FTT tensor manifold. The new adaptive algorithms are designed to improve computational efficiency, accuracy and robustness in numerical integration of high-dimensional PDEs. In particular, they allow us to overcome well-known computational challenges associated with dynamic tensor integration, including low-rank modeling errors and the need to invert the covariance matrix of the FTT tensor modes at each time step. Numerical applications are presented and discussed for a four-dimensional Fokker-Planck equation.

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MS118

Signature-Based Representation of Events in Video Streams

Summarising a given path by computing its signature remains a seminal approach for many real-world applications (i.e handwriting recognition, landmark-based action recognition, etc.) due to its invariant characteristics to reparameterization. The challenges, however, remains on how we can deal with stream-like and high dimensional data such as images and video streams without the necessity of the presence of explicit temporal paths. In this talk, we introduce a framework for mapping objects in video streams as a stream of paths highlighting the order in which events take place. This temporal representation gives a descriptive summary for video contents which we can maximise: 1) data anonymity, and 2) systematic readability of large-scale video streams. This low dimensional representation of data allows retrieving information with minimal memory footprint and computational requirements. We also demonstrate how a single image can be transformed to streams with multiple channels. These streams are parameterized by spatial directions. We used open-access video datasets in cities to show the significance of the presented framework in mapping multi-agents and anomaly detection in cities.

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MS118

Signature Features with Visibility Transformation

In this talk, I will introduce the visibility transformation and show that this transform is able to embed the effect of the absolute position of the data stream into signature features in a unified and efficient way. The generated feature set is particularly useful in pattern recognition tasks, for its simplifying role in allowing the signature feature set to accommodate nonlinear functions of absolute and relative values.

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MS118

Neural CDEs - How to Make the Most of Them in Applications

In recent years, differential equation-inspired structures for neural networks have exploded in popularity. Neural ODEs, neural CDEs, and neural SDEs have achieved state-of-the-art performance across multiple domains. However, a lot of experiments may have limited scope. One recent development enables neural CDEs to be deployed for online applications, how practical is this? In this talk, we look at applications of neural CDEs on reinforcement learning and control problems, in particular, sequence-to-sequence learning. In combination with using path signatures as features to encode information of the historical path, we discuss the applicability of these methods.

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MS119

Nonlinear Elastic Instabilities in Parallel Shear Flows

In this talk, I will discuss the stability of viscoelastic flows in pipes and channels. I will show that the flow of a dilute viscoelastic fluid in straight microchannels (L=100 μm) can become unstable to finite amplitude disturbance even in the absence of inertia (i.e. low Re). Remarkably, the transition to the unstable flow state for the viscoelastic fluid in the microchannel is subcritical and is akin to the transition from laminar to turbulent flows in ordinary Newtonian fluids where the control parameter is the Reynolds number. Taking together, these results show that complex fluids can give rise to rich and potentially useful behavior even under relatively simple flow conditions.

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MS119

Active Particles in Complex Fluids

Active particles are self-driven objects, biological or otherwise, which convert stored or ambient energy into systematic motion. The motion of small active particles in Newtonian fluids has received considerable attention, with interest ranging from phoretic propulsion to biological locomotion, whereas studies on active bodies immersed in complex fluids are comparatively scarce. In this talk I will discuss a theoretical formalism for understanding the motion of active particles in fluids of arbitrary rheology and then discuss the effects of viscosity gradients, viscoelasticity and shear-thinning rheology in the context of biological locomotion and the propulsion of colloidal Janus particles.

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MS119

Vortex-Waves in Viscoelastic Fluids

Elastic stresses in viscoelastic fluids can result in torques on fluid elements, giving rise to regions of concentrated vorticity. Regions of vorticity formed in this way can propagate as a wave, and are referred to as vortex-waves. From an energy viewpoint, vortex-waves are the result of the conversion of elastic energy to kinetic energy. In this talk, I will discuss a linearized theory which indicates the existence of these waves. The model predicts that vortex-waves exhibit a period of growth, followed by a period of wave translation and viscous decay. Wave speeds are predicted to be proportional to the square root of the initial fluid tension, analogous to waves on a stretched string. Numerical simulations using a pseudo-spectral code are shown to give excellent agreement with theoretical predictions. For example, wave speeds obtained from the numerical simulations are generally within one percent of the predicted values. Results discussed in this talk have been obtained in whole or in part from: Handler, R.A.; Buckingham, M.J. Numerical Simulation and Linearized Theory of Vortex Waves in a Viscoelastic, Polymeric Fluid. Fluids 2021, 6, 325. https://doi.org/10.3390/fluids6090325

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MS119

Exact Coherent State in Purely Elastic Pressure-Driven Channel Flow

Dilute polymer solutions do not flow like Newtonian fluids. Their flows exhibit instabilities at very low Reynolds numbers that are driven not by inertia, but rather by anisotropic elastic stresses. Further increase of the flow rate results in a chaotic flow, often referred to as purely elastic turbulence. The mechanism of this new type of chaotic motion is poorly understood. In this talk we present the first coherent state in purely elastic parallel shear flows. We consider a model shear-thinning viscoelastic fluid driven by an applied pressure gradient through two- and three-dimensional channels. By starting from a linearly unstable mode recently discovered by Khalid et al. (arXiv:2103.06794) at very large flow rates and very low polymer dilution, we demonstrate that this instability subcritically connects to significantly higher values of polymer concentration and lower flow rates, rendering these structures experimentally relevant. We explain the physical mechanism of their stabilization and discuss their relevance to purely elastic turbulence.

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MS120

Stochastic Multiscale Simulation Method for Heterogeneous Catalysts: Concurrent Coupling of Kinetic Monte Carlo and Fluctuating Hydrodynamics

A concurrent coupling approach based on domain decomposition is applied to develop a stochastic multiscale simulation method for heterogeneous catalytic systems at the micron or submicron scale. Kinetic Monte Carlo (KMC) is employed to accurately describe complex reaction mechanisms on the catalytic surface, whereas fluctuating hydrodynamics (FHD) is used to effectively describe transport behavior in the bulk gas region. Under the reasonable assumption that interactions between the gas and surface phases occur only through adsorption and desorption processes, a flux-based coupling of KMC and FHD is constructed by modeling these processes and defining how to update each phase accordingly. Based on the Langmuir model of adsorption, a Markov process modeling of adsorption and desorption processes is developed, through which discrete (Poisson) fluctuations in KMC and continuous fluctuations in FHD are incorporated. For a prototype reactor setting, the effects of the coupling of hydrodynamic transport and surface chemistry and the effects of thermal fluctuations across the interface are analyzed.

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MS120

Heterogeneous Moment Closure Approximations in On-Lattice Chemical Kinetics

We present extensions of simple moment closure approximations to chemical reactions whose rates are nonuniform. The effects of static disorder in the rate constants and short-range correlation in the densities of reactants can be captured by considering representative sites or clusters of sites in a bath of the average environment. However, accurate treatment of long-range correlation remains elusive. We explore the potentials of machine learning moment closure (MLMC) to capture the effects of long-range correlation in on-lattice chemical kinetics. Using the lattice Lotka-Volterra model (LLVM) as a model system, we demonstrate a procedure to construct an accurate moment closure using the results of kinetic Monte Carlo (KMC) at select values of rate constants and initial conditions. Solving the kinetic equations with MLMC gives drastic improvements in the simulated kinetics and descriptions of the dynamical regimes. We discuss the challenges and the potential solutions in applying MLMC to realistic systems.

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MS120

Multilevel Adaptive Sparse Grids for Parametric Stochastic Models

A common research question is the dependence of a stochastic model's output on its input parameters. A particular challenge is the often high-dimensional parameter domains, the high costs of Monte Carlo (MC) sampling and the non-linear nature of the response. We address these issues with a new multilevel adaptive sparse grid (ASG) interpolation of the parameter dependence of the expected values. Here, ASG serve to approximate these functions over high-dimensional domains without being much affected by the dimensionality. As common in ASG, we utilize the hierarchical structure of the employed sparse grids basis to drive the adaptive grid refinement, i.e. to determine for which parameters MC sampling needs to be run. Additionally, we exploit the intrinsic multilevel decomposition of sparse grids to introduce different levels of MC sampling accuracy. We find that in every refinement step the sampling variance can be doubled for the new grid points. This is in contrast to the standard approach, where all grid points would be sampled with the same accuracy. Besides low- and high-dimensional toy models, we demonstrate the approach on a MC model from the field of catalysis. In all cases, the multilevel and the standard approach are indistinguishable in terms of accuracy. However, the multilevel approach achieves the required accuracy at significant lower costs - often by orders of magnitude.

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MS120

Bayesian Uncertainty Quantification for Particle-Based Simulations

A number of problems of interest in applied mathematics and biology involve the quantification of uncertainty in computational and real-world models. A recent approach to Bayesian uncertainty quantification using transitional Markov chain Monte Carlo (TMCMC) is extremely parallelizable and has opened the door to a variety of applications which were previously too computationally intensive to be practical. In this talk, we first explore the machinery required to understand and implement Bayesian uncer-

tainty quantification using TMCMC. We then describe dissipative particle dynamics, a computational particle simulation method which is suitable for modeling biological structures on the sub-cellular level, and develop an example simulation of a lipid membrane in fluid. Finally, we apply the algorithm to a basic model of uncertainty in our lipid simulation, effectively recovering a target set of parameters (along with distributions corresponding to the uncertainty) and demonstrating the practicality of Bayesian uncertainty quantification for complex particle simulations.

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MS122

Approximation of Fractional Harmonic Maps

This talk addresses the approximation of fractional harmonic maps. Besides a unit-length constraint, one has to tackle the difficulty of nonlocality. We establish weak compactness results for critical points of the fractional Dirichlet energy on unit-length vector fields. We devise and analyze numerical methods for the approximation of various partial differential equations related to fractional harmonic maps. The compactness results imply the convergence of numerical approximations. Numerical examples on spin chain dynamics and point defects are presented to demonstrate the effectiveness of the proposed methods.

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MS122

Generalized Exponential Time Differencing for Fractional Diffusion-Reaction Equations

Fractional subdiffusion-reaction equations are effective models for many complex phenomena in science and engineering. Spatial discretization of such models generates large ODE systems that are often stiff. Exponential time differencing schemes are known for their robust stability properties and accuracy for stiff systems. In this talk, we present a class of high-order generalized exponential time differencing schemes with efficient implementation using partial fraction decomposition of global rational approximations of Mittag-Leffler function.

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MS122

Numerical Solutions of Fractional Order Models with Application in Pattern Formation

Nonlocality and spatial heterogeneity of many practical systems have made fractional differential equations very useful tools in Science and Engineering. However, solving these types of models is computationally demanding. In this talk, I will present an overview of fractional calculus and some of my recent results on solving fractional diffusion-reaction problems. The talk will focus on the numerical solution of nonlinear reaction-diffusion fractional models using exponential time differencing. Different approaches to spatial discretization of the reaction-diffusion fractional systems which are very important in reducing computational time will be discussed. Generally, the mechanisms of cell motility and/or the generation of chemical pre-patterns are modeled using ideas of biological pattern formation. Several models for pattern formation have been proposed to explain the regenerative properties of hydra which have been experimentally observed in various transplantations. Invoking the intrinsic properties of fractional calculus is therefore apparent in biological and biochemical systems due to these complexities. I will present some applications of fractional calculus in biological pattern formation.

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MS122

Numerical Methods for Nonlocal Heterogeneous Problems

In this talk, I will introduce the recently developed meshfree methods based on the radial basis function to solve problems with the variable-order fractional Laplacian. The proposed methods take advantage of the analytical Laplacian of the radial basis functions so as to accommodate the discretization of the classical and variable-order fractional Laplacian in a single framework and avoid the large computational cost for numerical evaluation of the fractional derivatives. Moreover, our methods are simple and easy to handle complex geometry and local refinements, and their computer program implementation remains the same for any dimension d. The effects of variable-order fractional Laplacian will also be discussed.

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MS123

Simulation-Based Multi-Objective Optimization of Monoclonal Antibody Capture Chromatography Platforms

A major hurdle in the implementation of simulation-based optimization for process design are the computational resources constraints. In this work we discuss the use of surrogate functions and hybrid optimization algorithms to create an efficient and robust computational framework for process design. Our model process is the capture operation for monoclonal antibody (mAb) purification, an important step in biopharmaceutical manufacturing. The simulation of this operation involves approximating a nonlinear PDE with finite elements to generate a breakthrough curve. A new breakthrough curve is needed for every change in de-

sign parameters, meaning a new finite element simulation. To reduce the computational time, we create a library of curves to generate surrogate functions used by the optimization algorithm. This strategy yielded accurate results with a 10-fold decrease in processing time. Our case study considers two objective functions, each defined using two design variables. We demonstrate the performance of our hybrid optimization method, which uses MATLABs built-in tools, by comparing its performance against individual optimization algorithms. The comparison includes scenarios involving integer, continuous and mixed-integer variables. We show efficiency metrics for our test cases and discuss the increased flexibility of our approach. We also propose a generalization based on the number and type of variables.

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MS123

Hybrid Modeling and Analysis of Multicomponent Adsorption applied to Coalbed Methane

In this talk we present non-standard models of multicomponent adsorption with applications to adsorption in coal-beds. We take a thermodynamically consistent approach via the ideal Adsorbate Solution (IAS) theory at the macroscale level and a mean-field equilibrium approach at the pore-scale. The models we consider do not have a simple algebraic form, and therefore their analysis and numerical simulation present challenges. We present several mathematical analysis results and numerical solutions to illustrate the issues. This is joint work with Dr. Malgorzata Peszynska, Oregon State University.

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MS123

Towards Higher Order Methods for Nonlinear Adsorption Problems

The production of monoclonal antibodies, increasingly an important component of the biopharmaceutical industry, requires separation of proteins from a carrying fluid. Rapid and efficient separations processes improve the time to market of these drugs, ensuring their availability when needed. We are collaborating with a team of chemical engineers to evaluate the performance of adsorption mechanisms driven by membrane technology. In this work, we analyze the performance of second-order methods for generating approximate solutions to the nonlinear equation used to model changes in the transport of both the liquid and solid phase concentrations. Our results indicate simple extrapolated methods can be used to construct inexpensive approximations with convergence behavior on the same order as more complicated higher order schemes.

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MS124

Helical Organization of DNA-Like Liquid Crystal Filaments in Cylindrical Viral Capsids

We study equilibrium configurations of ds-DNA in a cylindrical viral capsid. We assume that the state of the encapsidated DNA consists of a disordered inner core enclosed by an ordered outer region, next to the capsid wall. In our approach, a DNA configuration is described by a unit helical vector field, tangent to an associated center curve, passing through properly selected locations. We postulate an expression for the energy of the encapsulated DNA based on that of columnar chromonic liquid crystals. A thorough analysis of the Euler-Lagrange equations yields multiple solutions to the corresponding boundary value problems. We demonstrate that there is a trivial, non-helical solution, together with two other solutions with nonzero helicity of the opposite sign. Using bifurcation analysis, we derive the conditions for local stability of such solutions and determine when the preferred coiling state is helical. The relevant bifurcation parameters are the ratio of the twist versus the bend moduli of DNA and the ratio between the sizes of the ordered and the disordered regions.

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MS124

Ionically Charged Topological Defects in Nematic Fluids

Controlling the electric charge in liquid electrolytes is of

prime importance in a range of applications such as supercapacitors, or the self-assembly of particles in colloidal or biological settings. However, realizing localised charge profiles in the bulk of such electrolytes generally requires the presence of surfaces which poses a fundamental constraint on the material design. Here, we show using numerical modelling that nematic topological defects in nematic electrolytes can perform as regions for local charge separation, forming charged defect cores and, in some geometries, even electric multilayers, analogous to electric double layers found in isotropic electrolytes. Specifically, we show that flexolectricity and ion solvability perform as the main mechanisms for the effective charging of the nematic. Different bulk and surface geometries will be discussed, including flat interfaces and colloids. More generally, the relevance of this work is for possible applications where topological defects act as diffuse ionic capacitors or as ionic charge carriers.

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MS125

Axisymmetric and Non-Axisymmetric Critical Points of the Onsager Functional

The talk will discuss critical points of the Onsager functional for liquid crystals, giving in particular a simple proof of their axisymmetry in the case of the Maier-Saupe molecular interaction, a classical result of Fatkullin & Slastikov (2005) and Liu, Zhang & Zhang (2005). For general molecular interactions the smoothness of critical points is proved, and for a wide class of interactions the existence of non-axisymmetric critical points established.

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MS125

Colloidal Rocket Propulsion, and Other Surprises in Soft Matter at the Nanoscale

If there is one thing that is clear from the work of Mark Warner, it is that surprising physical phenomena need not have complicated explanations. In my talk I will discuss a few examples of non-trivial physical phenomena that, at least to me, were a surprise. My examples focus on numerical studies of non-equilibrium phenomena in soft matter, but sometimes the insights seem relevant for equilibrium systems as well.

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MS125

Chain Whip Dynamics

Chains, consisting of jointed rigid segments, can exhibit fascinating and unexpected dynamical phenomena; one example is the chain fountain. Whips, formed from continuously deformable soft materials, also show interesting dynamical phenomena, such as supersonic tip velocity. In this talk, I will describe the processes responsible for the unusual response of these two mechanical systems and demonstrate astonishing dynamics when these are combined in a chain whip.

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MS125

Three Generations of Liquid Crystalline Elastomers

LCEs are a unique class of materials with over 30 years of history, with their remarkable properties utilizing two key effects: the spontaneous shape change due to the equilibrium relation between the state of local LC order and the macroscopic shape and the soft elasticity that arises due to the internal degeneracy of local order orientation during mechanical deformation. LCEs were anticipated in a little-known paper by De Gennes, but their real discovery is recognized to be due to Warner and Finkelmann in the late 1980s. Since then, there were two revolutions in the material science, when first the cheap di-acrylate mesogens and the robust click chemistry of thiols were introduced, making LCE materials readily available to almost anyone. Secondly, the introduction of dynamic bond exchange into the networks allowed the 'exchangeable LCE (xLCE) to be molded and programmed into any shape or orientation profile during their plastic-flow regime at high temperature. There was only one similar breakthrough in theoretical understanding of LCEs: the one based on the Trace formula or the equivalent quasi-convexification of the elastic energy. The second advance, to match the introduction of xLCEs and incorporate the elastic-plastic transition into the LCE elastic theory, is overdue and is sure to occur shortly. This talk will overview the key concepts behind the xLCE materials developed so far, and illustrate their emerging uses in applications.

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MS126

Divide-and-Conquer Methods for Functions of Matrices with Banded Or Hierarchical Low-Rank Structure

This talk is concerned with approximating matrix functions for banded matrices, hierarchically semiseparable matrices, and related structures. We propose new divide-and-conquer methods which exploit the fact that these matrices can be (recursively) decomposed as a sum $A = D + R$ of a block diagonal matrix D and a low-rank correction

R. While the update $f(A) - f(D)$ often has low numerical rank and can be approximated via (rational) Krylov subspace projections, the block diagonal part $f(D)$ is computed recursively for each diagonal block. We present a convergence analysis that relates the accuracy attained by the algorithm with best polynomial or rational approximations of the function. For the special case of a banded matrix, we show that the divide-and-conquer method reduces to a much simpler algorithm, which proceeds by computing matrix functions of small submatrices of A. The numerical results demonstrate that, most of the time, the proposed methods outperform state-of-art techniques with respect to time consumption and offer a comparable accuracy.

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MS126

On Estimating the Trace of a Matrix Function

The development and analysis of randomized techniques for estimating the trace of a large, symmetric matrix B is a topic with a long history that has recently seen increased attention and new exciting developments. This talk presents new results when B is a matrix function, that is, $B = f(A)$ for some function f and a symmetric matrix A. This includes log-determinant estimation, a task that features prominently in statistical learning, for instance in maximum likelihood estimation for Gaussian process regression. We present novel error bounds that are turned into an improved and adaptive variant of Hutch++, a recently developed combination of randomized low-rank approximation with stochastic trace estimation. For an important subclass of functions, we derive and analyze a new approach that can significantly faster.

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MS126

Computing Functions of Matrices via Composite Rational Functions

Most algorithms for computing a matrix function $f(A)$ are based on finding a rational (or polynomial) approximant $r(A) \approx f(A)$ to the scalar function on the spectrum of A. These functions are often in a composite form, that is, $f(z) \approx r(z) = r_k(\cdots r_2(r_1(z)))$ (where k is the number of compositions, which is often the iteration count, and proportional to the computational cost); this way r is a rational function whose degree grows exponentially in k. I will review algorithms that fall into this category and highlight the remarkable power of composite (rational) functions.

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MS126

From Esprit to Espira: Function Approximation by Exponential Sums

We consider exponential sums of the form

$$f(t) = \sum_{j=1}^{M} \gamma_j \, \mathrm{e}^{\phi_j t} = \sum_{j=1}^{M} \gamma_j z_j^t,$$

where $M \in \mathbb{N}$, $\gamma_j \in \mathbb{C} \setminus \{0\}$, and $z_j = \mathrm{e}^{\phi_j} \in \mathbb{C} \setminus \{0\}$ with $\phi_j \in \mathbb{C}$ are pairwise distinct. The recovery of such exponential sums from a finite set of possibly corrupted signal samples plays an important role in many signal processing applications, as signal approximation, sparse deconvolution in nondestructive testing, model reduction in system theory, etc.. We introduce a new method for Estimation of Signal Parameters based on Iterative Rational Approximation (ESPIRA) for sparse exponential sums. Our algorithm uses the AAA algorithm for rational approximation of the discrete Fourier transform of the given equidistant signal values. We show that ESPIRA can be interpreted as a matrix pencil method applied to Loewner matrices. These Loewner matrices are closely connected with the Hankel matrices which are usually employed for recovery of sparse exponential sums. ESPIRA achieves similar recovery results for exact data as ESPRIT and the matrix pencil method (MPM) but with less computational effort. Moreover, ESPIRA strongly outperforms ESPRIT and MPM for noisy data and for signal approximation by short exponential sums.

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MS127

A Principal-Agent Mean Field Game Approach to REC Market Design

A novel framework is presented that combines Mean Field Game (MFG) theory and Hybrid Optimal Control (HOC) theory to obtain a unique ϵ-Nash equilibrium for a non-cooperative game with switching and stopping times. We consider the case where there exists one major agent with a significant influence on the system together with a large number of minor agents constituting two subpopulations, each agent with individually asymptotically negligible effect on the whole system. Each agent has stochastic linear dynamics with quadratic costs, and the agents are coupled in their dynamics and costs by the average state of minor agents (i.e. the empirical mean field). It is shown that for a class of Hybrid LQG MFGs, the optimal switching and stopping times are state-invariant and only depend on the

dynamical parameters of each agent. Accordingly, a hybrid systems formulation of the game is presented via the indexing by discrete events: (i) the switching of the major agent between alternative dynamics or (ii) the termination of the agents' trajectories in one or both of the subpopulations of minor agents. Optimal switchings and stopping time strategies together with best response control actions for, respectively, the major agent and all minor agents are established with respect to their individual cost criteria by an application of Hybrid LQG MFG theory.

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MS127

Equilibrium Model of Limit Order Books A Mean-Field Game View

In this paper, we propose a continuous time equilibrium model of the (sell-side) limit order book (LOB) in which the liquidity dynamics follows a non-local, reflected mean-field stochastic differential equation (SDE) with state-dependent intensity. To motivate the model, we first study an N-seller static mean-field type Bertrand game among the liquidity providers. We shall then formulate the continuous time model as the limiting mean-field dynamics of the representative seller, and argue that the frontier of the LOB (e.g., the best ask price) is the value function of a mean-field stochastic control problem by the representative seller. Using a dynamic programming approach, we show that the value function is a viscosity solution of the corresponding Hamilton-Jacobi-Bellman equation, which can be used to determine the equilibrium density function of the LOB, in the spirit of [Ma et al., 2015].

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MS127

Superposition and Mimicking Theorems for Conditional McKean-Vlasov Equations with Application in Stochastic Control

We consider conditional McKean-Vlasov stochastic differential equations (SDEs), such as the ones arising in the large-system limit of mean field games and particle systems with mean field interactions when common noise is present. The conditional time-marginals of the solutions to these SDEs satisfy non-linear stochastic partial differential equations (SPDEs) of the second order, whereas the laws of the conditional time-marginals follow Fokker-Planck equations on the space of probability measures. We prove two superposition principles: The first establishes that any solution of the SPDE can be lifted to a solution of the conditional McKean-Vlasov SDE, and the second guarantees that any solution of the Fokker-Planck equation on the space of probability measures can be lifted to a solution of the SPDE. We use these results to obtain a mimicking theorem which shows that the conditional time-marginals of an Ito process can be emulated by those of a solution to a conditional McKean-Vlasov SDE with Markovian coefficients. This yields, in particular, a tool for converting open-loop controls into Markovian ones in the context of controlled McKean-Vlasov dynamics.

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MS127

A Portfolio Choice Problem under Risk Capacity Constraint

This work studies a retirement portfolio problem by reformulating into an optimal portfolio choice problem. The model is under the framework of Merton (1971) but with the constraint that the investment dollar amount in the risky asset is always bound from above by a fixed constant, which is named by risk capacity constraint. The existing literature (e.g. Zariphopoulou and Vila (1997)) mainly focus on the leverage constraint which does not include our case. We solve the problem by characterizing the value function as the unique viscosity solution of an HJB equation and shows that the constraint is binding at some free boundary, which is a positive constant W^* in our model. After characterizing the region, we solve the HJB equation as ODEs in both constrained and unconstrained domain. In addition, we get the numerical solution for this HJB equation. This is a joint work with Weidong Tian.

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MS128

Hybrid Iterative Refined Restarted Lanczos Methods

Large sparse eigenvalue and singular value problems are some of the most important and profoundly studied areas in numerical linear algebra. These problems have been historically studied and possess a wealth of applications with numerical features that make them attractive for developing new innovative routines. We have developed hybrid restarted Lanczos methods that combine restarting with Ritz vectors with restarting with iterative refined Ritz vectors to compute the extreme eigenpairs of large sparse symmetric matrices or singular triplets of large sparse general matrices. The computation of singular triplets exploits the well-known relationships between singular triplets of a matrix and eigenpairs of the symmetric matrices A^TA or $[0\ A; A^T\ 0]$. The methods are designed to use at little storage space as possible and only require the evaluation of matrix–vector products with A (and A^T when computing for singular triplets). The iterative refined Ritz vectors is a new strategy based on refined Ritz approximations that has proven via numerical examples to perform better than the standard computation process for refined Ritz approximations. Some theoretical results are provided, along

numerous computed examples illustrating the performance of the new methods.

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MS128

Recycling Invariant Subspaces for a Sequence of Eigenproblems

We present a warm-started Krylov-Schur algorithm for solving a sequence standard eigenvalue problems (SEP) of the form $\mathcal{A}^{(k)}y = \mu y$, $k = 1, 2, \ldots, N$. When computing invariant subspaces for such a sequence, we can recycle the approximate invariant subspace computed for one matrix to warm-start the eigensolver for another matrix in the sequence, rather than starting the eigensolver from scratch. This recycling technique reduces the total number of matrix-vector products required in the eigensolver. An additional complication emerges when solving the sequence of eigenvalue problems that arises in a numerical simulation of brake squeal [Grabner et al., Numerical methods for parametric model reduction in the simulation of disk brake squeal, Z. Agnew. Math. Mech, 96 (2016)]. Here, a sequence of generalized eigenvalue problems (GEP) of the form $A^{(k)}y = \mu B^{(k)}y$ are solved as SEPs with coefficient matrix $\mathcal{A}^{(k)} = (B^{(k)})^{-1}A^{(k)}$. The matvecs in the eigensolver now require a linear solve, so an iterative linear solver (e.g., GMRES) can be used to efficiently compute them. We can improve convergence of the iterative linear solver by using a Krylov subspace recycling method, such as GCRO-DR, thus further reducing the total number of matvecs in the eigensolver. A theoretical analysis of this method will be discussed in another presentation in this minisymposium; see E. de Sturler, "Analysis of a Warm Start Krylov-Schur Method".

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MS128

Communication-Efficient Distributed Eigenspace Estimation

Distributed computing is a standard way to scale up machine learning and data science algorithms to process large amounts of data. In such settings, avoiding communication between machines is paramount for achieving high performance. A common practice for avoiding communication is to compute local solutions or parameter estimates on each machine and then combine the results. However, simple averaging schemes do not work well when the local solutions are not unique, such as in spectral methods where solutions are only unique up to rotations and reflections. In this talk, I will present a communication-efficient distributed algorithm for computing the leading invariant subspace of a data matrix. The algorithm uses a novel alignment scheme that minimizes the Procrustean distance between local solutions and a reference solution and only requires a single round of communication. For the importance case of principal component analysis (PCA), it achieves an error rate similar to that of a centralized estimator at a fraction of the required communication. This work is joint with Austin R. Benson and Anil Damle from Cornell CS.

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MS129

Discontinuous Galerkin Schemes for Diffuse Interface Models

Discontinuous Galerkin Finite Element Methods for the solution of Cahn-Hilliard-type systems will be presented. Analysis of the schemes will be performed. Numerical tests verifying the theoretical results will be presented.

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MS129

A High-Order Immersed C0 Interior Penalty Method for Biharmonic Interface Problems

In this talk, an immersed C0 interior penalty method is proposed to solve biharmonic interface problems on unfitted mesh. The immersed P2 and P3 finite element spaces are constructed to match biharmonic interface conditions in a least-squares sense. Basic properties of these new spaces such as unisolvence and partition of unity are analyzed. The new proposed spaces are also used in a symmetric C0 interior penalty scheme to solve the biharmonic interface problems. The well-posedness of discrete solution is also proved. Extensive numerical experiments show optimal convergence of proposed method in L2, H1 and H2 norms. This is a joint work with Dr. Xu Zhang.

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MS129

Multiscale Finite Element Methods for an Elliptic Optimal Control Problem with Rough Coefficients

The solution of multiscale elliptic problems with non-separable scales and high contrast in the coefficients by standard Finite Element Methods (FEM) is typically pro-

hibitively expensive since it requires the resolution of all characteristic lengths to produce an accurate solution. Numerical homogenization methods such as Localized Orthogonal Decomposition (LOD) methods provide access to feasible and reliable simulations of such multiscale problems. These methods are based on the idea of a generalized finite element space where the generalized basis functions are obtained by modifying standard coarse FEM basis functions to incorporate relevant microscopic information in a computationally feasible procedure. Using this enhanced basis one can solve a much smaller problem to produce an approximate solution whose accuracy is comparable to the solution obtained by the expensive standard FEM. Based on the LOD methodology, we investigate multiscale finite element methods for an elliptic distributed optimal control problem with rough coefficients.

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MS129

Recent Advances in Structure-Preserving Hybridization

Hybrid finite element methods are a classical topic in finite element analysis. There are several numerical and implementational advantages to *hybridization*, i.e., writing an existing method in hybrid form; this has been done for conforming, nonconforming, mixed, and (more recently) discontinuous Galerkin methods. In this talk, I will discuss some recent work on hybridization of structure-preserving methods, with a particular focus on the vector Laplacian and related problems arising in finite element exterior calculus (FEEC).

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MS130

Asymptotic Convergence from Inverse Helmholz to Inverse Liouville

Light has wave-particle duality. The Helmholz equation and the radiative transfer equation (RTE) are both used to describe light propagation, and they are asymptotically equivalent in the high frequency regime. We investigate the corresponding inverse problems in this talk. In particular, we evaluate the asymptotic convergence of inverse scattering problem of the Helmholtz equation, to the inverse scattering problem of the Liouville equation (a simplified version of RTE). The two inverse problems are connected through the Wigner transform that translates the wave-type description to the phase space, and the Husimi transform that extracts data that is concentrated both in location and direction. The finding suggests a stable reconstruction of the unknown medium using the information from data generated by a single light frequency. This is in contrast with the unstable reconstruction in the inverse Helmholtz where plain waves are used.

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MS130

Reduced Basis Methods for the Radiative Transfer Equation

Due to the high dimensional nature of radiative transfer equation, reduced order models (ROMs) utilizing the underlying low rank structure to decrease the number of degree of freedoms are highly desired. In this talk, we use the reduced basis method to construct such a ROM with a greedy offline algorithm. Techniques to utilize the low rank structure with respect to the angular direction and time will be discussed.

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MS130

Adjoint DSMC Method for Boltzmann-Constrained Optimization Problems

Applications for kinetic equations such as optimal design and inverse problems often involve finding unknown parameters through gradient-based optimization algorithms. Based on the adjoint-state method, we derive two different frameworks for approximating the gradient of an objective functional constrained by the nonlinear Boltzmann equation. While the forward problem can be solved by the Direct Simulation Monte Carlo (DSMC) method, it is difficult to efficiently solve the high-dimensional continuous adjoint equation obtained by the "optimize-then-discretize" approach. This challenge motivates us to propose an adjoint DSMC method following the "discretize-then-optimize" approach for Boltzmann-constrained optimization. We also analyze the properties of the two frameworks and their connections. Several numerical examples are presented to demonstrate their accuracy and efficiency.

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MS130

Bi-Fidelity Methods for Uncertainty Quantification in Kinetic Equations

Designing efficient methods for uncertainty quantification in kinetic equations represents a challenge due to the high dimensionality and computational costs of the models. On the other hand, there are many simplified models capable of providing approximate solutions at a computationally reduced cost in the field of kinetic equations. It is, therefore, natural to take advantage of such models in a multi-fidelity setting where the original kinetic equation represents the high-fidelity model, and the simplified models define the low-fidelity models. In this talk, we will discuss some recent results about bi-fidelity methods for kinetic equations that are able to accelerate the uncertainty quantification computations by combining high-fidelity and low-fidelity model evaluations.

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MS131

Elastic Flow Instabilities in Disordered Porous Media

Many energy, environmental, industrial, and microfluidic processes rely on the viscous flow of polymer solutions through porous media. In many cases, the macroscopic flow resistance abruptly increases above a threshold flow rate in a porous medium—but not in bulk solution. The reason why has been a puzzle for over half a century. By directly visualizing the flow in a transparent three-dimensional (3D) porous medium, we have experimentally demonstrated that this anomalous increase is due to the onset of an elastic instability in which the flow exhibits strong spatio-temporal fluctuations reminiscent of inertial turbulence, despite the vanishingly small Reynolds number. We find that the transition to unstable flow in each pore is continuous, arising due to the increased persistence of discrete bursts of instability above an onset flow rate; however, this onset value varies from pore to pore. Thus, unstable flow is spatially heterogeneous across the different pores of the medium, with unstable and laminar regions coexisting. Guided by these findings, and using a power density balance for viscous-dominated flows, we quantitatively establish that the energy dissipated by unstable pore-scale fluctuations generates the anomalous increase in flow resistance through the entire medium. Thus, by linking the onset of unstable flow at the pore scale to transport at the macroscale, our work yields generally-applicable guidelines for predicting and controlling polymer solution flows.

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MS131

Critical Limits and the Stability of Yield Stress Fluid Flows

Yield stress fluids are idealized simple models (e.g. Bingham, Casson, Herschel-Bulkley), describing fluids for which there is no deformation wherever the deviatoric stress lies below the yield stress. This simple rheological change results in hydrodynamic stability features that are quite different from those of purely viscous fluids. We can classify the flows into those that have a non-zero base flow $\mathbf{U}$, and those for which $\mathbf{U} = 0$. Unlike purely viscous fluids, flows with $\mathbf{U} = 0$, have meaningful applications beyond hydrostatics. It is these flows that we explore here, focusing on general features of stability, control and determining the critical limit of static stability.

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MS131

Particle Suspensions in Elastic Fluids: Toward a Swimming Rheometer

Rigid or flexible particles suspended in viscoelastic fluids are ubiquitous in the food industry (e.g. pastes), industrial molding applications (all composites and 3-D printed parts), the energy industry (e.g. fracking fluids), and biological fluids (i.e. swimming of bacteria in mucous). The mathematical description of these suspensions is remarkably still in its infancy, but the real breakthrough in this area has been the development of 3D computational simulations of such viscoelastic suspensions including particle motion and particle level resolution of the elastic flow fields. These simulations will allow the principles which govern the simplest flows of such suspensions, which are now generally not understood, to become elucidated in the next decade. I will describe two problems that have been recently analyzed using these computational methods – inluding the shear thickening of such suspensions and the design of a mechanical swimmer that is sensitive to elastic fluid rheology.

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MS131

On the Elastic Turbulence in Viscoelastic Shear Flows

In Newtonian parallel shear flows, turbulence starts at large Re via a non-normal mode bifurcation due to finite-size perturbations. At sufficiently large amplitudes, the fastest algebraically growing non-normal modes, mostly stream-wise rolls and streaks, saturate. These exact coherent structures (ECSs) are self-organized into cycling self-sustained process (SSP) of emerging and decomposing ECSs during a period. This by-pass route to turbulence is identified numerically and confirmed experimentally. Here I present a recent discovery of a pure elastic instability into a chaotic flow in viscoelastic shear flows at Re ¡ 1 and Wi ¿¿ 1, Wi is the Weissenberg number. The elastically driven chaotic flow reveals ECSs similar to those in the Newtonian case. Moreover, ECSs are accompanied by elastic waves emerging above the onset and playing a key role in supporting ECSs. As a result, ECSs are self-organized into a cycling SSP synchronized by the elastic waves. It is also verified that with increasing Wi, the ECSs and their dynamics depend on the intensity of the elastic waves and are found in three flow regimes, namely transition above the onset, elastic turbulence, and drag reduction. Thus, the observed similarity in the flow dynamics in Newtonian and viscoelastic parallel shear flows suggests the universality in stochastically steady state of ECSs, self-organized into cycling SSP in random states that occurred via non-normal mode instability, otherwise linearly stable flows.

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MS132

Simulating Complex Biological Systems Using the Stochss Suite of Software

A striking outcome of the past decade of Systems Biology research is the insight that stochasticity plays an important role in many biological processes. As a result, discrete stochastic simulation is now an important and widely-used tool for modeling of biological systems. However, these tools are often challenging to use, not user friendly, and requiring extensive specialized training before they can be used effectively. To address this and accelerate the pace of scientific discovery, we have built a powerful platform for

the development, simulation and analysis of biochemical models: StochSS (Stochastic Simulation as-a-Service). In addition, we have developed a complete suite of tools for simulation and analysis. StochSS supports models ranging from ODEs to well-mixed discrete stochastic models to spatial reaction-diffusion models. It also features an easy-to-use WebUI, scalable tools for parameter inference and model exploration that enables researchers to utilize semi-supervised human-in-the loop machine learning. Finally, host *StochSS Live* as a computational service at: https://live.stochss.org/, see https://stochss.org for more info.

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MS132

Stochastic Modeling of Metabolic Enzyme Complexes

Enzymes in glucose metabolism have been shown to spatially organize into multienzyme complexes. These multienzyme complexes regulate metabolic flux in living human cells. We hypothesize that metabolic enzyme complexes are formed by liquid-liquid phase separation, which is determined by macromolecular interaction and crowding as other biomolecular condensates do. In this talk, I will introduce a stochastic model for metabolic enzyme complexes and their spatial organization using the Langevin dynamics. The model is simulated by the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), revealing the effects of concentration, size, and shape of enzymes on the formation of metabolic enzyme complexes.

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MS132

Performance-Efficiency Trade-Off of Stochastic Directional Search Process

Intercellular signaling has important role for organism development, but not all communications form by the same mechanism. Here, we analyze the energy efficiency of the intercellular signaling for two canonical mechanisms: the diffusion of signaling molecules via extracellular space and the direct transport mediated by signaling cellular protrusions. We show that the efficient contact formation for direct transport can be established by an optimal projection initiation rate and identifying the location information of the target cell. This predicts that the direct transport mechanism can be observed as responding signals with target location information. The optimal projection rate can differ if involving signaling molecule transport along the protrusion. We find that this depends on the ratio of the energy cost for contact formation and molecule synthesis. Also, we compare the energy efficiency of the two models with various model parameters. We find that the direct transport mechanism is favored over the diffusion mechanism when transporting a large amount of signaling molecules because of discounting the contact formation cost per molecule. This shows the existence of the critical number of molecules that the efficiency of the two mechanisms are the same. In particular, the critical number is small when the distance between cells is far, which justifies why protrusion-based mechanisms are observed in long-range cellular communications.

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MS132

Identifiability of Stochastically Modeled Reaction Networks

When an underlying reaction network is given for a biochemical system, the system dynamics can be modeled with various mathematical frameworks such as continuous-time Markov processes. In this presentation, the identifiability of the underlying network structure with a given stochastic system dynamics will be discussed. We will see that some data types related to the associated stochastic dynamics can uniquely identify the underlying network structure as well as the system parameters. We also talk about the accuracy of the presented network inference when given dynamical data is obtained via stochastic simulations.

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MP1

Minisymposterium: Local Compatibility Boundary Conditions for High-Order Accurate Finite-Difference Approximations of PDEs

We describe a high-order numerical boundary conditions method for finite-difference (FD) approximations of PDEs. The novel Local Compatibility Boundary Conditions method uses boundary conditions, derivatives of the governing equations, interior and boundary grid values to construct a local interpolating polynomial centered at each boundary point. Such polynomial gives a discrete formula for the solution at ghost points near the boundary. Ghost values are then used in the implementation of high-order accurate centered FD schemes.

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MP1

Minisymposterium: Periodicity of Mixed-Integer Programming Gap Functions

A critical measure of the quality of a mixed-integer programming (MIP) model with fixed data is the difference, or gap, between the optimal objective value of the linear pro-

gramming relaxation and that of the corresponding MIP. In many contexts, only an approximation of the right-hand sides may be available, or there may be multiple right-hand sides of interest. However, there is currently no consensus on appropriate measures for MIP model quality over a range of right-hand sides. This poster provides an overview of absolute and relative MIP gap functions over finite discrete sets, and conditions under which absolute MIP gap functions are periodic.

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MP1

Minisymposterium: Modeling Public Transportation Networks with Queues

Efficacy of new roads is a significant issue due to rapid city expansion. This has led to escalating traffic around city centers and necessitates the adoption of more efficient public transportation networks to help prevent congestion and negative environmental factors. We propose an adaptation of a standard queuing model to analyze bus behavior and passenger interaction. This process allows us to suggest infrastructure changes that benefit a bus company and avoid negative impacts on passengers.

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MP1

Mathematical Analysis of Pulmonary Hypertension and Ventricular Interaction

This study utilizes 0D cardiovascular system models to study cardiovascular function in patients with pulmonary hypertension (PH). We focus on understanding under what conditions ventricular interaction (VI) play a role for hemodynamic predictions. Ventricular interaction can be modeled by introducing a nonlinear equation representing the elastic septal wall separating the left and right ventricles. In control patients, the ventricular wall bows to the right as the pressure in the left ventricle is significantly higher than the right, but for PH patients with high right ventricular pressure the wall is pushed towards the left ventricle eventually reducing left heart function. The systems level model forms a nonlinear differential algebraic system, which is challenging to solve. To study this equation in detail we conduct three simulations comparing pressure volume predictions for control and PH patients assuming 1) no interaction, 2) linearized VI, and 3) nonlinear VI. Since VI is a phenomenon that is not easily detected in routine right heart catheterizations, we are particularly interested in whether each model can capture physiologically accurate ventricular and septal dynamics; i.e. negative septal volume is considered an indication that the septum is bowed opposite to its natural position. Using modeling and sensitivity analysis, the goal is to test under what conditions VI are important and if a simple linear model is adequate.

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MP1

Champ: A High-Order Accurate Partitioned Scheme for Conjugate Heat Transfer

A fourth-order accurate partitioned scheme for solving conjugate heat transfer problems with advection is presented. The solutions are advanced in each material domain independently with an implicit method, and domains are coupled at the interface using a new high-order accurate CHAMP (Conjugate Heat Transfer Advanced Multi-domain Partitioned) interface conditions. These conditions are based on interface jump conditions involving continuity of temperature and heat flux, together with additional compatibility conditions derived from the governing equations. The CHAMP conditions are implemented numerically using an optimized Schwarz approach, with a Taylor expansion leading to an effective domain overlap, which significantly improves the convergence. The overall partitioned scheme is stable and accurate with just one implicit solve in each domain for a wide range of material parameters. The approach is analyzed to determine the optimal coupling coefficients and the scheme is verified using several numerical examples.

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MP1

Minisymposterium: Kempe Equivalent List Colorings

An α, β-Kempe swap in a properly colored graph interchanges the colors on some component of the subgraph induced by colors α and β. Two k-colorings of a graph are k-Kempe equivalent if we can form one from the other by a sequence of Kempe swaps (never using more than k colors). Las Vergnas and Meyniel showed that if a graph is $(k-1)$-degenerate, then each pair of its k-colorings are k-Kempe equivalent. Mohar conjectured the same conclusion for connected k-regular graphs. This was proved for $k = 3$ by Feghali, Johnson, and Paulusma (with a single exception $K_2 \square K_3$, also called the 3-prism) and for $k \geq 4$ by Bonamy, Bousquet, Feghali, and Johnson. In this paper we prove an analogous result for list-coloring. For a list-assignment L and an L-coloring φ, a Kempe swap is called L-valid for φ if performing the Kempe swap yields another L-coloring. Two L-colorings are called L-equivalent if we can form one from the other by a sequence of L-valid Kempe swaps. Let G be a connected k-regular graph with $k \geq 3$. We prove that if L is a k-assignment, then all L-colorings are L-equivalent (again with a single exception $K_2 \square K_3$). When $k \geq 4$, the proof is completely self-contained, so implies an alternate proof of the result of Bonamy et al.

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MP1

Minisymposterium: Dirac's Theorem for Hamiltonian Berge Cycles in Uniform Hypergraphs

Dirac's Theorem gives an exact bound on the minimum degree of an n-vertex graph guaranteeing the existence of a hamiltonian cycle. We prove exact bounds of similar type for both hamiltonian Berge cycles and Berge cycles of length at least k in r-uniform, n-vertex hypergraphs for all $3 \leq r < n$.

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MP1

Acyclic Graphs with at Least $2l + 1$ Vertices are l-recognizable

The $(n - l)$-deck of an n-vertex graph is the multiset of subgraphs obtained from it by deleting l vertices. A family of n-vertex graphs is l-recognizable if every graph having the same $(n - l)$-deck as a graph in the family is also in the family. We prove that the family of n-vertex graphs having no cycles is l-recognizable when $n \geq 2l + 1$ (except for $(n; l) = (5; 2)$). It is known that this fails when $n = 2l$.

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MP1

Minisymposterium: Inferring Dynamics of Biological Systems

Biological networks are complex and constructing dynamics for large systems can prove difficult. We will explore utilizing data-driven techniques to uncover the dynamics of a biological network from data provided. Several sparse identification algorithms will be presented and discussed. We will apply these methods to data obtained for the Mitogen-Activated Protein Kinase (MAPK) pathway. The MAPK pathway is of particular interest in studying cancer mutations.

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MP1

Modeling and Tracking Biofilm-Mediated Bacteria within a Water Supply Network

Surprisingly, water-borne illnesses are still a common problem in developed countries. Most water-borne illnesses are caused by foreign bacteria that have entered a water distribution network. Despite this problem, little research has been done to develop methods to track the source of foreign bacteria that cause these illnesses. Currently, mainly brute force methods are used within the field to track and clean out foreign bacteria within a water distribution network. Our objective is to create an efficient method to find the source of foreign bacteria after it is reported downstream within a community. This poster will present the network model used to simulate the transport and growth of bacteria in a water distribution network. Then, we will present how data assimilation methods can be used to predict the source of foreign bacteria within the network.

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MP1

Dynamical Systems Modeling of Inflammation for a Continuous Administration of Endotoxin

Sepsis, a severe inflammatory illness with a high mortality rate, is characterized by sustained, abnormal inflammation. Several studies have investigated short-term inflammation using data collected during a bolus administration of lipopolysaccharide (LPS). However, inflammation in sepsis is better represented by a continuous infusion of LPS. We propose a mathematical model calibrated to experimental data that investigates inflammatory dynamics during a prolonged administration of LPS. A sensitivity analysis and parameter estimation are performed on the model.

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MP2

An Immersed Peridynamics Model of Fluid-Structure Interaction Accounting for Material Damage and Failure

This work develops an immersed peridynamics method that enables fluid-structure interaction simulations of the deformation, damage, and failure of hyperelastic materials. The immersed peridynamics method uses Eulerian and Lagrangian descriptions for the fluid-structure system and immersed structures, respectively. The coupling between Eulerian and Lagrangian variables is achieved by integral transforms with Dirac delta function kernels as in standard immersed boundary-type methods. The major difference between our approach and conventional immersed-type methods is that we use peridynamics, instead of using classical continuum mechanics, in computing the internal body forces of the immersed structure. We focus on non-ordinary state-based peridynamic material descriptions that allow us to use well characterized nonlinear constitutive models of soft materials. The convergence and accuracy of our approach are compared to classical finite element methods using standard benchmark problems of nonlinear incompressible elasticity that are widely used in the computational mechanics literature. We demonstrate that the proposed method yields comparable accuracy with similar numbers of structural degrees of freedom for a variety of choices of horizon size. We also demonstrate that the method can generate grid-converged simulations involving damage growth, crack formation and propagation, and rup-

ture under large deformations by solely fluid driven forces through several numerical tests.

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MP2

An Immersed Lagrangian-Eulerian Method for Rigid-Body Fluid-Structure Interaction Involving Geometries with Sharp Features

Our recently developed immersed interface algorithm for discrete surfaces is revisited. Previously, we used an L2 projection of the space spanned by Lagrangian basis functions to construct continuous jump conditions along the C0 representation of smooth interfaces with applications of such surfaces in nature and biology. In engineering applications, however, the design and manufacturing of devices with one or more sharp features, immersed in the surrounding fluid, are sometimes desired. Examples range from mechanical heart valves to turbine blades to airfoils and so on. Resolving the fluid flow around these structures described by a piecewise parametric representation may require introducing dense local elements with sizes that are much smaller than the average element size in the bulk mesh. Resolving fluid around these sliver elements proves to be challenging, particularly in a fluid-structure interaction (FSI) framework using immersed methods for which the Eulerian grid size needs to be comparable to the Lagrangian element size. We present an alternative approach using discontinuous basis functions with element-local support for the projection that allows us to effectively capture the fluid flow around these sharp features, without any regularization or additional mesh refinement. These basis functions are similar to the Lagrange family but without inter-element continuity. We demonstrate how our choice significantly improves our FSI previous results for problems involving objects with sharp features.

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MP2

A Nodal Immersed Finite Element-Finite Difference Method

The immersed finite element-finite difference (IFED) method is a computational approach to modeling interactions between a fluid and an immersed structure. The IFED method uses a finite element (FE) method to approximate the stresses and forces on a structural mesh and a finite difference (FD) method to approximate the momentum of the entire fluid-structure system on a Cartesian grid. The fundamental approach used by this method follows the immersed boundary framework for modeling fluid-structure interaction (FSI), in which a force spreading operator prolongs structural forces to a Cartesian grid, and a velocity interpolation operator restricts a velocity field defined on that grid back onto the structural mesh. Evaluating either coupling operator requires solving a matrix equation at every time step. Constructing the coupling operators also requires determining the locations on the structure mesh where the forces and velocities are sampled. We show that sampling the forces and velocities at the nodes of the structural mesh is equivalent to using lumped mass matrices in the IFED coupling operators. If these approaches are combined, the IFED method permits the use of lumped mass matrices derived from nodal quadrature rules for standard interpolatory elements. Our theoretical results are confirmed by numerical benchmarks, including standard solid mechanics tests and examination of a dynamic model of a bioprosthetic heart valve.

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PP1

Modelling the Delays in Reporting Disease Incidence with an Application to Forecasting Covid-19 Cases

Effective monitoring of infectious disease incidence remains a major challenge to public health. Difficulties in estimating the trends in disease incidence arise mainly from the time delay between case diagnosis and the reporting of cases to public health databases. However, predictive models usually assume that public data sets faithfully reflect the state of disease transmission. In this paper, we study the effect of delayed case reporting by comparing data reported by the Johns Hopkins Coronavirus Resource Center (CRC) with that of the raw clinical data collected from the San Antonio Metro Health District (SAMHD), San Antonio, Texas. An insight on the subtle effect that such reporting errors potentially have on predictive modeling is presented. We use an exponential distribution model for the regression analysis of the reporting delay. The proposed model for correcting reporting delays was applied to our recently developed SEYAR (Susceptible, Exposed, Symptomatic, Asymptomatic, Recovered) dynamical model for COVID-19 transmission dynamics. Employing data from SAMHD, we demonstrate that the forecasting ability of the SEYAR model is substantially improved when the rectified reporting obtained from our proposed model is utilized. The methods and findings demonstrated in this work have ample applicability in the forecasting of infectious disease outbreaks. Our findings suggest that failure to consider reporting delays in surveillance data can significantly alter forecast

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PP1

Investigation of Intervention Efforts to Combat High Drop-Out Rates in Milwaukee Public Schools

Several studies and on-going research have reported COVID-19 having negative mental and physical health outcomes for students. It is well known that ACES (adverse childhood experiences) impact how quickly a student can learn, their ability to preserve through challenges, and control emotional reactions and stress levels. Additionally, these experiences could drive higher drop-out rates, which is the focus of this talk/poster. The investigation builds on a study by Amdouni et.al. that likened the influence of failing students to a contagious disease and used a modified SEIR (susceptible-exposed-infected-removed) model that also incorporated the role of parental involvement in the students education. The current model adds explicit intervention at various points in the process. We investigate the resulting dynamics and relate it to data collected

by the Wisconsin Department of Public Instruction.

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PP1

Dynamic Bootstrap-Based Extensions of Sparse Partial Least Squares Regression

Since the early 2000s, methods based on partial least squares regression (PLSR) have been developed for performing variable selection and have gained much attention in analyzing high-dimensional single or multi-omics datasets. Most of these techniques rely on tuning parameters often determined by cross-validation (CV) based methods, which raises essential stability issues. We created a new dynamic bootstrap-based method for significant predictor selection to overcome this. It is suitable for both PLS regular and generalized (GPLSR) linear regression models. It relies on establishing bootstrap confidence intervals, which allows testing of the significance of predictors at preset type I risk a, and avoids CV and its known low stability. Our new dynamic bootstrap-based method has the property of best separating random noise in y from the relevant information, leading to better accuracy and predictive abilities, especially for non-negligible noise levels. We have also developed adapted versions of sparse PLS and sparse GPLS regression, using a recently introduced non-parametric bootstrap-based technique to determine the numbers of components. We compare their variable selection reliability and stability concerning tuning parameters determination and their predictive ability, using simulated data for PLS and real microarray gene expression data for PLS-logistic classification. We implemented the related code in the bootPLS R package recently published on the CRAN.

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PP1

A Convergent Quadrature Based Method for the Monge-Ampre Equation

The Monge-Ampre equation is a fully nonlinear Elliptic Partial Differential Equation that arises in applications such as Optimal Transport, Machine Learning, Image Processing, and Seismology. Due to the nonlinear nature of this problem, standard numerical techniques are not suitable as they are not guaranteed to converge. Provably convergent methods have been developed in recent years using wide stencil schemes. However, these algorithms can have low accuracy and are not fast enough for current large scale applications. The goal of this project is to introduce a new integral representation of the Monge-Ampre operator, which can be efficiently discretized with a suitable choice of quadrature. The benefits of this new discretization are seen within two separate solvers. The first is a fixed stencil size scheme in which we discretizatize our domain with triangular or hexagonal tilings to exploit the spectral trapezoid rule. Although this method will not completely converge, we observe higher orders of accuracy and very efficient solve times. The second method is a wide stencil scheme on a uniform cartesian mesh using a higher order quadrature rule. The result is a provably convergent scheme which allows for more narrow stencils and better accuracy than existing methods.

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PP1

Computational Advances for Cancer Detection Through Electrical Impedance Tomography and Optimal Control Theory

Electrical Impedance Tomography (EIT) is a non-invasive medical imaging technique recently gaining popularity in various medical applications for detecting changes in tissues suspicious for any type of cancer. EIT-based screening is an attractive alternative to current detection methods, such as X-rays or MRIs, because it is non-invasive and cost-effective, providing benefits for both patients and medical practitioners. In this talk, we present an elegant and computationally efficient solution to the inverse problem for cancer detection through EIT. A mathematical framework is formulated as a highly nonlinear optimization problem constrained by sets of PDEs. This problem is solved computationally by our in-house open-structure multifaceted software package EIT-Opt utilizing both adjoint-gradient and non-derivative approaches. Increased computational performance and reliability of the new engineering design procedure applicable to real models are achieved by adding novel numerical techniques for proper regularization, parameter space upscaling, and re-parameterization. Computational results for 2D synthetic models will be presented to demonstrate the efficient performance of the new computational framework and its high potential for minimizing possibilities for false-positive screening and improving the overall quality of the EIT-based procedures. Future applications to clinical data and enhancements of the framework functionality to full 3D capability will be also discussed.

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PP1

Parking with Varying Rate

In the classical parking problem, unit intervals ("car lengths") are placed uniformly at random without overlapping. The process terminates at saturation, i.e. until

no more unit intervals can be stowed. We present a generalization of this problem in which the unit intervals are placed with an exponential distribution. We show that the mathematical expectation of the number of intervals present at saturation satisfies a certain integral equation. We investigate the asymptotic behavior of this function. We also show that the corresponding limits converge to the uniform case as the parameter vanishes, yielding the well-known Renyi constant. Finally, we reveal the asymptotic behavior of the variance of the intervals at saturation (Journal of Statistical Physics 182(2), 2021).

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PP1

Constant-Coefficient Fractional Differential Equations

We consider l^{th}-order linear fractional differential equations with constant coefficients

$$D^{\alpha}u(x) + \lambda D^{\beta}u(x) + \sum_{i=0}^{m-2} p_i D^{\alpha_i}u(x) = 0,$$

where $\alpha > \beta > \alpha_{m-2} > \ldots > \alpha_1 > \alpha_0 = 0$ and $l = \lceil \alpha \rceil$. The current theory requires $\alpha - \beta \geq l - 1$ for the existence of l linearly independent solutions and, thus, at most one derivative may have order greater than one but all other derivatives must be between zero and one. We remove this essential restriction and elaborate the multi-sum fractional series approach to construct l linearly independent solutions for constant coefficients and Riemann-Liouville and Caputo fractional derivatives of arbitrary orders.

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PP1

Modeling and Numerical Analysis of Cholesteric Shells

Liquid Crystals (LCs) are a key component of our life in the modern world, appearing in various technologies, such as LC displays and temperature sensors. A classic, yet sophisticated, model is the Landau-de Gennes (LdG) model, which utilizes a 3×3 tensor as the order parameter (the so-called "Q-tensor"). This model has many advantages over others, such as the Oseen-Frank model, which we briefly review. Next, we show how the standard LdG model can be extended to model cholesteric shells, which have applications as droplet lasers, novel bio-sensors, and anti-counterfeiting markers. In particular, we describe the various energetic terms in the Landau-de Gennes free energy, and discuss its variational formulation. Furthermore, we give a numerical discretization of LdG using a finite element method. Since the LdG energy is non-convex, we use an L^2 gradient flow to compute equilibrium points (minimizers). We also discuss various time step and mesh size conditions to ensure stability, some of which are not well-known in the LC literature, particularly when simulating cholesteric LCs that exhibit "twist". Finally, we present various numerical simulations in 3-D, on both slab geometries and spherical shells, and connect these results with experiments.

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PP1

Predicting the Non-Trivial Zeros of the Riemann Zeta Function

SAS (SAS/STAT, 2018) programs solve for the non-trivial zeros of the Riemann zeta function. The Riemann hypothesis is a conjecture that all non-trivial zeros of the zeta function have real part one-half. If the hypothesis is correct all of the non-trivial zeros lie on the critical line + ti. The first few nontrivial zeros occur at Re() and Imaginary coefficients t = 14.134725, 21.022040, 25.010858, 30.424876, 32.935062 and 37.586178. We provide a program that uses a search grid to find the imaginary coefficients as we zoom into the non-trivial zeros of the Riemanns zeta function. We examine the residuals and predicted values of models fit to fine-tune a process so that predicted values of the zeros of the Riemann Zeta function become accessible for large n and become more precise/accurate within the process. Sectional quadratic models are developed which use closer to end-points of the search grid. We find these models perform well in the prediction.

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PP1

Inference of Multiple Physical Quantities with Uncertainty Quantification on a Thermal-Fluid System

In this work, we discuss the development of a method to infer the local value of heat flux boundary conditions in a simulated forced convection problem based on a limited number of point-wise temperature measurements. We show that it is possible to efficiently reconstruct a steady-state heat flux boundary condition solution using a physics-based mapping with an appropriate polynomial basis. In addition, the method can also be used to estimate the inlet mass flow rate, if unknown. The uncertainty of the heat flux reconstruction is also analytically estimated. We considered the uncertainty arising from the modeling of turbulence (i.e., through wall function and eddy diffusivity) and noise in the temperature measurements (as sources of error). We derive the sensitivity coefficient of each error source and apply the uncertainty propagation equation. In the future, the established inference method will be applied to an actual thermal-fluid experiment to understand its impact and applicability.

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PP1

Boundary Layer Flow Around an Immersed Plate In a Yield Stress Fluid

Completing a well to isolate fluids involves pumping cement slurry down through the casing, under pressure into the annulus, which is the space between the steel pipe casing

and the formation. Cement slurries are yield stress fluids that can exhibit non-linear behavior, such as thixotropy; they can be modeled through a dependence of the viscous stress on a structural parameter that describes the degree of the aggregation. In most applications, the rheological behavior of cement slurries is often characterized either as Bingham or Herschel-Bulkley visco-plastic fluids. Here we study the boundary layer flow and the solid-like behavior of the fluid, away from the boundaries, expected to take place along the solid boundaries of the wellbore and the casing. To assess the models, we simulate a plate slowly immersed into a Carbopol gel, with properties similar to cement, characterized as a Herschel-Bulkley visco-plastic fluid. This problem has been studied experimentally, and detailed velocity profiles measurements are available in the literature. The numerical solutions of the mass and the linear momentum equations, along with the constitutive relations, are calculated by relying on the regularization methods implemented as customized by the non-Newtonian viscosity libraries in OpenFOAM (a CFD code). The results show that the boundary layer thickness is satisfactorily predicted against the measurements, and that both fluid and solid regions are favorably captured by the models.

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PP1

Improving Variable Selection for Finding Robust Model-Based Classifications

Variable selection has become one of the critical challenges in statistics. Many methods have already been proposed in the literature. In a context where the number of variables far exceeds the number of observations or in a highly correlated setting, their performances are generally limited in recall and precision. Taking this correlation structure into account is the fundamental strength of our approach, which allows for the selection of reliable variables in parsimonious or non-parsimonious classification problems. Thanks to correlated resampling techniques, it is possible to improve the performance of existing classification models, typically those based on regression approaches. For instance, we have succeeded in increasing the performance of glmnet logistic models, of variable selection models using variational approximation methods for a binary response, of sparse partial least-squares discriminant analysis models and sparse generalized partial least squares models. The performance increase was demonstrated on both simulated and real datasets using a comprehensive simulation benchmark.

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PP1

Complete Characterization of Two-Site Adsorption / Desorption Processes: Finite System-Size Effect on Equilibrium and Time-Transient Surface Coverage

Lattice modeling is a useful tool in computational chemistry to simulate the kinetics of surface reactions. In realistic surface chemistry simulations, periodic boundary conditions are usually employed to mimic an infinite system. Nevertheless, there may exist a significant finite system-size effect, where the equilibrium position and time-transient behavior of surface coverage obtained from simulations are different from those of the infinite system. This presentation reports significant finite system-size effects observed in two-site adsorption/desorption processes, particularly when the adsorption and desorption rates of the chemical system are very different. We completely characterize them using analytical, computational, and theoretical approaches. We first demonstrate the effects using kinetic Monte Carlo (KMC) simulations. We then analytically investigate the equilibrium surface coverage obtained from each system size using the chemical master equation (CME) approach, demonstrating that the finite system size effect is greater when we choose an even number of sites compared with an odd number of sites. We also apply the mean-field approximation (MFA) to predict the equilibrium position of surface coverage and confirm that this theoretical approximation gives the exact value of the infinite system size limit. However, the MFA as well as the pair approximation (PA) fail to make accurate predictions for the time-transient behavior.

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PP1

A Computational Package for Measuring Topological Entanglement in Polymers, Proteins and Periodic Systems (TEPP)

Many materials, like polymer melts, solutions, biopolymers and textiles, are composed of entangled filaments. The entanglement in these systems significantly affects their mechanical properties. We introduce the Topological Entanglement in Polymers, Proteins and Periodic systems (TEPPP) software, that enables to compute the topological and geometrical com- plexity in such systems. In particular, this software enables the computation of the Writhe, the Average Crossing Number (ACN) and the Jones polynomial of each filament in the system, whether it is open or closed. In particular, the software uses rigorous definitions of the Writhe, ACN and of the Jones polynomial of linear (open) chains that do not require any closure scheme. The software also enables the computation of the Gauss linking integral for all pairs of chains (open or closed) in 3-space and in systems employing Periodic Boundary Conditions. In addition, a new source-file and command in LAMMPS is introduced, that enables the computation of topological parameters in a simulation using LAMMPS. We provide examples of how the code is used and we present results

on the entanglement effect in polymers obtained using this package.

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PP1

Characterizing the Growth Rate and Fractal Dimension of Marine Aggregates Formed Through Brownian Dynamics

Microorganisms and particulates present near the ocean surface tend to form clusters when coming into contact with each other. The resulting marine aggregates exhibit a fractal structure and play a fundamental role in the oceanic carbon cycle. Our research aims to numerically characterize the formation of aggregates using Brownian dynamics. Our approach improves on the well-known Diffusion-Limited Cluster Aggregation (DLCA) model, in which aggregates undergo random translation only, by also incorporating random rotations and settling under gravity. We measure the fractal dimension of the resulting aggregates for both constant and more realistic size-dependent diffusivities. Furthermore, we quantify the impact of rotation and settling on their growth rate, allowing the lifespan of the aggregates to be compared to the time scale of other biological and physical processes. The flexibility of our formulation allows for the future integration of more complex features, such as disaggregation, hydrodynamic interactions, and charges.

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PP1

Significant Gene Array Analysis and Cluster-Based Machine Learning for Breast Cancer Prediction

Gene expression analysis plays an essential role in disease risk assessment and prediction. This study evaluates the use of several machine learning (ML) approaches in identifying the relative importance/differentially expressed (DE) genes among breast cancer patients. We have incorporated clusters of genes that showcase an effective biologically driven ML approach to uncover DE genes. In this regard, Significant Analysis of Microarrays (SAM), followed by five machine learning models; (a) random forest, (b) random forest with Gene eXpression Network Analysis (RF-2), (c) RF++, (d) LASSO, and (e) Bayesian Neural Networks (BNN) have been investigated on two breast cancer data sets obtained from Gene Omnibus Database (GSE 2034 and GSE 2990). We have incorporated the Automatic Relevance Determination prior with BNN to assess the relative importance of genes. RF-2 had shown appealing results with an average area under the receiver operating characteristic curve (AUC) value of 70% and 78%, respectively, on GSE 2034 and GSE 2990. This was followed by BNN with average AUCs of 55% and 64%, respectively. As per SAM, a protein-encoding gene TRAF5 had shown a significant up-regulation (log-fold change:2.27, q-value: 0.00) among relapsed subjects. Several other genes including SERPINA3, ID1, RSBN1, MAD2L1, SPAG16, and PCLAF were consistently ranked within the top 25 based on the mean decrease in accuracy, by at least two ML methods.

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PP1

Topology Optimization Through Machine Learning

Topology Optimization (TO) is a powerful computational design method for automatically generating a structural layout to determine the optimal material layout in a design domain with maximum performance under relevant design specifications. In recent years, considerable research efforts have been made in the advancement of TO procedures. Although structural TO has great potential for creating innovative structural designs without prior knowledge, it is a time-consuming task. In this study, we investigate the application of neural networks and convolution neural networks to conduct TO directly from the finite element solver. In this approach, a neural network is used to represent the density field function independent of finite element mesh. A Fourier space projection has been implemented within the machine learning model to control the minimum and maximum length scales to meet the manufacturing and other functional requirements. We have adapted the high-performance Google automatic differentiation library JAX to build an end-to-end differentiable network model. The sensitivity computations are automated by using the built-in backpropagation functionality in JAX. The performance of the proposed framework is demonstrated by solving several elastic and thermoelastic compliance minimization problems and comparing the results with the optimized structures obtained from other optimization techniques.

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PP1

A Multiscale Method for the Heterogeneous Signorini

In this work, we develop a multiscale method for solving the Signorini problem with a heterogeneous field. The Signorini problem is encountered in many applications, such as hydrostatics, thermics, and solid mechanics. It is well-known that numerically solving this problem requires a fine computational mesh, which can lead to a large number of degrees of freedom. The aim of this work is to develop a new hybrid multiscale method based on the framework of the generalized multiscale finite element method (GMsFEM). The construction of multiscale basis functions requires local spectral decomposition. Additional multiscale basis functions related to the contact boundary are required so that our method can handle the unilateral condition of the Signorini type naturally. A complete analysis of the proposed method is provided and a result of the spectral convergence is shown. Numerical results are provided to validate our theoretical findings.

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PP1

A New Efficient Numerical Scheme for the Q-Tensor Model of Nematic Liquid Crystals

Liquid crystals are an intermediate phase of matter possessing qualities of both a liquid and a solid. One particular phase of liquid crystals is the nematic phase of which the constituent molecules flow freely, but align themselves with partial orientational order. Observations of topological defects within the material is a top priority to engineers although the microscopic behavior is difficult to study in the lab. For this reason, simulations of liquid crystals is an important contribution to the design of these materials. In this poster we present a finite element numerical scheme for the simulation of nematic liquid crystals using the LandaudeGennes Q-Tensor theory. This theory relies on using a symmetric and traceless tensor which allows for the proper characterization of topological defects. To reduce the computational cost, we propose a numerical scheme based on decoupling the computation of the variables into several smaller substeps which allows us to significantly reduce the size of the linear system to be solved. We show this decoupled scheme is energy stable. In addition, we implement an adaptive time-stepping algorithm by varying the time-step at each iteration based on the numerical dissipation introduced in the discrete energy law. This allows us to accurately capture the dynamics of the system while reducing the number of discrete time steps. We compare these results with the nonadaptive time-stepping algorithm to measure computational savings.

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PP1

A Multiphase, Embedded Boundary Method for Solving the Stress Balance Equation of Ice Sheet Dynamics

Projecting contributions from marine ice sheets to future sea level rise requires an accurate treatment of the region of ice neighboring the grounding line. The grounding line marks the location where ice that was formerly sitting directly on bedrock flows into floating ice shelves, making it an area of dynamic activity. Floating ice balances the force of gravity through internal deformation, while grounded ice can additionally balance gravity by sliding on bedrock. This abrupt change in governing equations at the grounding line is a source of costly numerical error in ice sheet models. Our solution to this problem is to treat grounded and floating ice as distinct phases coupled by matching conditions at the grounding line. We utilize recent advances in Embedded Boundary (EB) methods, which are finite volume schemes that intersect an irregular geometry with a regular Cartesian mesh. By considering the grounding line to be an embedded boundary, we build upon least-squares interpolation techniques that were previously developed for single phase problems in complex geometries. These methods provide a way to impose constraints on the solution at the grounding line through stencil modification. We present the mathematical formulation of our scheme as well as numerical results from idealized test problems.

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PP1

Refit: Data-Driven Algorithms for Computing with Trigonometric Rational Functions

The poster describes rational approximation schemes for reconstructing periodic signals from samples with poorly separated spectral content are described. The methods introduced are automatic and adaptive, requiring no tuning or manual parameter selection. Collectively, they form a framework for fit- ting trigonometric rational models to data that is robust to various forms of corruption, including additive Gaussian noise, perturbed sampling grids, and missing data. Our approach combines a variant of Pronys method with a modified version of the AAA algorithm. Using representations in both frequency and time space, a collection of algorithms is described for adaptively computing with trigonometric rationals. The MATLAB software system REfit, based on these algorithms, is used to illustrate our ideas with synthetic and practical examples drawn from applications including biomedical monitoring, acoustic denoising, and feature detection.

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PP1

Diagonalization of Schrödinger Operators with Piecewise Constant Potentials

We provide a numerical method for computing the solution of the *parabolic equation*, a partial differential equation (PDE) which models propagation of sound waves in the ocean, and arises from factoring the Helmholtz Equation. The solution is a function of variables indicating depth and range, as opposed to space and time. The spatial differential operator in the PDE is a Schrödinger Operator, which has a potential α^2 that is approximated by a piecewise constant function, to account for variation in sound speed. This project primarily deals with the 3-piece case; however, a generalization is made to the case of n pieces. The Uncertainty Principle will be used to obtain accurate estimates for the eigenvalues of the operator. Then, the estimated eigenvalues are used as initial guesses for the Secant Method to find the exact eigenvalues, and an eigenfunction expansion of the solution is constructed. The accuracy, efficiency, and scalability of this method is shown through numerical experiments in comparison with other methods. Efforts to improve the efficiency even further leads to an investigation of a change of basis matrix that could circumvent the need for constructing eigenfunctions explicitly. The sparsity of this matrix suggests that variable-coefficient PDEs can be solved almost as rapidly as their constant-coefficient counterparts, through an FFT-like operation.

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PP1

Spectrum Adaptive Preconditioning for Kernel Matrices

We present a spectrum adaptive preconditioning technique for solving linear systems associated with covariance matrices from Gaussian process. The spectrum property of covariance matrices varies dramatically as the hyperparameters in the kernel function change. The optimization to find the optimal kernel requires solving linear systems with hyperparameters within a wide range. In order to tackle this challenge, we propose to first apply a sampling technique to reorder the matrix into the block 2-by-2 form where the leading block reveals the rank of the covariance matrix. We then sparsify the leading block in a systematic way and construct a sparse preconditioner for this block. We can show that the proposed method scales almost linearly with respect to the matrix size for all hyperparameters. Numerical experiments are provided to demonstrate its performance on several real datasets. This is joint work with Luke Erlandson, Edmond Chow and Yuanzhe Xi.

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IP1

Opening Remarks and Presentation: Preparing and Supporting Teachers to Include Mathematical Modeling in Their Curriculum

Students clearly deserve stimulating problem-solving opportunities in which they create and explore mathematical models to address situations relevant and meaningful to them. Yet despite calls to incorporate more modeling activities in our classes, teachers at all levels struggle to put recommendations into action. Since undergraduate mathematics serves as a confluence in the teacher preparation stream, it must include model mathematical modeling pedagogy. In this talk, I will share insights my collaborators and I have gained from designing and implementing data driven mathematical modeling activities in undergraduate courses. I will further detail various strategies for engaging undergraduate mathematics faculty as well as prospective and professional secondary teachers in mathematical modeling focused professional development.

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IP2

Research on Learning and Teaching University Mathematics: Where We Are and Where We Might Go Next

In this talk I begin with a brief overview of what we know about the teaching and learning of calculus in the United States. In particular, I highlight findings from two large US national studies of the precalculus through calculus sequence . Next, I review what we know about the effects and uptake of research-based instructional strategies at the university level. I then reflect on new directions for the broader field of research in university mathematics education. These new directions include expanding the notion of inquiry, research related to departmental and institutional change, and research that centers issues of equity and social justice.

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IP3

Education, Data, and Social Justice

While the importance of data science training has been highlighted by stakeholders across the mathematical sciences, the fusion of data skills with core parts of the curriculum has yet to be fully realized. In parallel to this challenge, the mathematical sciences are struggling with issues of equity, diversity, and inclusion. This talk presents pathways for incorporating data skills into undergraduate mathematics education in ways that support social justice. One pathway is through the classroom. I will present selected examples of course activities such as creation of computational art designed to celebrate artists from marginalized identity groups. A second pathway is through undergraduate research. I will showcase data-intensive student projects, including work on incarceration policy on Rikers Island. Finally, I will highlight resources for instructors who themselves want to grow their data skills and/or their understanding of social justice.

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IP4

Closing Remarks and Presentation: Toward a Culturally Relevant and Historically Responsive Data Science

In the expanding discourses around data science and statistical data analysis, less work has been done to make culturally- and historically- centered pedagogies a central area of investigation. To this end, this invited talk will examine seminal theories in education focused on the role of culture and history in teaching and student learning. Within the development of inquiry-based classrooms, these frameworks support our collective knowledge around the role of culture and history in relation to applied mathematics, statistics, and data science education in k-12, postsecondary, and community settings. Moreover, these frameworks can be used to support the ongoing development of data science programs and research-practice partnerships that advance actionable and critical data science practices.

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JP1

Joint Plenary with the SIAM Annual Meeting AN22: Building Mathematical Communities of Students, Faculty, and the Public to Create Pathways from K-12 to Graduate Programs

Given the large percentage of Latino and first-generation college students in the Rio Grande Valley, the University of Texas Rio Grande Valley serves as a vital pipeline for preparing the nations leadership in STEM disciplines from underrepresented groups. In this talk, we describe efforts to build communities in mathematics involving public schools, universities, students and faculty, and the UTRGV Center of Excellence in STEM Education (C-STEM). We will discuss how we have built communities of undergraduates and K-12 students through summer camps and mobile STEM labs through the C-STEM. Additionally, we will discuss how communities of faculty through university collaborations have created pathways to graduate programs via REUs, team-teaching of advanced math courses and boot camps aimed at preparing students to effectively apply for graduate programs. At the departmental level, we will describe how we have built communities within our student population through collaborative problem-solving sessions. A crucial component in many of these programs is the inclusion of professional development workshops to guide students along the path to success in graduate school.

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CP1

Bagel Institute: A Simple Web-Based App for Anxiety-Free Student-Instructor Interaction

Bagel Institute (https://bagel.institute) is a free web-based app for in-person or online teaching. The app has a 2-minute learning curve. There are two simple functions only,

letting students ask and answer questions in class without having to reveal who they are. The app has Latex support. We will report on experiences using Bagel Institute in several applied mathematics classes, ranging from introductory to graduate level. The main benefit is to give instructors a clearer picture, in real time, of their students' thinking. This definitely results in slower teaching. Of course we hope that it also results in more effective and more inclusive teaching, but more data will be needed to support that.

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CP1

Confidence-Based Marking (CBM) in Online Mathematics Instruction: How to Involve Students in Assessment-for-Learning?

This paper addresses the need for developing Self-regulated Learning (SRL) as the holy grail in online instruction. A collaborative action research, aiming at embedding self-and-peer assessment into mathematics learning, was carried out over 14-weeks in a master program in mathematics and computer sciences at university of Passau, Germany. Students were engaged in Student-generated Questions (SGQ) and Confidence-based Marking (CBM): they were asked to conduct inquiry-based learning, develop relevant questions, ask their peers to answer the questions and rate their confidence in their answers throughout the online course. Data were triangulated from three sources: (a) assessment artifacts, i.e. SGQ and CBM, as evidence of learning,and (b) students attitude captured through Task Perception Questionnaire. Assessment data were analysed by three experts based on their judgement of quality. Kappa measure was used to assess consistency among raters. Quantitative analysis of questionnaire data indicated positive attitudes towards CBM (engaging, fair, easy, or useful) among students. Analysis of field-notes and observation made by instructors provided complementary evidence about real-time reactions and experiences (confusion, frustration, bewilderment) of students as they were performing CBM tasks. We examine the limitations as well as implications of this project and conclude with a discussion of future action plans to improve such classroom research.

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CP1

Functional and Fourier Analysis Learning Trajectories for Engineering Mathematics Education

Fourier and functional analysis are critical for engineering mathematics education with its diverse applications in control theory, signal analysis, electromagnetics, vibration, and acoustic. Learning trajectories are used here as a pedagogical tool to build bridges between mathematics and engineering courses. Towards building a scholarship of teaching and learning of applied mathematics for engineers for applied mathematics and engineering students, interdisciplinary faculty from applied Mathematics and Engineering collaboratively worked on development of Fourier and Functional Analysis ideas across mathematics and engineering courses. The design research, as described in Prediger, Gravemeijer, Confrey, (2015) and Streefland (1994) is conducted to explicate learning trajectories for Fourier and Functional Analysis to support local instructional practices. Using concept maps, the Fourier and Functional analysis learning trajectories are depicted as spanning across the following courses: Trigonometry, Calculus III, Complex Analysis, Ordinary Differential Equations, Linear Algebra, Control Theory, Signal Processing, Electromagnetics. Engineering and applied mathematics instructors reflected and articulated these pathways from their disciplinary perspectives, highlighting the critical transitions such as the transition from subspace to inner product spaces in Linear Algebra, and Fourier transform with Maxwells equations in Electromagnetism in the frequency domain.

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CP2

Research Projects in Data-Enabled Industrial Mathematics: from a Course to NSF REU Site

Undergraduate research projects with industrial partners combine the essence of academic research and hand-on practice in the real world by building a bridge between them. The real-world problems have an educational impact that cannot be replicated in the traditional mathematics classroom setting. In this talk, we will discuss the challenges of bringing collaboration with real business, industry, or government (BIG) into the undergraduate research. We highlight differences and challenges compare to traditional undergraduate research. We will share our experience from a course to nationwide NSF REU site at Embry-Riddle Aeronautical University.

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CP2

Computation and Programming - Why Aren't We Teaching This to Everyone?

The computational world impacts almost every academic, industrial and business enterprise. It stands on its own as an experimental world of new concepts and fascinating phenomena. It is a world of active learning and investigation. It promotes abstraction in its data structures and operations, while being the most concrete of venues. The numerical, the algebraic, the visual are integrated into one computing system, empowering the user on their own to conceptualize, execute, and display virtually any computation. Modern software, most particularly MATLAB, is easily accessible, includes a general purpose programming language, a stunningly efficient set of data structures and operations based on arrays, and full visualization capability. What could students accomplish with computation as one of the pillars of their academic education, something which can be easily introduced and fully appreciated even in high school. So why aren't we teaching this to everyone? Having taught a basic course in programming and computation using Matlab for more than ten years, the most compelling way to present this viewpoint, it seems,

is through example. These are not specifically motivated by a topic in the standard mathematics curriculum which speaks to our larger point - but rather by curiosity, or by applying a new programming concept. Having seen the result, one is prompted to go further, to explain it using mathematics, or simply to sit in wonder.

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CP2

Experiences in Offering a New Undergraduate Course in Mathematical Foundations of Data Science

This presentation will summarize experiences developing and delivering a new undergraduate course covering foundational topics in data science and data-driven mathematical modeling. The target audience for this course is junior and senior undergraduates pursuing majors or minors in mathematics or applied mathematics at a large STEM-focused public university. Course prerequisites included vector calculus, a first course in linear algebra and some familiarity with Matlab. Strategies and reflections will be shared regarding selection of course topics and source materials, modes for delivery of course content, design of homework sets and group projects, and integration of data into the curriculum. Student feedback as well as experiences with integrating this course into existing degree paths and data science initiatives will also be discussed.

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CP2

Applied Honors Calculus at Michigan

Applied Honors Calculus (Math 156) at Michigan is a 2nd semester calculus course for STEM majors who took AP calculus in high school. The course started in 1994 in response to a request from the College of Engineering, and it emphasizes the science applications of calculus and math topics relevant to the students' subsequent STEM classes. This talk will describe the course and the teaching strategies that have been found to work well.

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CP2

Industrial Applied Mathematics and Data Science Education at Metropolitan State University

In response to an alumni survey conducted in 2017, the Mathematics Statistics Department at Metropolitan State University in Minnesota is transforming its applied mathematics education and offering pre-professional opportunities to support career readiness. The University serves students of diverse backgrounds, with a particular focus on adult learners and communities of color. The initiatives undertaken by the department are designed to support the diverse challenges and interests of these students. Initiatives include the creation of an Industry Advisory Board with representation from a range of Twin Cities-based companies, programmatic additions and changes, course development and redesign, and pre-professional opportunities including job shadowing, mentoring, supervised consulting, and internships. The department recently launched the Industrial Applied Mathematics BS integrating mathematical, statistical, and computational skills with increased emphasis on modeling, exposure to complex open-ended problems, technical communication skills, and teamwork. Collaboration with the Computer Science and Management Information Systems Departments has resulted in the creation of a Data Science BS with many of the same emphases. This presentation will describe these initiatives.

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CP2

The Effect of Repetition Learning in Data Analysis Projects

Repetition learning has been considered as an efficient tool to help students to master the knowledge, but it is seldom applied in subjective assignments, like a data analysis project. In practice, we believe that project assignments are less likely to be reviewed after grading, thus it is hard to know whether students have learned from their mistakes. Moreover, because of the flexibility of topic/methodology choices, there may exist more than one correct answer/approach, thus students are always encouraged to view the questions from different perspectives even with the same data. In this work, we want to know what if a student gets a second chance to do the exact same project assignment, can they self-improved the work quality? Between the two submissions, we add a group reflection activity that students will be asked to read the peers work, to reflect on what their peers have done great, but they need to improve. This is slightly different from the normal peer review which we focus more on giving suggestions to the peers. Group reflection requires students to think more about how to improve their own work, thus may also be able to improve their self-learning ability. Wed like to quantitatively measure how the repetition project and group reflection may affect students learning outcomes in different project settings through both their project scores and word choices in the final analysis report.

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MS1

The Graduate Student Mathematical Modeling Camp

In recent years, the need for increased opportunities for training graduate students in industrial mathematics has become clear. Much of this training is extracurricular, taking place at summer workshops. We present results from the first half of a two-part approach. At the three-day Graduate Student Mathematical Modeling Camp (GSMMC), students work together in teams under faculty guidance on interdisciplinary problems typically inspired by industrial applications. The problems are carefully chosen to promote a rich set of analytical and nu-

merical problem-solving skills. "Soft skills" are promoted via lively discussions about the solution process, as well as oral and written presentations. After the Camp, students travel to the Mathematical Problems in Industry Workshop (MPI). There, they use their new-found skills to join teams of faculty, postdocs, and industrial scientists to solve open-ended, real-world problems. We will discuss our successful outcomes, as well as the challenges of administering such a program, both before and during the pandemic.

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MS1

Logistics of Running a Hybrid Problem-Solving Workshop Involving Graduate Students

Due to the pandemic, the Mathematical Problems in Industry workshop in 2020 and 2021 was hosted online. One advantage of this format was the ability to bring in academic participants from different continents (mostly America and Europe) without incurring significant expenses. It also allowed some participants the flexibility to contribute only part of their time to the workshop, which, for some, was an incentive to participate. The online format also introduced or made more prominent a number of challenges. Following below is a list of some choices that needed to be made to address those challenges.

- A platform that would allow the interaction among participants to mimic that in an in-person workshop; MS Teams was chosen for the task.
- A schedule that would accommodate participants from time zones differing by as much as 8 hours.
- A means of maintaining continuity among groups working in different time zones.
- Of paramount importance for both online and in-person workshop is the commitment of industrial participants to guide their academic group. This puts the responsibility on the organizers to convey this importance to the industrial participants.

These issues will be addressed in detail in this talk.

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MS1

Math Industry: Running An Industrial Mathematics Research Experience for Undergraduates

In the Worcester Polytechnic Institute (WPI) Center for Industrial Mathematics and Statistics (CIMS) Research Experiences for Undergraduates (REU) Program in Industrial Mathematics and Statistics, students work in teams on research problems of industrial and mathematical significance that come directly from industry, and which are of immediate interest to the companies involved in the program. They work closely with company representatives to define the problem and develop solutions, and they work closely with faculty advisors to maintain a clear focus on the mathematics and statistics at the core of the project. This nine-week, summer research provides challenges not faced in standard undergraduate programs and develops skills not always developed in traditional educational programs. It also provides a glimpse of the many career possibilities that are open to students with a strong mathematical background. This NSF-funded REU Program has been held at WPI during the summers of 1998–2015 and 2018–present. In this talk, I discuss the structure, planning, and implementation of this summer program, and its broader impacts.

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MS2

RTG: Randomized Numerical Analysis

We report on the research, educational, and outreach activities of the NC State RTG award on Randomized Numerical Analysis. Our research activities are organized across the three interconnected themes of sensitivity analysis, randomized numerical linear algebra, and nonlinear equations. Our graduate fellows are expected to complete an internship during their studies. These internships typically take place at national labs and have resulted in career opportunities, research collaborations, and new partnerships. The program has generated an extensive amount of new research and results; it has provided an enriching environment for our students, postdocs, and faculty participants.

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MS2

RTG: Modeling and Computations for Complex Systems at Southern Methodist University

As this RTG starts its fourth year, I will provide a list of activities, accomplishments and challenges we have faced during the first three years. With 3 core topics running in parallel: Computation-enabled investigations into circuits and cognition, Nonlinear dynamics and the modeling of large systems and Modeling complex transport processes in nanoscale manufacturing, specific educational activities focused on vertically integrated training of undergraduate students, graduate students, and postdoctoral fellows have worked well. A bigger challenge has been developing cross-fertilization. For this we have found that the postdocs have played a critical role in facilitating this. With this in mind, the presentation will highlight successes and upcoming plans, with a summary of the overall impact the RTG has had in our general PhD program.

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MS2

RTG: Applied Mathematics and Statistics for Data-Driven Discovery

The Data Driven Discovery RTG at the University of Arizona (UA) is a group of a dozen faculty spanning mathematics, applied computational math, and statistics, with a comparable number of graduate students and postdocs. The RTG is dedicated to vertically integrated training in the use of data driven modeling techniques in the mathematical sciences, with applications ranging from medical imaging to fluid dynamics. In this session, we will report on our experience and many lessons learned starting and running the RTG and the associated Research Experience for Undergraduates program during the COVID-19 pandemic, and our plans for the future.

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MS2

RTG: Mathematics of Information and Data with Applications to Science

I will provide an overview of the educational activities of the research training group "Mathematics of Information and Data with Applications to Science" at Brown University. The central theme of this RTG is the mathematical foundations of data science and their applications, and we approach this topic with a strong interdisciplinary flavor. The educational activities focus on vertically integrated training of undergraduate students, graduate students, and postdoctoral fellows. Concrete training activities include first-year seminars (e.g. on data science and social justice), enhanced undergraduate and graduate curricula, summer research experiences for undergraduates, graduate students, and postdoctoral fellows, and semester working groups for advanced graduate students and postdoctoral fellows. Our goals for workforce development center around the recruitment, retention, and training of a diverse cohort of applied mathematicians trained in data science.

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MS3

Addressing the Need for Stem Teachers in Rural and Urban High-Need Schools

Economically disadvantaged communities face unique challenges to engage and retain talented K-12 teachers, especially those with aptitude in STEM. STEM teacher shortages that exist in K-12 schools across the country are even more prevalent in high-need school districts. A range of factors contribute to the barriers that limit the applicant pool: lower teaching salaries, fewer resources, lack of access to materials and programming, and often the need to teach multiple subjects because there are fewer faculty. Early field experiences that engage undergraduate STEM students in mentoring and teaching K-12 students, through educational outreach programs, competitions and design challenges, after-school tutoring, and peer mentoring programs, provide enhanced K-12 STEM learning opportunities in high-needs school districts while simultaneously planting seeds for undergraduate students to consider careers in STEM education. Among our MAT applicants we have observed a high preponderance of students who participated in some type of early field experience, and students whose experiences were in high-needs schools are particularly drawn to working in similar situations. A combination of early field experiences in high-needs schools, together with additional coursework that helps develop cultural competence and equity literacy, helps to ensure a successful transition as our students move into their early careers.

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MS3

Graduate Pre-Service Teacher Preparation for High-Need Schools

In preparation for their work in high-need schools, the Clarkson University Noyce Program provides scholars with opportunities to learn more about the environments and communities that they will be working in. As a part of their Masters of Arts in Teaching program, they complete a full-year residency as part of their program and complete an action research project, in addition to other coursework. The Noyce scholars also reflect on their teaching, focusing on equity and how they respond and relate to their students. The program provides students opportunities to talk to current teachers in both rural and urban schools to find out what is unique about working in their district in addition to equity-focused activities. In this session, we share about the aspects of the program we find to be successful, and also raise questions and ideas on how to improve the program for future scholars.

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MS3

Undergraduate Experiences and Training with High-Need K12 Students

Much like any profession, good educators require both formal education and firsthand experiences with teaching to grow to their full potential. Through experiences in formal settings and more informal work with students, educators are better able to build their confidence, learn better practices, and develop a strength in connecting with their students. The Noyce program provides participants with both aspects: a strong understanding of equity and best teaching practices in high-need settings as well as a plethora of opportunities to work with middle and high-school level students. A previous student and Noyce scholar describes how the program helped to shape his current mathematics teaching practices and how these experiences with multi-

ple levels of education built the foundation of his teaching practices.

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MS3

Cultural Explorations and Experiences: Immersive Experiences to Better Serve a Diverse Population of Students

A recent Clarkson graduate shares her experience participating in the Noyce program while completing her MAT in secondary math education. She describes how the Noyce program enhances a STEM students experience in the MAT program by providing real opportunities to understand the benefit of working in a high-needs district and build the competency to do so. She shares how meeting with veteran teachers in both urban and rural high-needs districts allows students to learn the challenges and rewards of working in both settings, providing insight into which environment would be best suited for each individual. In addition she shares how the Noyce program builds a community of graduates and faculty that support each other through the graduates year-long student teaching experiences, action research projects, the job search process, and even current teaching positions. It is these experiences collectively that build the graduates competence to work in a high-needs district and ultimately supports them in succeeding as an educator in any setting.

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MS4

Mathematical Modeling Education: Developments in the Russian Federation

Two teams from Russia have been participating in IMMC every year since its first edition. Initially, only two schools were involved in the selection, but step by step, the number of schools and teams increased, and lately we have about 30 teams from the places scattered all over the country, from Siberia through Urals to Caucasus and to Moscow, competing for a pass to the international round. To popularize IMMC and related activities, we use various events for high school students and teachers, most notably, the international Mathematical Modeling Tournament (MMT) conducted annually by the Kolmogorov School of MSU. MMT comprises four contests, one of which is similar to IMMC and the other three are closer to traditional olympiads in terms of their format and to applied mathematics in terms of content, which makes them easier accessible for unprepared students. Sample problems from MMT will be presented. More generally, we will discuss the reasons why Russian teams are not as successful at IMMC as could be expected judging by their results at IMO and other traditional olympiads.

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MS4

Mathematical Modeling Education: Developments in Spain

Despite the fact that the Spanish educational programmes include modelling as a content to be worked on in Mathematics in secondary education, the reality is that mathematical modelling has not yet effectively entered the classrooms. In 2019, after contacting some of the organisers of the IMMC, a group of Spanish mathematicians with different profiles, we started the selection phase of the competition in Spain. The development of the competition has been a challenge that has involved different agents and in which the work of dissemination has been crucial, but also that of teacher training. In order to choose the two teams that will represent Spain in the IMMC, we open the registration phase for teams in November. The organisers of the IMMC-Spain competition set a modelling problem common to all participants. A key aspect of our way of working is the correction; we do not limit ourselves to just qualifying the productions, but we also provide the participants with a qualitative evaluation. This is certainly a motivation for the participants as well as for the teachers. The teams with the best productions are invited to solve the problem in the international phase and the two best productions are selected to participate in the IMMC. This presentation will present the details of the selection of teams in Spain and will focus on the difficulties and the impact of modelling in the Spanish education system.

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MS4

Mathematical Modeling Education: Developments in Chile

The mathematics curriculum in Chile has modeling as one of the fundamental skills to be developed by students. Even though for primary and middle school this was introduced almost a decade ago, the evidence we have and our own personal experience suggest that teachers are not being prepared to teach it and that students have little opportunities to work with real-world mathematical modeling problems. In this talk we will present an overview of different initiatives the Laboratory of Math Education of the Center for Mathematical Modeling (CMM-Edu) of Universidad de Chile has developed to help to improve this situation. The first one is the selection process for the International Mathematical Modeling Challenge (IMMC), which is an annual school-level team-based contest. We will describe what we have learned from running the process, particularly some findings of a study that focuses on the changes on students conceptions about the nature of mathematics that could be triggered when working autonomously in modeling problems. We will also present other two initiatives that focus on improving teacher preparation to teach modeling: a course of mathematical modeling for a pre-service teacher education program and an online course for in-service teachers which is run nationwide. In both cases we will describe the instructional model, give examples of activities and present some results of the implementation.

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MS4

Mathematical Modeling Education: Developments

in the Netherlands

In 1985, two new programs were introduced in Senior High School, replacing the existing mathematics program: Mathematics A, preparing for social sciences and Mathematics B for natural sciences. New in both programs was explicit attention for applications and aspects of modeling. Because modeling is hard to assess in time-limited national exams, the Freudenthal Institute developed the Mathematics A-lympiad and Mathematics B-day, a one-day modeling experience for teams of four students. About one-third of all schools use these tasks every year for all students in grade 11, as mandatory part of their school exam. All teacher-training institutes prepare students for these aspects of their future job. All commercial textbooks have to pay attention to applications and modeling, because the national curriculum prescribes so. Seen from this perspective, there is no need for institutional change in the Netherlands, although sometimes back-to-basics movements try to influence policymakers. IMMC is promoted in the Netherlands, because we believe that students and teachers deserve the possibility of working on a realistic problem to experience how mathematics can be used to attack and solve real life problems. We promote IMMC by doing workshops at teacher conferences, publish articles in the national mathematics teachers journal and through personal networks.

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MS5

Tapia Camps for K12 Students at Rice University

The Tapia Center for Excellence and Equity at Rice University has been delivering STEM summer camps to middle and high school students. Since 2017, over a thousand students have participated, of which 47% were women and 70% were from underrepresented racial groups in STEM. The programs focus on STEM, communication, and equity, and they build a community of young scientists from all over Texas, the country, and the world. The students interact with university students and faculty, including Dr. Richard Tapia, winner of the National Medal of Science. In this presentation, the camp director Dr. Paul Hand will share stories from the programs.

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MS5

The History and Future of Lathisms: Latinxs and Hispanics in the Mathematical Sciences

In this talk I will discuss the history of Lathisms, from its creation to our hopes for the future. I will also share some of the current challenges and opportunities we face when building inclusive communities that uplift those who are most marginalized in the mathematical sciences. Lastly, I will give a variety of ways in which those who are interested can get involved with Lathisms. Its goals and programming aim to be community driven, and it needs the support of our community members to grow and thrive.

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MS5

Building Resilient Math Communities in the Classroom and Research Lab

At the University of Texas Rio Grande Valley (UTRGV), we have worked to build communities of faculty and students both in the classroom and the research lab. These communities have created a critical mass of support for students on the path to graduate school. A component of these efforts is flipping upper-level courses so that lecture is structured around group work and communication. This helps to build a more resilient community of undergraduate students. Through an NSF and Sloan Foundation grant, some of the courses have been co-taught by faculty from UTRGV and UT Dallas, who have then collaborated on summer programs for undergraduate students intended to create a pathway to graduate programs. In this way, faculty with a shared commitment to widening this path toward research also form a collaborative community. Additionally, through summer research opportunities for undergraduates, we extend the concept of a community of students to the research lab. By creating a pathway for talented students from the Texas-Mexico border to research participation, we can contribute to the diversity of tomorrows set of leaders and mathematicians. During this talk I will share the lessons I have learned from being a part and helping to build these diverse research communities.

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MS6

Sharing Resources and Facilitating Community Conversations About QuantCrit

As new fields, like mathematics for social justice and QuantCrit, are explored and defined, it is important to identify where current work is happening. We do this in order to be more efficient (stop reinventing the wheel) and to build quickly on the work already done. In this active, participant-driven session, we will work on compiling resources and sharing experiences from our session speakers and participants.

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MS6

Questioning Dogma - How P-Values Can Hide In-

equities

Scholars, largely women of color, have used qualitative methods to show the inequities that Black women and other women of color face during their STEM education. Quantitative discipline-based education research (DBER), however, largely fails to engage in similar intersectional work to complement this qualitative research. "Mindless statistics" (Gigerenzer, 2004) stand in the way intersectional quantitative research through a dogmatic dedication to $p < 0.05$. Dogmatic, because the American Statistical Association calls for "Moving to a world beyond '$p < 0.05$'" (Wasserstein, Schirm, and Lazar, 2019). This dedication to statistical significance pushes researchers to aggregate data across demographic groups. We argue researchers should instead focus on disentangling and informing the intersecting power structures of racism, sexism, and classism. We will discuss common statistical practices in DBER, how these practices obscure inequities, and solutions to these issues.

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MS6

A QuantCrit Investigation of Societys Educational Debts in Stem

This talk offers an example research project that is grounded in QuantCrit and followed the methods proposed in the prior two talks. The American Chemical Society holds supporting diverse student populations engaging in chemistry as a core value. We analyzed chemical concept inventory scores from 4,612 students across 12 institutions to determine what inequities in content knowledge existed before and after introductory college chemistry courses. We interpreted our findings from a Quantitative Critical (QuantCrit) perspective that framed inequities as educational debts that society owed students due to racism, sexism, or both. Results showed that society owed women and Black men large educational debts before and after instruction. Societys educational debts before instruction were large enough that women and Black mens average scores were lower than White mens average pretest scores even after instruction. Society would have to provide opportunities equivalent to taking the course up to two and a half times to repay the largest educational debts. These findings show the scale of the inequities in the science education systems and highlight the need for reallocating resources and opportunities throughout the K-16 education system to mitigate, prevent, and repay societys educational debts from sexism and racism.

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MS6

How Statistical Model Development Can Obscure Inequities in Stem Student Outcomes

Researchers often frame quantitative research as objective, but every step in data collection and analysis can bias findings in often unexamined ways. In this investigation, we examined how the process of selecting variables to include in regression models (model specification) can bias findings about inequities in science and math student outcomes. We identified the four most used methods for model specification in discipline-based education research about equity: a priori, statistical significance, variance explained, and information criterion. Using a quantitative critical perspective that blends statistical theory with critical theory, we reanalyzed the data from a prior publication using each of the four methods and compared the findings from each. We will discuss how these practices can obscure inequities and which methods are best suited for research into issues of equity in the STEM disciplines.

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MS7

RTG: Data-Intensive Research and Computing at the University of California, Merced

Since summer 2019, the University of California Merced campus has been running the Data-Intensive Research And Computing (DIRAC) RTG. In this presentation, we will describe the research foci of our program and present the structure we put in place to enhance and support mentoring at all levels. In particular, we formed small Mentoring and Research Training (SMaRT) teams that are vertically integrated, combining faculty, postdocs, graduate students, and undergraduate researchers to establish a community of researchers that can serve to support each other at various points of their careers. We will discuss successes and challenges encountered over the last three years of this project.

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MS7

NSF Research Training Groups in the Mathematical Sciences

This will be a short presentation about the NSF Research Training Groups in the Mathematical Sciences (RTG). We will discuss a brief overview of the RTG program solicitation, followed by a QA.

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MS7

RTG: Computational Mathematics for Data Science

The Emory RTG is designed unify and further develop the mathematical theory and computational tools used in applications ranging from data assimilation to machine learning. This comprehensive approach will be based on knowledge from, and make novel contributions to mathematics, computational science, and data science. Particular focus will be on the mathematics of deep learning and data assimilation and their application in impactful areas of medicine (cardiac modeling, medical imaging), the weather and environment (hurricane storm surge modeling), and disease outbreak modeling. Common threads in these areas are their mathematical foundations, most importantly differential equations, optimization, linear algebra and advanced techniques from computational science, such as parallel and distributed computing. This RTG program is anchored around year-long research themes that include one or more of the above mentioned core research themes. Training will by multi-faceted, to include education, potential career skills and experiences, soft skills, scientific integrity, and promoting an appreciation for diversity.

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MS8

Research in Mathematical Modeling for Secondary Teacher Education

Research in prospective teachers development of mathematical modeling knowledge for teaching is gaining momentum. We found that project-based mathematical modeling experiences provide opportunities for prospective secondary teachers to develop foundational knowledge in modeling and a vision for teaching and learning mathematical modeling. We designed modeling problems for the MODULE(S2) Project with a variety of social contexts that allow prospective teachers to examine critical social issues to consider in their future teaching. We describe two modeling projects: (1) the use of sandbags as emergency barriers for damage-causing flooding, and (2) the use of historic maps to examine the shrinking land of the Sioux Reservation. The first problem focuses on the arrangement of sandbags as standard protocol by safety guidelines, and the latter explores different methods for finding the area of land in connection to the injustice deeply rooted in the treatment of indigenous people. Both problems call for explicit attention to pedagogical knowledge in structuring discussions around the contextualization of the mathematical results. Our work informs teacher preparation programs for inclusion of mathematical modeling with authentic social contexts that embrace meaningful curriculum.

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MS8

Mathematics Education as a Mathematicians Research Discipline

Applied mathematicians often participate in collaborative projects with investigators from disciplines close to mathematics as well as more distant disciplines such as medicine and social sciences. In some cases the collaborators may be experimentalists or field workers who provide a complementary and synergistic approach to the mathematics. Mathematicians who are involved in the teaching and learning of mathematics at the university level develop effective teaching practices through experience. These experiences are a starting point (akin to a conjecture) that can be assessed through research studies that take into account students cognitive development, learning environments, social contexts and other factors in which mathematics educators have expertise that mathematicians typically do not. It pays off to view mathematics education as any other discipline sufficiently distant from mathematics that collaborative partnerships are necessary in order to have broad impact beyond anecdotal evidence of effective teaching. We describe collaborative projects designed to inform teacher preparation programs on ways to include mathematical modeling in their curriculum.

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MS8

Implementing Mathematical Modeling with Prospective Elementary Teachers

Over the last two decades, the mathematics education community increased research on and attention to the education of prospective teachers in mathematical modeling. Much research is devoted to better preparing future and current middle and high school teachers in teaching modeling within teacher education. Yet, standards across the United States include mathematical modeling in elementary grades. The Guidelines for Assessment and Instruction in Mathematical Modeling Education (GAIMME) report (2016) emphasizes modeling in elementary grades to help students develop skills in modeling for later grades. To better understand elementary teachers conceptions of mathematical modeling, research was conducted using mathematical modeling curricular units that were implemented in mathematics content courses for prospective elementary teachers. The curricular units emphasized the mathematical modeling process focusing on the various elements of and approaches to modeling rather than solely on the final models. In addition to student-created mod-

els and reports, questionnaires assessing conceptions and reflections on the modeling process were collected during two modeling units across the course of a semester. In this colloquium, we discuss the findings from implementing these mathematical modeling curricular units and their impact on prospective elementary teachers conceptions of mathematical modeling.

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MS9

Fourier's Heat Equation: Miniprojects for a Course in Differential Equations

It is often said that Joseph Fourier gave birth to modern climate science. His 1827 paper "Memoire sur les Temperatures du Globe Terrestre et des Espaces Planetaires" (translated to English as "On the Temperatures of the Terrestrial Sphere and Interplanetary Space" in [Pierrehumbert, 2004]) contained influential observations concerning climate and energy. Its analysis was based on mathematical results, establishing the diffusion equation, in his earlier "Analytical Theory of Heat." We present a historically based project for a course in differential equations [Monks, K. M., Fourier's Heat Equation and the Birth of Modern Climate Science, 2021. Differential Equations. 5. https://digitalcommons.ursinus.edu/triumphs_differ/5]. The goal of the project is to give the reader an insight into the techniques Fourier employed in his work in climate, as it has become the basis of modern thermodynamics and has been enormously consequential in mathematics.

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MS9

Historical Developments of ODE Techniques : The Laplace Transform

The Laplace Transform $\mathcal{L}\{f(s)\} = \int_0^\infty f(t)e^{-st}dt$ had a long and convoluted history before it arrived in the form students see in a standard Ordinary Differential Equation textbook. Indeed, Deakin in 1981 and 1982 identified over 30 well-known mathematicians that made important contributions to its development. While utilizing history and primary sources in teaching mathematics has pedagogical benefits, this history of the Laplace Transform is much too complicated to be of use in the classroom. Today, we present a simplified version that traces the history form Euler, to Laplace, and then to Oliver Heaviside and his Operational Calculus. We will present their contributions along with some historical examples, both of which can be used in an Ordinary Differential Equations course.

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MS9

Historical Experiments in a Mathematical Modeling Course

Experiments in optics and the understanding of matter have contributed to advances in mathematics. We describe historical experiments that may be replicated in classrooms as part of introductory courses in mathematical modeling.

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MS9

Historical Reflections on Teaching The Fundamental Theorems of Vector Calculus

This talk explores some history of the fundamental theorems of vector calculus, namely, Green's Theorem, Stokes' Theorem, and the divergence theorem. The historical development informs the teaching of these theorems and establishing connections to applications.

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MS10

Deconstructing Whiteness and Bias in Applied Mathematics Classrooms

The majority of applied mathematics and applied mathematics education involves some use of data. However, required courses in statistics or applied mathematics rarely focus on the ethical repercussions of using that data in a meaningful way. Inside the classroom, there is a growing need to discuss and address issues of how whiteness has influenced the development of mathematical education, models, and algorithms. By having students share their own experiences, connect the material on a personal level, and discussing the ethical considerations of presented content, we can begin to deconstruct whiteness and address bias in the mathematical content we teach as well as the data we use. This talk will primarily focus framing whiteness in applied mathematics classrooms and on practical approaches to incorporate examples, discussions, and assignments on addressing bias in data and creating a community in applied mathematics classrooms.

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MS10

A Retrospective Look at MSRIs 2021 Math and Racial Justice Workshop

The Mathematical Sciences Research Institute (MSRI) hosted the inaugural [Online] Workshop on Mathematics and Racial Justice (`https://www.msri.org/workshops/1012`) over six days in June 2021. The workshop included sessions on Bias in Algorithms and Technology; Fair Division, Allocation, and Representation; Public Health Disparities; and Racial Inequities in Mathematics Education. In this talk we will present a retrospective look back at the 2021 workshop in order to share lessons learned, to highlight and amplify its successes and to look forward to future activities that build upon this event to advance racial equity in the mathematical sciences community.

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MS10

Promoting Effective Practices in JEDI for Applied Mathematics Education

In this talk, we will share some experiences and lessons learnt from sharing best practices in JEDI for Applied Mathematics. The ideas helped identifying persistent racial injustices and inequalities in the community that have led to renewed concern and interest in addressing the need to promote JEDI in teaching, learning and research in Applied Mathematics. Thoughts and ideas evolved from collaborations with the SIAM Diversity Advisory Committee that helped to develop authentic partnership with members in the United States who were also concerned about the most impacted by the inequities caused by systemic racism. We hope to share some of the lessons learnt around systemic barriers to opportunities and benefits for students and faculty, and how these barriers impact access to, retention in, and success in Applied Mathematics Education, research, and workforce development both in Mexico and the United States.

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MS11

Quantitative Education for Life Science Undergraduates: Lessons from 40 Years of Efforts

I will summarize briefly a range of activities over the past several decades to enhance the quantitative conceptual and skill development of undergraduate life science students. These have included formal quantitative courses with emphasis on biological examples, as well as approaches that incorporate quantitative concepts within life science courses. Discussion will include a few case studies to illustrate how biological examples might enhance insight about several different areas of mathematics. I will point out the limited evidence regarding the effectiveness of examples in learning mathematical concepts, discuss progress on a BioCalculus Concept Inventory to assess student's mathematics abilities as affected by the use of real-world examples from the life sciences, and present a novel approach to the problem of prioritization of quantitative topics taking account of local faculty expectations.

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MS11

Teaching Discrete Modeling Topics First in Mathematics for the Life Sciences

In our Mathematics for the Life Sciences course, we use the Rule of Five for different learning styles to meet needs of diverse students: Symbolically, Graphically, Numerically, Verbally, Data-driven. The concepts and skills in our course help students to appreciate the components of the modeling process, including assessing hypotheses based on data, formulating a mathematical description of a system based on assumptions, and by analyzing the resulting model. We begin our course with discrete mathematics involving analyzing data and discrete time modeling, instead of starting with calculus. We have incorporated MATLAB to introduce basic computer coding and the concepts of algorithms that are applied throughout computational methods in science. We have also developed an assessment tool to begin to evaluate the impact of biological examples on mathematics comprehension in courses for life sciences majors.

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MS11

The IUSE Project: Implementing Quantitative Biology Modules Across Institutions

Calls for transforming biological curricula have spurred a flurry of activity in interdisciplinary STEM education, particularly quantitative biology. A previous HHMI-funded UMBC project developed competency-based modules to facilitate quantitative reasoning in biology courses. Increases in quantitative competencies resulted, but a discrepancy in achievement gains between direct entry and transfer students. To address this, UMBC joined with four community college partners to develop a consortium to facilitate quantitative module development in core biology courses and to facilitate large-scale implementation. Funded by an NSF IUSE grant, the consortium tracks student achievement with the intention of both mitigating the achievement gap between direct entry and transfer students, as well as understanding the effect of increased exposure to quantitative modules. Three years into the project, modules have been created, implemented and assessed across all five institutions and all four courses of the Biology core, creating a rich data set. Pre-post tests from multiple modules show significant gains in student understanding at the end of the module. We will also present data from student surveys about the modules and from a global assessment test given to students in their first course of the Biology core (at all institutions) and again to graduating seniors at UMBC. Finally, we will discuss lessons learned in this challenging, pandemic-straddling, multi-institutional project.

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MS11

Educational Frameworks for Engaging the Next Generation Workforce at the Interface of Mathematics and Biology

In this talk, we discuss some novel educational frameworks including experiential learning, inquiry-based learning, challenge based learning and interdisciplinary problem-based learning that provide the opportunity to engage students to represent, understand, analyze and solve real world problems at the interface of mathematics and biology. These approaches can help students to become life-long learners going beyond a content-based education in mathematical biology to also include a competency-based training. The talk will present examples of authentic tasks that can help to incorporate a shared collaborative experience with innovative pedagogical practices to advance teaching and learning. The session will also introduce participants to potential funding opportunities available at the interface of mathematics and biology.

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MS12

Interdisciplinary Mentoring: Mentoring Undergraduate in Biology and Mathematics on Modeling Plant-Virus-Vector Interactions

In this seminar, I will describe our two institutional mentoring approach of biology and mathematics undergraduate students. Our team consist of two groups of undergraduate students, each group had two mathematics students and one biology student with three faculty mentors from two institutions within 45 mins drive of each other. The groups were set up this way to provide the undergraduate students a first-hand overview of interdisciplinary research experience on modeling plant-virus-vector interactions. I will report how the group concept is used to support undergraduate research in mathematical biology and the mentoring challenges we experienced.

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MS12

Math-Bio Undergraduate Research in Ecology

Interdisciplinary research provides solutions to problems in multiple disciplines and can sometimes be challenging. In this talk, we will discuss two recent math-bio projects undertaken with Samford undergraduate students. The mathematics and biology students involved in these projects were able to apply the theories they learned in their classes. Also, the students developed multifaceted competency in collaborative science.

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MS13

Addressing Academic Status via Authentic Mathematical Modeling Tasks

Mathematical modeling is a process for describing the world with mathematics, as well as a practice for learning mathematics in the K-12 classroom. In this study, I implemented modeling materials from the MODULE(S)^2 Project in a senior-level content course for secondary mathematics pre-service teachers. The diversity of contexts and math concepts in the modeling tasks led to collaborative instructional practices that highlighted students' mathematical strengths and created an equitable learning environment. In particular, the authenticity of the tasks and creativity of projects allowed students to draw on their funds of knowledge and mathematical knowledge bases to decrease issues of academic status. In this presentation, I will share examples of student work to illustrate the benefits of incorporating modeling tasks in undergraduate curricula for mathematics teacher preparation.

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MS13

Math Modeling and Social Justice

In the Spring 2022 semester, the University of Utah hosted a "datathon4justice" modeled after a datathon organized by QSIDE in Fall 2021. This event gathered undergraduates interested in ways that computational methods can address social justice questions, and for many was the first time they realized such connections could be used in fruitful ways. I'll talk about the route we followed to put on this event, from QSIDE's (excellent) 2021 datathon4justice through getting support from the university through some specifics about the organization process.

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MS13

Modeling with Data: the Good, the Sparse and the Imperfect

Biological data is tremendously valuable, often difficult to obtain, sparsely sampled and imperfect. In this talk we will examine the great opportunities and challenges of working with real data in mathematical modeling.

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MS13

(Mis)Adventures in Experiential Learning: 10+ Years of Hands-On Learning in College Algebra

10+ years ago, college algebra classes at BYU-I were transformed from a traditional, lecture-based course to an experiential learning approach that relies heavily on basic mathematical modeling of real-world phenomena. I share the original vision of the course, recent changes, student

reactions and our vision for the future of the class.

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MS14

A Simiode Textbook Example: Hot Potatoes and Parameter Estimation

A modeling-driven approach to motivate the study of ODEs works best when we "close the loop' in the modeling process, by validating our model against real data. This frequently involves the estimation of unknown parameters in the ODE. We introduce this approach using data concerning the cooling of a hot potato. This data can easily be collected in the classroom and modeled with variations of Newton's Law of Cooling. The important parameters can be estimated using a least-squares approach. We also discuss the Akaike Information Criterion, a means for determining how many and which parameters can reasonably be estimated.

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MS14

Implementing SIMIODE Activities in Teaching Differential Equations

SIMIODE Modeling Scenarios and Technique Narratives, articles providing project activities and teaching guides, provide tangible connections to course content and can motivate students to learn at a deeper level. This talk focuses on the efficient implementation of two projects in a Differential Equations course from SIMIODE publications which develop and analyze mathematical models of a problem based upon known data and real-life situations. Logistical pitfalls and insights are highlighted as well as several key implementation resources. Student feedback demonstrates a positive correlation between the use of projects and an enhanced understanding of the course topics when logistical issues are reduced. Best practices learned over the years will be shared along with example student work on the projects.

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MS14

A Modern Undergraduate Experience in Modeling Differential Equations: SCUDEM

SCUDEM (SIMIODE Challenge Using Differential Equations Modeling) offers coaches, students, and judges a modern approach to teaching, learning, and mentoring, respectively, modeling differential equations. I have experienced each of these perspectives and wish to share my SCUDEM journey with you. We find that the SCUDEM challenge is both a rich undergraduate mathematical challenge outside the classroom for all students and potentially replicates how researching applied mathematics with colleagues and advisors is in graduate school as an undergraduate level experience. This presentation will introduce the SCUDEM challenge, describe a coach's experience and resources, show examples of a few student responses, and discuss the benefits of engaging in SCUDEM.

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MS14

What Does the Simiode Community of Practice Offer?

We introduce the SIMIODE (Systemic Initiative for Modeling Investigations and Opportunities with Differential Equations) community and its many features and offerings, first among them are Modeling Scenarios, teaching materials to permit faculty to support classroom endeavours in applying modeling to motivate teaching differential equations. We illustrate the offerings of SIMIODE and demonstrate the principles in several Modeling Scenarios.

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MS15

Advancing Racial Equity Through Inclusion

How can instructors encourage underrepresented students to pursue further studies in statistics? Three major pioneers in our field promoted eugenics! Even generations later, the statistics discipline can appear hostile to those who are not white and male. This talk provides three tangible ways for instructors to overcome this apparent barrier. First, formulate a course policy that - up front - explicitly recognizes past exclusions. Such a statement addresses concerns that a student may not "belong" in the field. Second, institute a practice that nurtures respect for every individual. Asking a daily question allows students to open up to their peers and provides opportunities for student validation. Third, incorporate a biographical assignment that exposes students to contributions from underrepresented individuals. Such an assignment helps students to recognize that inherent, immutable characteristics are not predictors of a successful future in statistics. Attendees will receive daily, tangible methods to enfold inclusion into their classroom and foster an environment that explicitly encourages underrepresented students. The session seeks to empower instructors - to assist them in their vital mission to ensure underrepresented students do not self-exclude from a future in the field of statistics.

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MS15

Cultivating Inclusion Through Broader Engagement at SIAM Conferences (be@siam)

Racial equity in applied mathematics requires an understanding of the forces which have resulted in inequity as well as techniques to transform curriculum, policies, practices, and the community. Inclusion is an essential ingredient in advancing racial equity in applied mathematics. The Broader Engagement program at the SIAM Computational Science and Engineering conferences has been an effort to increase the participation of students and professionals from underrepresented groups in the society as well as catalyze the normalization of inclusion by engaging, educating, and including the broader community. In

this session, we will review the approach, components, and reflections from BE@CSE programs beginning in 2015.

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MS15

Panel: How Can We Advance Racial Equity in the Applied Mathematics Commuinity?

The final event in the minisymposium on advancing racial equity in the applied mathematics community will be an opportunity for the organizers and speakers in the two sessions to dialogue with each other and the broader community about concrete steps that can be taken to advance racial equity in the mathematical sciences. This panel will be online and accessible to all registered attendees of AN22 and ED22.

TBA TBA
na
na

MS15

Using Place-Based Education in Precalculus

Indigenous cultures have been using mathematics in their lives for generations. In this talk, we present methods of using place-based examples in a precalculus classroom using Native Hawaiian culture. Through these examples, we hope to increase student participation in the classroom from both Indigenous and non-Indigenous students as well as spread awareness of various cultures.

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MS16

Research with First-Year STEM Students

Motivated by evidence correlating undergraduate research (UR) with better retention and engagement, Northern Kentucky University facilitates two programs that provide first-year students with UR opportunities in STEM. In this talk, we discuss math-focused UR for students in these programs. The UR-STEM program provides summer UR opportunities for students early in their college careers. Initiated with NSF funds and now sustained through NKUs Center for Integrative Natural Science and Mathematics, the paid UR program utilizes an open application and prioritized selection model to include students at-risk of leaving a STEM major. Data from 2017-2021 indicates student participants have been retained at significantly higher levels than non-participants (94% in STEM major, 98% at NKU). Supported by NSF funds, the STEM Ready program seeks to improve mathematics preparation and retention of students interested in STEM. During the two-week summer bridge program, STEM Ready participants complete three guided UR projects: one in biology, chemistry, and data science. Preliminary data suggest participants benefit from the program. The cumulative GPA and grades in participants first math course for the summer 2020 cohort (N=22; 50% PEERs, first-generation, and low-income; ACT mean 22.2, median 23) were equivalent to other first-year STEM majors (ACT mean 24.6, median 25) and their retention at NKU into spring semester was slightly higher (91% vs 77%).

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MS16

Research from the Sidelines with Sports Analytics

Sports analytics has gathered tremendous momentum as one of the most dynamic fields. Diving deep into the numbers of sports can be game changing or a framework for data analytics research. What questions can be explored? What actionable insights can be gleaned for teams? From March Madness to national media broadcasts, analytics are becoming increasingly indispensable. Dr. Tim Chartier will discuss outlooks that help with successful analytics, and the variety of questions that can be tackled. He will also share how he leads students to dig into sports using math and computer science, and their success across the NBA, NFL, NASCAR, ESPN and his own college teams.

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MS16

Bridging the Gap Between High School and Undergraduate Mathematics by Exploring Problems in Ecological Modeling: Training Tomorrows Leaders in Stem Mentorship

Training and appreciation of quantitative sciences in both high school and undergraduate biology and ecology is lacking, but this type of training is crucial to collecting and using data to fully understand how such systems behave. I will discuss a project for which I have incorporated predictive modeling into high school summer curriculum on watershed management/environmental science, where undergraduates outside mathematics (from fields such as biology, environmental science, psychology, and data science) were recruited as program mentors - the idea being to develop a trained workforce through a feedback mechanism where trainees become trainers. The program, Project WHIRL (Protectors of the Watershed in the Indian River Lakes), originally run as a volunteer program established in 2019 by the Indian River Lakes Conservancy (Upstate NY). In the pilot 2021 program, high school students collected field data from local lakes and input these into a predictive model that tested weevils' efficacy (a biocontrol) at reducing a local invasive aquatic, Eurasian Watermilfoil. Students learned how to collect field data, clean and analyze data in excel, the basics of supervised machine learning (how the model was developed by my team), and how to use predictive modeling to make predictions of biocontrol success. I will discuss the overall theme of the project, its results, and its success in initiating training of a skilled workforce in both quantitative fields and watershed management.

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MS17

Enhancing Student Learning Through Projects and

Presentations in a Mathematical Modeling Class

Classes such as *Mathematical Modeling* and *Nonlinear Dynamics* offer unique opportunities to enhance student learning through group or individual projects. When I first included student projects in these classes I was anxious about whether students learning and interest in the material would decline. I was also concerned with student motivation and work quality without the more regular and standardized homework and exams. On the contrary, I have found students worked much harder and seemed to master the material involved in their project at a deeper level than they did with homework or exam questions. Additionally, both in conversation with me and in their course evaluations, a large majority of students commented on how much they enjoyed and learned from their projects. Several of these students mentioned that they wish they had more time for their projects. In this talk, I discuss the guidance I give and the structure I provide students for their project. I also focus on what I have learned and changed over the last few years of assigning student projects.

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MS17

Walking in Brunelleschis Footsteps

The dome of the Cathedral of Florence is designed as the upper halves of four intersecting cylinders. It was engineered by Filippo Brunelleschi and completed in 1436. Before modern construction techniques, it was the largest dome in the world and remains the largest brick dome in the world today. In this Calculus project, students extend the techniques of calculating volumes of solids of revolution as well as arc length and surface area. They begin by first calculating the volume of a Roman Vault, a structure designed as two intersecting cylinders. Students then calculate the volume of the inner dome of the Cathedral of Florence by developing an appropriate integral and evaluating it. They also calculate the arc length of the cylinder intersections of the cathedral dome. Once the computations are complete, students present their findings with posters in groups. This project encourages students not only to work collaboratively on an application of what they learned in class, but also to practice their soft skills of communicating their findings in an engaging and visually appealing manner.

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MS17

Laboratory Modules for Numerical Methods

Education research has suggested that students who receive a wider variety of sensory inputs during the learning process will be able to make more connections and more deeply understand course content. To this end, three laboratory learning modules were designed for a numerical methods course to help students develop intuition for physical systems, to allow for a comparison of real data against numerical solutions of physics equations, and to increase student engagement. These modules were designed to reinforce specific topics covered in the numerical methods curriculum, including numerical differentiation and numerical solution of ordinary differential equations (ODEs) and partial differential equations (PDEs). In this talk I will discuss our development and implementation of these modules.

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MS17

Building Mathematical and Scientific Communication Skills in Statistics Using Projects

Careful written and verbal communication is of critical importance in the field of statistics. Unlike mathematical proof-writing, the audience for writing about statistics may frequently have little experience with the formal mathematics underlying the results. Thus, being able to carefully and accurately explain statistical conclusions to a non-expert audience is a necessary skill for students to develop. This is not a skill that they are frequently asked to practice. Long-term projects give students a chance to dedicate time to this valuable skill. In this talk, I present several projects that aim to develop these skills at the introductory, intermediate, and advanced levels. At the introductory level, long-term projects give students time to write extensively about mathematics, which might be a new experience for them. At the intermediate level, students practice writing and presenting in the forms expected for scientific communication. At the advanced level, students continue to refine their scientific writing and presenting, but also are pushed to practice explaining statistical ideas to other audiences, for example with "popular science' articles. I will share resources and rubrics related to these projects, as well as my reflections on them.

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MS18

Role of Guided Reflections in Teaching Proofs

An interventional course in Introduction to Mathematical Reasoning was developed to mitigate the difficulty of learning to write proofs in a content-based upper level math course. As part of the interventional course, enrolled students were asked to write weekly self-reflections guided by the mechanical, structural, creative, and critical modalities of thinking in proof writing. We categorized the quality of the students responses, and within each category calculated average course grades in the interventional course, the prerequisite math course, and the advanced core course. Results demonstrated that high quality self-reflection responses were significant predictors of higher average course grades in the interventional course and the advanced course, but not in the prerequisite course. When reflecting on their mastery of the modalities on a rubric-based Likert scale, students self-reported scores approached those of an expert graders over the duration of the semester. The resulting correlation suggests that repeated exposure to guided-self-reflection may support growth in students awareness of their own abilities pertaining to proof writing using the lens of the modalities. Together, these results support the potential power of repeated, modality-based self-reflections as a strategy to improve student outcomes in future advanced math courses.

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MS18

Investigating Explanation in Proof-Based Mathematics

Proof has several roles in mathematical practice and in the mathematics classroom. One of those roles is to explain why a given proposition holds (as opposed to, for example, demonstrating that it does). Indeed, explanation is a particularly important role of proof in the mathematics classroom, but not one that it always fulfills. Philosophers of mathematics and mathematics educators have struggled for decades to identify what makes a proof explanatory, or what makes a proof of a given proposition more explanatory than another one. While there have been promising, recent developments in this area, explicit criteria for what makes a proof (more or less) explanatory are still being debated. In this presentation, I illustrate a novel empirical approach to investigating the notion of explanation in proof-based mathematics. In particular, I report on a couple of studies aimed at investigating the extent to which mathematicians and undergraduate students share a notion of explanatoriness in proof-based mathematics (both among and between themselves). Results from these studies suggest this is a fruitful approach for studying what makes a proof (more or less) explanatory in mathematics.

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MS18

Teaching and Operationalizing Authentic Proof-Based Activity in the University Classroom

Educators often advocate for students to engage in authentic mathematical activity. However, we have found that such activity has not yet been operationalized to allow for meaningful analysis of student activity in proof-based courses. As part of a larger research project, we developed the Authentic Mathematical Proof Activity (AMPA) framework to both operationalize the nature of this activity and to address the ways in which student activity may be more or less authentic. Leveraging the extant literature on how research mathematicians go about their work, we identify a set of tools and motives that characterize the reported proof-related activities. Further, we document classroom activity from an authentic-to-the-disciplinary perspective (accounting for the variety, complexity, and accuracy of tool use) and an authentic-to-the-student perspective (accounting for who has agency in generating tools, authority to evaluate contributions, and whose contributions are taken up). Using data from a design-based research project focused on undergraduate abstract algebra, we illustrate the utility of the AMPA framework. In particular, we share evidence of ways that students engage in authentic mathematical proof activity, as well as the ways that tensions between disciplinary and student authenticity shape activity.

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MS18

Proof Comprehension: What Does It Mean to Understand a Proof and How Can This Understanding Be Measured?

We first describe the development of a model of proof comprehension through interviews with mathematicians. We use this to highlight different ways in which a proof can be understood. We then describe the development and validation of proof comprehension tests. We argue that we have 12 item multiple choice proof comprehension tests that can validly and reliably measure students' ability to understand proofs. Finally, we use these instruments to show proof comprehension is predictive of students' academic performance in proof-oriented mathematics courses, even when factors such as math SATs and grades in prior mathematics courses are accounted for.

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MT1

Introduction to Comaps Certificate in Modeling (CiM) Program for Educators Part I of II

During this workshop, we will introduce participants to the CiM program as well as the opportunity to obtain the Modeling Educator Certificate (MEC). Workshop participants will participate in two hour-long sessions where COMAP will expose participants to the material contained within the first two modules of the Modeling for Education course. During module 1, participants will trace a bit of history of educational practices from traditional/computational (#1-15 odd), to "word" problems, to applied problem solving, to "modeling problem." After completing module 1, every participant will have a better understanding of the philosophy of teaching/learning and framework for applied problem solving and modeling. During module 2, participants will explore a Showcase of (Modeling) Examples to learn how to expose students to various fields, levels of solutions, and types of mathematics involved. In addition to being exposed to the course in-class activities, workshop participants will also experience some of the pre- and post-class activities planned as part of the program. Following the completion of module 2, the workshop will conclude with a discussion about the workshop experience and opportunity to obtain the modeling certificate.

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MT2

Introduction to Comaps Certificate in Modeling (CiM) Program for Educators Part II of II

During this workshop, we will introduce participants to the CiM program as well as the opportunity to obtain the Modeling Educator Certificate (MEC). Workshop participants will participate in two hour-long sessions where COMAP will expose participants to the material contained within the first two modules of the Modeling for Education course. During module 1, participants will trace a bit of history of

educational practices from traditional/computational (#1-15 odd), to "word" problems, to applied problem solving, to "modeling problem." After completing module 1, every participant will have a better understanding of the philosophy of teaching/learning and framework for applied problem solving and modeling. During module 2, participants will explore a Showcase of (Modeling) Examples to learn how to expose students to various fields, levels of solutions, and types of mathematics involved. In addition to being exposed to the course in-class activities, workshop participants will also experience some of the pre- and post-class activities planned as part of the program. Following the completion of module 2, the workshop will conclude with a discussion about the workshop experience and opportunity to obtain the modeling certificate.

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SIAM Conference on the Life Sciences (LS22)

July 11–14, 2022

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IP1

Opening Remarks and Presentation: Multi-scale Modeling can Unravel Mysteries about the Immune Response and Treatment in Tuberculosis

Tuberculosis (TB), caused by infection with Mycobacterium tuberculosis (Mtb), is one of the worlds deadliest infectious diseases and remains a significant global health burden even in the face of COVID. TB disease and pathology presents clinically across a spectrum of outcomes, ranging from total sterilization of infection to active disease. Much remains unknown about the immunobiology that drives an individual towards various clinical outcomes as it is challenging to experimentally address specific mechanisms driving outcomes. Furthermore, it is unknown whether numbers of immune cells in the blood accurately reflect ongoing events during infection within human lungs. We have utilized a myriad of multi-scale approaches and analyses to study the host immune response to Mtb across multiple physiologic and time scales. The models we developed range from molecular scale to whole-host scale and we used a hybrid approach combining differential equations and agent-based modeling at multiple scales. We use extensive analyses to predict mechanisms in the system driving different outcomes via parameters. Additionally, a key goal is to improve antibiotic treatment for TB. Currently multiple drugs are used simultaneously over a 6-9 month period which is a burden on the patient and medical system. We use our models to predict regimens that can improve clinical treatment of TB.

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IP2

Mathematical-based Microbiome Analytics for Clinical Translation

Traditionally, human microbiology has been based on laboratory focused cultures of microbes isolated from human specimens in patients with acute or chronic infection. These approaches primarily view human disease through the lens of a single species and its relevant clinical setting however such approaches fail to account for the surrounding environment and wide microbial diversity that exists in vivo. Given the emergence of next generation sequencing technologies and advancing bioinformatic pipelines, researchers now have unprecedented capabilities to characterise the human microbiome in terms of its taxonomy, function, antibiotic resistance and even bacteriophages. Despite this, an analysis of microbial communities has largely been restricted to ordination, ecological measures, and discriminant taxa analysis. This is predominantly due to a lack of suitable computational tools to facilitate microbiome analytics. In this talk I will introduce the available and emerging analytical techniques including integrative analysis, microbial association networks, topological data analysis (TDA) and mathematical modelling. I will then present our recently developed approach to the multi-biome that integrates bacterial, viral, and fungal communities in the context of several clinically relevant applications to patients with bronchiectasis.

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IP3

Data-driven Mathematical Models for Malaria Response

The effect of malaria on the developing world is devastating. Each year there are more than 200 million cases and over 400,000 deaths, with children under the age of five the most vulnerable. Ambitious malaria elimination targets have been set by the World Health Organization for 2030. These involve the elimination of the disease in at least 35 countries. However, these malaria elimination targets rest precariously on being able to treat the disease appropriately; a difficult feat with the emergence and spread of antimalarial drug resistance. In this talk, I will introduce several statistical and mathematical models that can be used to monitor malaria transmission and to support malaria elimination. For example, Ill present statistical models that allow the emergence and spread of antimalarial drug resistance to be monitored, mechanistic models that capture the role of bioclimatic factors on the risk of malaria and optimal geospatial sampling schemes for future malaria surveillance. I will discuss how the results of these models have been used to update public health policy and support ongoing malaria elimination efforts.

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IP4

Leader, Follower, and Intermediate: Modeling Collective Cancer Invasion

A major reason for cancer treatment failure and disease progression is the heterogeneous composition of tumor cells at the genetic, epigenetic, and phenotypic levels. While tremendous efforts have tried to characterize the makeups of single cells, much less is known about interactions between heterogeneous cancer cells and between cancer cells and the microenvironment in the context of cancer invasion. Clinical studies show that cancer invasion predominantly occurs via collective invasion packs, which invade more aggressively and result in worse outcomes. In vitro non-small cell lung cancer spheroid experiments show that the invasion packs consist of leaders and followers and that leaders and followers engage in mutualistic social interactions during collective invasion. Many fundamental questions remain: What is the division of labor within the heterogeneous invasion pack? How does the leader phenotype emerge? Are phenotypes plastic? How does the invasion pack interact with the stroma? Can the social interaction network be exploited to devise novel treatment strategies? I will present the recent experimental and modeling efforts that try to address these questions. I will try to convince you that analyzing this social interaction network can potentially reveal the weak-links, which when perturbed can disrupt collective invasion and potentially prevent malignant progression of cancer.

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IP5

The Noisy Homunculus

There are two defining features of cortical activity. First, neuronal population response to a sensory stimulus or motor action is complex and diverse, with neurons showing very heterogeneous activity. Second, neurons are notoriously unreliable, where the trial-to-trial responses of populations of neurons are exceedingly variable. In this talk I will outline modeling and analysis from my group that argues that both of these features arise from the known structure of synaptic wiring in cortical circuits. We will explore how the spatial and temporal wiring of strongly coupled recurrent networks of excitatory and inhibitory neurons can produce emergent low dimensional population-wide variability that captures the salient features of real neuronal response. Our general modeling approach has given insights into: how subject attention shifts population responses, the propagation and communication of activity across layers of neurons, the learning of attractor dynamics in neuronal circuits, the distribution of stimulus tuning in early visual areas, and how the brain does inference in complex sensory worlds.

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IP6

Data Driven Uncertainty Quantification, Validation, and Credibility of Multiscale Models of Cardiac Electrophysiology

Cardiac electrophysiological (CEP) action potential cell models have been enormously successful as a scientific tool to develop and test mechanistic hypotheses. CEP models are now being used in safety-critical clinical applications which require rigorous validation and credibility assessment for their context of use. Incorporating experimental uncertainty in cell simulations results in a variety of action potential behavior including: normal repolarization (NR) and abnormal oscillations and/or failure to repolarize. How this cellular uncertainty affects action potential spatial heterogeneity and behavior in tissue is unknown but very important. Here simulations are used to study the impact of cellular coupling. Uncertainty data was extracted from 16 studies and incorporated into all repolarization parameters in the context of 8 transmembrane current submodels. The method of pooled variance was used to incorporate uncertainty from multiple studies. In control cells (C), 26% exhibited abnormal behavior and this number increased to 71% when an important potassium current was blocked (B). Results from one- and two-dimensional simulations for both C and B will be presented in which the coupling strength is varied. Surprisingly the cellular abnormalities that occur when experimental data uncertainty is incorporated into simulations does NOT translate into unphysiological behavior in simulations in tissue for both C and B.

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IP7

Closing Remarks and Presentation: The Geometry of Decision-Making

A central challenge for animals when alone, or when grouping with others, is deciding where to go. Running, swimming, or flying through the world, animals are constantly making decisions while on the movedecisions that allow them to choose where to eat, where to hide, and with whom to associate. Despite this most studies have considered only on the outcome of, and time taken to make, decisions. Motion is, however, crucial in terms of how space is represented by organisms during spatial decision-making. Employing a range of new technologies, including automated tracking, computational reconstruction of sensory information, and immersive holographic virtual reality (VR) for animals, experiments with fruit flies, locusts and zebrafish (representing aerial, terrestrial and aquatic locomotion, respectively), I will demonstrate that this time-varying representation results in the emergence of new and fundamental geometric principles that considerably impact decision-making. Specifically, we find that the brain spontaneously reduces multi-choice decisions into a series of abrupt (critical) binary decisions in space-time, a process that repeats until only one optionthe one ultimately selected by the individualremains. Due to the critical nature of these transitions (and the corresponding increase in susceptibility) even noisy brains are extremely sensitive to very small differences between remaining options (e.g., a very small difference in neuronal activity being in favor of one option) near these locations in space-time. This mechanism facilitates highly effective decision-making, and is shown to be robust both to the number of options available, and to context, such as whether options are static (e.g. refuges) or mobile (e.g. other animals). In addition, we find evidence that the same geometric principles of decision-making occur across scales of biological organisation, from neural dynamics to animal collectives, suggesting they are fundamental features of spatiotemporal computation.

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SP1

Activity Group on the Life Sciences Early Career Prize Lecture - Model Order Reduction of Limit Cycle Oscillators Far Beyond the Weakly Perturbed Limit

In the decades since Art Winfrees pioneering work on phase models for nonlinear, high-dimensional oscillators, the overwhelming majority of theoretical analysis in this field has been performed in the weakly perturbed limit. Comparatively very little is understood about limit cycle oscillators in response to arbitrary, strong perturbations, mostly due to the lack of viable reduction strategies for considering large magnitude inputs. In this presentation, I will discuss recent work that uses isostable coordinates, which characterize level sets of the slowest decaying eigenmodes of the Koopman operator, in conjunction with phase-based techniques to yield analytically tractable reduced order models that are valid in the strongly perturbed regime. Applications involving phase resetting of circadian rhythms following rapid travel across multiple time zones, elimination of a cardiac arrhythmia that represents a precursor to cardiac arrest, and phase locking of neural rhythms in response to strong synaptic coupling illustrate the utility of these new methods in situations where standard, phase-only techniques fail. Data-driven methods for inference of phase-isostable-based models will also be dis-

cussed for use when the underlying dynamical equations are unknown or unavailable.

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JP1

Joint Plenary Speaker with the 2022 SIAM Annual Meeting (AN22): Machine Learning and Sparse Modeling for Scientific Discovery, with Examples in Fluid Mechanics

Accurate and efficient reduced-order models are essential to understand, predict, estimate, and control complex, multiscale, and nonlinear dynamical systems. These models should ideally be generalizable, interpretable, and based on limited training data. This work describes how machine learning may be used to develop accurate and efficient nonlinear dynamical systems models for complex natural and engineered systems. We explore the sparse identification of nonlinear dynamics (SINDy) algorithm, which identifies a minimal dynamical system model that balances model complexity with accuracy, avoiding overfitting. This approach tends to promote models that are interpretable and generalizable, capturing the essential physics of the system. We also discuss the importance of learning effective coordinate systems in which the dynamics may be expected to be sparse. This sparse modeling approach will be demonstrated on a range of challenging modeling problems, for example in fluid dynamics, and we will discuss how to incorporate these models into existing model-based control efforts.

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CP1

Modeling the Effects of Shed Targets on Efficacy of Immunotherapies

The therapeutic efficacy of cancer cell surface targeting antibodies can be affected by shedding of target cancer cell surface molecules which can escape targeted treatment by lowering the expression of target but also producing soluble targets that reduce the levels of free drug. The net effect of target shedding on drug efficacy is a complex interplay of several dynamical processes: a) the kinetics of drug action in lysis and hence removal of source of soluble targets, b) the drug pharmacokinetics, and c) the feedback loops that can dynamically affect target shedding rates. We investigate this interplay between drug and target using mechanistic mathematical models for both liquid and solid tumors. We showcase our modeling framework and analysis of the resulting dynamical system which explicitly tracks the distribution of the drug, the interaction of the drug with shed targets, the modulation of shedding by the drug, and the lysis of tumor cells in the presence of free drug. We also provide a proof that the fixed point in the two-compartment model of liquid tumors is a global attractor. Our research provides a theoretical platform for investigating the complex interactions of tumor growth, target shedding, and drug pharmacokinetics, and can be useful to understand the effects of shed target on the efficacy of immunotherapies and support dose optimization.

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CP1

Using the Inflection Point of the Verhulst Model to Predict Pregnancy Complications

Currently, pregnancy complications are detected after it is too late to turn the course of the pregnancy. This is because imaging of the fetus is ineffective using ultrasounds and no model effectively predicts adverse pregnancy outcomes based on placental ultrasound images. Nevertheless, ultrasounds have been deemed effective in imaging circular objects such as the placenta. Given ultrasound compatibility with the placenta and the modern correlation of fetal growth restriction with pregnancy complications, the Verhulst model was developed to track placental growth. This model exhibits placental volume as a function of time. The solution of the Verhulst model contains an inflection point. This inflection point could potentially give insight into the outcome of a pregnancy. I will use past pregnancy data to fit and analyze this model along with the resultant inflection points and will present my results. This information has a high potential to allow for early opportunities to predict adverse fetal-maternal outcomes.

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CP1

Mathematical Model of Triple-Negative Breast Cancer in Response to Doxorubicin and Paclitaxel

Triple-negative breast cancer (TNBC) is a heterogenous disease that is defined by its lack of estrogen hormone, progesterone hormone and human epidermal growth factor receptor 2 (HER2). The lack of receptors frequently results in poorer outcomes, higher rates of metastasis and recurrence since there are no viable targeted therapies. Combination chemotherapy treatments, radiation therapies, and surgery are the current standard-of-care for TNBC. We have built an ordinary differential equation model of TNBC and its response to a combination of chemotherapies, doxorubicin (DRB) and paclitaxel (PTX). This model was parameterized to longitudinal tumor volume and proliferation data, then validated using percent necrosis data for both

a human cancer mouse model (MDA-MB-231) as well as a syngeneic, mammary carcinoma (4T1) mouse model. This novel mathematical model can give insight to the ordering, dosing, and timing of DRB and PTX treatment. More importantly, this model can also give insight to vital immunotherapies for TNBC, that we would not otherwise receive, due to its calibration to the syngeneic, mammary carcinoma (4T1) mouse model.

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CP1

How Multiscale Modeling Can Help Us Understand Pots

Postural Orthostatic Tachycardia Syndrome (POTS) is characterized by an increase of heart rate of 30 beats per minute (40 bpm in patients aged 12-19 years) upon a postural change, combined with the presence of orthostatic symptoms. In addition to these criteria, recent studies have shown that POTS patients exhibit large low frequency 0.1 Hz heart rate and blood pressure oscillations upon a postural change when compared to control subjects. Moreover, several studies have hypothesized that POTS patients express autoantibodies binding to $\beta_{1,2}$ and M_2 receptors. These receptors are abundant on the sinoatrial node, while α_1 receptors are associated with smooth muscle cells. This study uses mathematical modeling to test if subjects expressing these antibodies experience augmented 0.1 Hz oscillations. To do so, we develop a multiscale model using a systems level five-compartment cardiovascular model, a baroreflex control regulating heart rate, cardiac contractility, and vascular resistance in response to changes in blood pressure. Specific attention is paid to the control of heart rate achieved by adding a sinoatrial node cell model. We demonstrate that by changing receptor sensitivity we can predict 0.1 Hz oscillations in POTS patients, Finally, we show that by varying system level model parameters we can simulate characteristic POTS phenotypes and study effects of POTS in patients with low blood volume, known to have more severe POTS symptoms.

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CP1

Quantifying Chaos in Experimental Cardiac Tissue Under Fast Periodic Stimuli; Leading Lyapunov Exponent and Unstable Periodic Orbits Including Period Three

Cardiac tissue is modeled as a nonlinear system that can exhibit chaotic dynamics. However, little experimental evidence has been collected to verify these dynamics. This study aims to both quantify and qualify the chaotic nature of cardiac tissue from a cardiac systems electrical response to a range of periodic forcing signals including high frequencies which emulate arrhythmias. Tissue response was recorded as the voltage signal from a single cell within a frog ventricle. The resulting action potential durations (APDs) were measured as a time series for analysis with Lyapunov exponents. Results have shown to give negative Lyapunov exponents for forcing frequencies around APD bifurcation events and positive exponents during complex response. In addition, stable period-three orbits, and several unstable periodic orbits of APDs were identified during the complex response, further suggesting that the tissue response is not random but in fact chaotic. This will facilitate the development of methods to control and terminate arrhythmias.

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CP2

Modeling Transcatheter Aortic Valve Replacement (TAVR): A Fluid-Structure Interaction Model

Transcatheter aortic valve replacement (TAVR) is the implantation of an artificial heart valve that is mounted on a stent, which is crimped in a catheter and guided through the patients arteries to the heart without an open-heart surgery. Computer modeling and simulation (CMS) is an emerging tool in the process of TAVR device design, regulatory approval, and indication in the care of specific patients, since there are still many open questions surround-

ing post-implantation complications. This talk will present a computational fluid-structure interaction (FSI) model of Medtronics *CoreValve Evolut R* TAVR device based on a hyperelastic finite element extension of the immersed boundary (IB) method. We then perform dynamic simulations of crimping and deployment of the CoreValve, as well as device behavior across the cardiac cycle in a patient-specific aortic root geometry reconstructed from CT image data of a patient at UNC hospital. We will demonstrate that our CoreValve model behaves realistically under physiological in vivo simulation conditions. All simulations are conducted in IBAMR, which is an open-source software developed and maintained by Boyce Griffiths Cardiovascular Modeling and Simulation laboratory at UNC Chapel Hill.

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CP2

Regularized Stokeslets Inside Spherical Geometries

We formulate a general mapping from singular image systems to regularized image systems for use with the method of regularized Stokeslets and apply it to biologically relevant flows within a fluid-filled, spherical cavity. The method of regularized Stokeslets has been heavily applied to micro-scale biofluids problems such as microorgianism locomotion. It is based on the boundary integral form of the Stokes equations where the singular fundamental solution (the "Stokeslet") is replaced with a smooth approximation. The method can be modified such that certain boundary conditions are satisfied automatically via the addition of an appropriate "image system" to the regularized Stokeslet. Here, we focus on the computation of fluid flows due to distributions of forces within a fluid-filled, spherical cavity because no regularized image system has been derived for this specific setting and because of its importance to flows driven by active structures within cells. We present two example problems in this context: the flow due to a translating particle and the flow due to a relaxing flexible filament contained in the cavity.

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CP2

Dynamics of Microtubule, Intracellular Fluid Interaction with Microtubule (de)Polymerization

During mitosis, ordinary cells with extra centrosomes fail to divide; however, cancer cells retain the ability to divide despite having supernumerary centrosomes. The clustering and movement of centrosomes can determine the viability of such cells. Existing force-balance models track the dynamics of centrosome movement, but they naively account for the fluid-structure interaction between organelles and extracellular fluid. The interaction of microtubules with centrosomes and other cellular structures is one of the main factors driving centrosome movement. This includes microtubule (de)polymerization, the interaction between individual microtubules and the interaction of microtubules with the cellular membrane or organelles. Thus, we are interested in modeling microtubule dynamics and the microtubule-fluid interaction. Using a Kirchhoff rod model and the method of regularized Stokeslets, we contribute a model of microtubule (de)polymerization. We also present a preliminary examination of the interaction between several microtubules, and the drag of a centrosome with attached microtubules in free space.

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CP2

Mathematical Modeling of Aqueous Humor Production in the Eye and Its Implication on Drug Therapies for Glaucomatous Patients

Glaucoma is a severe neuropathology of the eye representing the second major cause of blindness worldwide. Elevated value of intraocular pressure (IOP) is the established risk factor and is determined by the balance between production and drainage of aqueous humor (AH), a watery transparent fluid including electrolytes and low protein concentration. Reducing AH production (AHP) is one approach to reduce IOP. Herein we develop a mathematical model of AHP based on a lumped version of the 3D Velocity-Extended Poisson-Nernst-Planck differential system in stationary conditions. Model variables represent the compartment values of electric potential, ion molar densities and AH fluid pressure and are numerically determined by a fixed-point iteration designed to prevent spurious oscillations and negative ion concentrations. The proposed formulation is employed as a virtual laboratory to investigate the quantitative impact of Na+/K+ pump on AHP. Model predictions indicate that AHP reduction is maximal for intermediate levels of pump activity whereas a larger inhibition of ATPase activity does not significantly reduce AHP. These results demonstrate a non-linear relationship of ATPase to AHP and demonstrate how mathematical virtual laboratories may assist in best practices for design of IOP lowering medications.

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CP2

Biomechanics of Neural Tube Folding

Epithelial tubes are key building blocks of life, yet their morphogenesis is poorly understood. A particularly important example is the neural tube, a precursor for the central nervous system. Given the severe medical consequences of neural tube defects, which affect approximately 1:1000 births, it is pivotal to understand the biomechanics of mammalian spinal neurulation. The folding neural tube shows a transition from medial to dorsolateral bending sites ("hingepoints") along the embryo's body axis. These hingepoints are commonly considered active driving forces in neural tube closure, although the causation remains largely unclear. In this presentation, I will show how a recently developed biomechanical model has flipped this view upside down. In computer simulations combining mesoderm expansion, non-neural ectoderm expansion, zippering, and neural plate adhesion to the notochord, hingepoints emerge as passive mechanical byproducts in response to neural-plate-extrinsic forces. Our simulations are based on tissue dimensions measured in mouse and human, and recapitulate the different folding modes along the embryo's body axis, explaining their morphogenesis from a new perspective.

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CP3

A Second-Order Positive and Elementary Stable Nonstandard Numerical Method with Applications to a Chemostat Model

Nonstandard finite difference (NSFD) methods have been widely used to numerically solve various problems in biology, as they preserve many of the essential properties of the solutions of differential equations with no restriction on the time-step size. However, most NSFD methods developed to date are only of first-order accuracy. In this talk, we discuss the construction and analysis of a new second-order modified NSFD method for a chemostat model with microbial input and constant death rate. The proposed numerical method not only preserves the positivity of solutions and the local stability properties of equilibria, but is also of second-order accuracy. Numerical simulations are presented to support the theoretical results.

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CP3

The Shape of Aroma: Measuring and Modeling Citrus Oil Gland Distribution

From preventing scurvy to being part of religious rituals, citrus are intrinsically connected to human health and perception. From tiny mandarins to head-sized pummelos, citrus capability of hybridization provides a vastly diverse array of fruit sizes and shapes, which in turn corresponds to a diversity of flavors and aromas. These sensory qualities are tightly linked to oil glands in the citrus skin. The oil glands are also key to understanding fruit development, and the essential oils contained by them are fundamental in the food and perfume industries. We study the shape of citrus based on 3D X-ray CT scan reconstruction of 163 different citrus samples comprising 58 different species and cultivars, including samples of all fundamental citrus species. First, using the power of X-rays and image processing, we are able to compare and contrast size ratios between different tissues, such as the size of the skin compared to the rind or the flesh. Second, we model the fruit shape as an ellipsoidal surface, and later we study and infer possible oil gland distributions on this surface using principles of directional statistics. We finally compare and contrast these overall fruit shape models along their gland distributions across different citrus species. This morphological modeling will allow us later to link genotype with phenotype, furthering our insight on how the physical shape is genetically specified in DNA.

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CP3

Effect of Eye Deformations on Contact Lenses Comfort

About one in ten Americans wears contact lenses. The main reasons individuals stop using contact lenses are discomfort and dryness. To understand what makes contact lenses comfortable or not, it is essential to understand the interaction between the contact lens and the eye. We propose a mathematical model of the interaction between the contact lens and the eye that accounts for the deformability of the eye. The lens is modeled as a thin, axially symmetric, soft hydrogel contact lens that conforms to the

eye shape. The eye is model as a homogenous, isotropic, axially symmetric, linear elastic material. The eye and the lens are coupled via the non-linear suction pressure under the lens. The model is used to investigate the effect of eye deformability on the lens suction pressure by comparison to the rigid eye case for different lens shapes.

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CP3

Optimal Entrainment of Pinned Spiral Waves

Cardiac fibrillation is caused by self-sustaining spiral waves that occur in the myocardium, some of which can be pinned to heterogeneities such as blood vessels in tissue. These pinned spirals are a hinderance to the development of low energy methods for cardiac defibrillation; a small electrical voltage gradient applied across the heart is sufficient to unpin and eliminate these spirals, but only if it is applied at the correct phase which forms a unpinning window. When multiple pinned spirals exist these unpinning windows do not generally overlap. Using phase-based reduction techniques, we apply tools from control theory to design an energy optimal, externally applied voltage gradient to entrain a heterogeneous collection of pinned spirals. When the phases overlap they can be simultaneously unpinned by applying an external voltage gradient pulse at an appropriate moment. Numerical validation of this novel approach is also presented using bidomain model simulations. This method explicitly incorporates heterogeneity in the problem formulation and is guaranteed to entrain the spirals provided their phase response curves and nominal unperturbed frequencies fall within some prespecified window. Additionally, it requires no real-time feedback about the system state.

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CP3

Mathematical Modeling of TFPI Inhibition in Coagulation

Blood coagulation is a complex network of biochemical reactions necessary to form a blood clot. The process occurs in three stages (initiation, amplification propagation) in the presence of flow. Inhibition occurs at each stage to avoid over-clotting. Initiation in the tissue factor pathway begins when clotting factor VIIa in the plasma binds its cofactor, tissue factor (TF) forming an active enzyme complex (TF:VIIa). Next, clotting factor X in the plasma binds with TF:VIIa and is enzymatically cleaved into activated factor X (Xa). Xa is required for other reactions as coagulation progresses. Tissue factor pathway inhibitor (TFPI) is known to be a strong inhibitor during initiation, with the primary mechanism of binding to Xa in the plasma and then rebinding to TF:VIIa to form the quaternary complex TF:VIIa:TFPI:Xa. However, previous mathematical models show that flow itself is a more important inhibitor than TFPI. In this study, we re-investigate TFPI inhibition with and without the presence of flow. We consider previous static experimental studies of TFPI, where additional inhibitory reactions were suggested to be at play. We use mathematical models and constrained optimization to fit the new reaction schemes to multiple sets of data simultaneously. We find the new scheme for TFPI better fits the experimental data. Then, we put these new schemes into a simplified model of coagulation under flow to revisit the relationship between flow and TFPI inhibition.

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CP4

Extending Compartmental Models During the Covid-19 Epidemic: Lessons Learned from Two Years of Perpetual Model Development

Two years into the pandemic, the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) and its practical implications on day-to-day life don't warrant much introduction. At Ghent University, we developed and extended two compartmental epidemiological models for SARS-CoV-2 in Belgium and used them to present policymakers with counterfactual scenarios. Over the past two years, we incrementally extended our models to keep up with new scientific insights. First, the models had to be extended to account for the combined impact of novel variants of concern (VOCs) and vaccination of the general population. Then, the models had to be adapted to account for the waning immunity of the vaccines. Further, seasonal patterns emerged and variants started evading previously gained immunity. The gradual model extension required the introduction of additional degrees of freedom. Due to the risk of overfitting, it is no longer desirable to increase the model complexity even further. Instead, the model complexity should be reduced to the bare minimum needed to model the emergence of a novel VOC in near or distant future. To this end, crucial knowledge on key model parameters estimated during the pandemic must be retained while some degrees of freedom must be reestimated. We focus on the metametodology of model extension and complexity reduction to present policymakers with accurate counterfactuals during future outbreaks of SARS-CoV-2.

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CP4

The Impact of Information on the Spread of An Epidemic: a Qualitative Investigation

A large body of evidence shows that spontaneous behavioral changes deeply influence the course of an epidemic.

In particular, when the disease-protective tools are not mandatory, the individual choice to use them is determined by the circulating information and rumors. In the framework of the behavioral epidemiology of infectious diseases [Manfredi and dOnofrio (eds.), Springer 2013], the method of information-dependent models has been successfully applied to vaccine-preventable pediatric diseases and is increasingly being used. It is based on the introduction in the epidemic model of a new variable: the information index, which is defined in terms of a delay, a memory kernel and a function which describes the information that is relevant to the public in determining the choice to adopt the protective tool. We illustrate the basic idea of this approach and provide some recent applications related to (or inspired by) the ongoing COVID-19 pandemic. Precisely, we qualitatively investigate how the curbing of an epidemic can be affected by the information-dependent compliance to non-pharmaceutical interventions [Buonomo and Della Marca, Roy Soc Open Sci 2020] and hesitance about the vaccines [Buonomo et al., J Theor Biol 2022]. From a mathematical point of view, information-dependent quantities may lead to complex dynamical patterns, including sustained oscillations and hysteresis phenomena.

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CP4

Optimal Strategy for Lockdown and Deconfinement of Covid-19 Crisis

Most integrated models of the Covid pandemic have been developed under the assumption that the policy-sensitive reproduction number is certain. The decision to exit from the lockdown has been made in most countries without knowing the reproduction number that would prevail after the deconfinement. In this paper, we explore the role of uncertainty and learning on the optimal dynamic lockdown policy. We limit the analysis to suppression strategies. In the absence of uncertainty, the optimal confinement policy is to impose a constant rate of lockdown until the suppression of the virus in the population. We show that introducing uncertainty about the reproduction number of deconfined people reduces the optimal initial rate of confinement.

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CP4

A Novel Framework for Modeling Person-to-Person Transmission of Respiratory Diseases

From the beginning of the COVID-19 pandemic, researchers assessed the impact of the disease in terms of loss of life, medical load, economic damage, and other key metrics of resiliency and consequence mitigation. These studies included estimates of transmissibility, viral survivability, and other components of a disease transmission model at different levels of fidelity, resulting in analyses that were informative but, in many ways, incomplete. Using SARS-CoV-2 as a case study, we present a robust modeling framework that considers disease transmissibility from the source (characterization of the initial environment) through transport and dispersion (the effect the environment has on the initial source), and infectivity and severity (the effect that the presented environment has on the susceptible individual). The framework is designed to work across a range of particle sizes (from sub-micron up to 100 micron) and estimates the generation, environmental fate, deposited dose, and infection/severity, allowing for end-to-end analysis that can be transitioned to individual and population health models. Ultimately, we demonstrate how such high-fidelity models of disease transmission can advance and prioritize research efforts by conducting numerical simulations within this framework. This study was funded by Defense Threat Reduction Agency.

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CP4

Stochastic Models of Infectious Diseases in a Periodic Environment with Application to Cholera Epidemics

Seasonal variation affects the dynamics of many infectious diseases including influenza, cholera and malaria. The time when infectious individuals are first introduced into a population is crucial in predicting whether a major disease outbreak occurs. In this investigation, we apply a time-nonhomogeneous stochastic process for a cholera epidemic with seasonal periodicity and a multitype branching process approximation to obtain an analytical estimate for the probability of an outbreak. In particular, an analytic estimate of the probability of disease extinction is shown to satisfy a system of ordinary differential equations which follows from the backward Kolmogorov differential equation. An explicit expression for the mean (resp. variance) of the first extinction time given an extinction occurs is derived based on the analytic estimate for the extinction probability. Our results indicate that the probability of a disease outbreak, and mean and standard derivation of the first time to disease extinction are periodic in time and depend on the time when the infectious individuals or free-living pathogens are introduced. Numerical simulations are then carried out to validate the analytical predictions using two examples of the general cholera model. At the end, the developed theoretical results are extended to more general models of infectious diseases. This is joint work with Linda JS Allen.

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CP5

Gene Drives and Over-Suppression

Suppression gene drives (SGDs) spread a deleterious genetic cargo through a population by biasing their own inheritance. This technology offers a promising solution to the burden posed by crop pests and vectors of important human diseases. Presently, theoretical and experimental studies favor SGD constructs that quickly eradicate a population. If drive killing occurs faster than drive spreading, however, the target species can be locally eradicated. In the presence of migration from a non-controlled region, local eradication risks the re-invasion of wild-type immigrants, consequently undermining or even reversing suppression efforts. How might we balance drive lethality with target population permanence in the presence of bidirectional migration? In this work, we seek to answer this question for select SGDs. We use an agent-based model to account for heterogeneity in population density across a lattice landscape. Bidirectional migration is considered between a target and a non-target population. SGD performance is studied as migration levels vary, and we seek to establish under what conditions the drive persists in a suppressed target population while remaining robust to migration.

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CP5

A PDE Model for Protocell Evolution and the Origin of Chromosomes via Multilevel Selection

The origin of chromosomes was a major transition in the evolution of complex cellular life. In this talk, we model the origin of chromosomes by considering a simple protocell composed of two types of genes: a "fast gene' with an advantage for gene-level self-replication and a "slow gene' that replicates more slowly at the gene level, but which confers an advantage for protocell-level reproduction. Using a PDE to describe the effects of within-cell and between-cell competition, we find that the gene-level advantage of fast replicators casts a long shadow on the multilevel dynamics of protocell evolution: no level of between-protocell competition can produce coexistence of the fast and slow replicators when the two genes are equally needed for protocell-level reproduction. We find that introducing a "dimer replicator', a linked pair of the slow and fast genes, can allow for long-time coexistence under multilevel competition between fast, slow, and dimer replicators. Our results suggest that the formation of a simple chromosome-like dimer replicator can help to overcome the shadow of lower-level selection and work in concert with multilevel selection to promote coexistence of genes that compete under gene-level replication but are synergistic at a higher level of selection.

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CP5

Computational Models of *Kruppel* Enhancers Suggest Trade-Offs in Transcriptional Noise and Fidelity

Shadow enhancers are short regions of DNA that regulate developmental genes and ensure consistent expression patterns within the embryo. These multi-enhancer systems have been observed to drive more robust transcription than single enhancer systems. Nevertheless, it remains unclear why the arrangement of transcription factor (TF) binding sites happens across multiple enhancers rather than within a single large enhancer. In this work, we use a mathematical and computational approach to study enhancer systems with varying numbers of TF binding sites, enhancers, and distinct binding affinities. We model these systems as chemical reaction networks under stochastic dynamics and analyze the resulting trends in transcriptional noise and fidelity. The results of this work suggest that there may not be a strong selection pressure at the transcriptional level on having multiple enhancers. We also compare strategies for enhancer origins and present modeling results for the duplication and splitting of enhancers.

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CP5

Switching Gait Patterns in Hexapods Movement

The study of the synchronization patterns in biological processes is a growing discipline. Small networks of neurons model central pattern generators (CPG) that control insect locomotion (see doi 10.1137/17M1125571 and doi 10.1137/040607563). Here, we study small CPGs (6-neuron model) for insect locomotion where each neuron follows the Hodgkin-Huxley like model of Ghigliazza-Holmes (introduced in doi 10.1137/040607563). A first key point is the development of "roadmap' with exhaustive information on the dynamical behavior of a single neuron (see doi 10.1016/j.cnsns.2019.105047), using Spike-counting diagrams and bifurcation analysis. Then, we analyze the complete system, performing automatic detection techniques combined with quasi-Monte-Carlo sweeping methodologies and continuation techniques. These methods allow us to obtain a complete scheme of the patterns evolution on the movement gaits of the insect and to explain which bifurcations create and destroy the different routes leading to a global dominance of the tripod gait on the fast movement regime (see doi 10.1016/j.cnsns.2019.105047 and doi 10.1016/j.neucom.2020.06.151).

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CP5

Comparing the Evolutionary Difficulty of Intra-Organism and Inter-Organism Communication Problems

From an evolutionary perspective, is it harder to develop and maintain a communication system within a single organism, or one that works between individuals? Let us consider an artificial life simulation, in which individual agents (virtual organisms) have a bit string genome that encodes abstract chemical reactions. A selection-mutation process acting on a population of agents can evolve an artificial regulatory network that solves a computational problem. Two communication problems are of interest: Copy and PairCopy. Both require a two-bit word to be copied from a sender cell to a receiver cell over a one-bit channel. For Copy, the cells are genetically identical and part of a single agent. For PairCopy, they are from two genetically distinct agents. In experiments, a greater fraction of populations evolved complete solutions to PairCopy compared to Copy. Solving PairCopy is apparently easier because one agent with a sending mechanism and another with a receiving mechanism gain fitness from interacting; both mechanisms increase in popularity as soon as they arise. Solving Copy is harder, because if both mechanisms are present, their fitness cannot be realized until a single agent inherits them both. However, populations that solve the PairCopy problem show lower genetic diversity compared to Copy; population-wide homogeneity is favored and mutations are more likely to be deleterious, so maintaining a solution to PairCopy is harder.

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CP5

Planktos: An Agent-Based Modeling Framework for Small Organisms in Fluid and Around Structures

Most fluid dynamics work on organismal locomotion and dispersal has considered cases where either one organism actively locomotes in a quiescent fluid or many organisms passively drift with the fluid. Theoretical, computational, and experimental studies that consider both methods of transport are often limited to a small number of organisms across small scales or focus on fluid dynamic interactions between many microscopic individuals with simplified behavior. Agent-based simulations reveal complex emergent phenomena and collective behavior, but nearly all studies neglect background flows. Understanding the complex interactions between dynamic flows and small organism behavior for navigation, settlement, and dispersal has been a long-standing challenge. In this talk, I will introduce an open-source, computational framework for modeling the collective motion of microscopic organisms in 2D or 3D fluid flow near immersed structures. This library, Planktos, leverages high-performance numerical libraries to provide a complete agent-based environment in which to conduct and visualize simulations. Features include automated import of VTK data specifying time-varying fluid velocity fields, import of static mesh structures acting as solid barriers to agents, calculation of the FTLE field for generalized deterministic movement, an Ito stochastic differential equation solver and the ability to specify ad-hoc agent behavior, and native plotting.

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CP6

Separation of Na_V Subtypes in the Axon Initial Segment Can Impede Or Promote Backpropagation

We are interested in the biophysics of forward and backward propagation of action potentials (APs), as they are both important for learning. The axon initial segment (AIS) initiates APs in a variety of neurons. Pyramidal cells contain two subtypes of voltage-gated sodium channel: $Na_V1.2$ (high threshold) and $Na_V1.6$ (low threshold). These channels are nonuniformly distributed in the AIS: $Na_V1.2$ density is greatest near the soma, and $Na_V1.6$ density peaks in the distal AIS. The purpose of this spatially separated Na_V distribution remains unclear. We simulate a variety of hypothetical Na_V distributions in the AIS presumably available to evolution and compute the threshold for backpropagation. Counterintuitively, published simulations suggest that placing high threshold $Na_V1.2$ channels near the soma lowers backpropagation threshold [Hu et al., Distinct contributions of Nav1.6 and Nav1.2 in action potential initiation and backpropagation, 2009]. We find that this is true for axonal stimulation. However with somatic stimulation, we find that separating Na_V subtypes can impede or promote backpropagation. Modifying the right-shift of $Na_V1.2$ kinetics reveals that (I) Na_V availability and its time constant explain how proximal $Na_V1.2$ promotes backpropagation with axonal stimulation, and (II) steady-state activation explains how separating Na_V subtypes can impede or promote backpropagation with somatic stimulation.

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CP6

Cell Assembly Detection in Low Firing-Rate Spike

Train Data

Cell assemblies, defined as groups of neurons forming temporal spike coordination, are thought to be fundamental units supporting major cognitive functions. Detecting cell assemblies is challenging since they can occur at a range of time scales and with a range of precisions, from synchronous spikes to co-variations in firing rate. A recently published cell assembly detection (CAD) algorithm (Russo and Durstewitz, 2017) addresses this ambiguity in time scale and precision; however, it is limited to spike trains with a relatively high number of total spikes, a condition which is frequently not met by the low temporal resolution data produced by calcium imaging. We first show how the CAD method can be modified to apply to sparse spike train data. This allows us to detect assemblies in calcium imaging data of neuronal activity in the CA1 region of the hippocampus, a brain region critical for encoding and generalizing contextual memories, during contextual fear conditioning training and tests. We found that assemblies in hippocampus play a role in encoding and retrieving contextual memories. In particular, there exists a group of assemblies whose exploratory activities predict the animals ability to distinguish different contexts. Moreover, the mechanisms for processing contextual information are different between two genetically distinct strains of mice that are included in the experiments.

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CP6

Dynamical Effects of Electromagnetic Flux on Chialvo Neuron Map: Nodal and Network Behaviors

This is a study of the dynamical effects of the application of electromagnetic flux on discrete Chialvo neuron (https://arxiv.org/abs/2201.03219). I will talk about how the model manifests rich dynamical behaviors like multistability, firing patterns, antimonotonicity, closed invariant curves, various routes to chaos, and fingered chaotic attractors. I will next talk about how we have adopted the traditional techniques of bifurcation diagrams, Lyapunov exponent diagram, phase portraits, basins of attraction, and numerical continuation of bifurcations to confirm the dynamical behaviors exhibited by the system. Finally, I will shift my discussion from a single neuron to a network of Chialvo neurons and will end the talk by exploring how different dynamical regimes such as synchronous, asynchronous, and chimera states are revealed.

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CP6

Soma-Axon Electrical Separation Improves Coincidence Detection in Several Neuron Types Specialized for Sound Source Localization

Understanding how structure and dynamics of neurons impact their function is an essential neuroscience question. We use mathematical modeling techniques to study three specialized neuron types in the auditory brainstem: medial superior olive (MSO) and lateral superior olive (LSO) in mammals, and nucleus laminaris (NL) in birds. MSO and NL neurons are exquisitely sensitive to sub-millisecond time differences in their inputs. These time differences can reflect relative delays in arrivals of sounds at the two ears and thus carry sound source location information. Recent lines of evidence also indicate LSO neurons are time-difference sensitive. In short, these neurons act as coincidence detectors. We use a two-compartment structure to represent the electrical connection between synaptic input and integration regions of the neuron (soma and dendrite regions) and spike-generating regions (axon initial segment and axon), with compartment dynamics informed by physiological data. We systematically vary the connection between the regions (a two-parameter space) to identify effects of coupling configuration on dynamics and function. In all three cell types, we find that electrical separation between the two regions improves coincidence detection sensitivity. We will review our results and delineate how these different neuron types perform a similar neural computation (sound localization via coincidence detection) using distinct structural, synaptic, and dynamic features.

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CP6

Spontaneous Sleep-Wake Transition Induced by Synaptic Weight Dynamics

Understanding sleep has been a central topic in neuroscience. In order to explain experimental findings, researchers have raised different sleep hypotheses (Tononi Cirelli, 2014; Watson et al., 2016). To verify those hypotheses computationally, we first build models that can reproduce the neuronal pattern both in wake and sleep. We then simulate those models, in which sleep-wake transitions are achieved by alternating the electrophysiology of neurons in the network(Esser et al., 2007; Wei et al., 2020). However, in our model, we also observe spontaneous transitions in the entire network between sleep and wake states that occur based on simple Hebbian rules. This demonstrates a network-based way to achieve the sleep-wake transition. Our model for each neuron contains two important parts: a spiking cortical neuron model(Tatsuki et al., 2016) that includes calcium signaling, and a calcium synaptic plasticity model(Graupner Brunel, 2012; Inglebert et al., 2020) that regulates the synaptic weights within the network. We will show how to bridge those two models and attain sleep-wake transitions in networks of thousands of neurons as our main result. Our study shows that the dynamics of synaptic weights within the network is enough to change the overall behavior of the neuron network between sleep and awake. We hope our study can deepen the understanding that sleep or wake states are a network property, more than an enforced switch between two physiological states.

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CP7

Advances in Numerical Methods for Mathematical Models of Hepatitis C Viral Kinetics

Ordinary and partial differential equation models that are age-structured have been developed to study viral kinetics. The latter are nontrivial to solve and most importantly, when utilizing this type of models, parameter estimation becomes a challenging problem. It is shown that considerable gain in efficiency can be achieved by using adaptive stepsize methods and that those should be fully implemented in order to convincingly treat the problematic integral that is part of the age-structured model. Parameter estimation is then addressed directly from the model equations by the use of constrained and derivative free optimization methods. The implementation is supported by a simulator with a friendly graphical user interface that allows the user to perform parameter estimation in a realistic time of at most several minutes as compared to performing the optimization with standard methods that are costly because they require derivative evaluations. The simulator contains fully implemented numerical methods for both the model solution and parameter estimation of the model that are integrated, both are highly efficient based on linearizations at favorable instances of the outlined methods. In the next phase, machine learning of data from patients can be incorporated to model hepatitis C viral kinetics during antiviral therapy.

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CP7

An Agent-Based Model of Host-Phage Interactions for Demographic Control Scenarios

Bacteriophages ubiquitously shape microbial ecosystems by regulating the abundance, diversity, and activity of the resident bacterial community. The possibility of harnessing phages as control mechanisms for therapeutic applications to the human microbiome has understandably captured the scientific imagination. Despite substantial progress towards this goal in recent years, designing effective phage therapies still requires a better understanding of phage-bacteria interactions at the fundamental level. In particular, effective therapies often require the control of the resident bacterial community rather than its eradication. We developed an agent-based model of interacting phage and bacteria populations to investigate the coexistence and control mechanisms underlying these dynamics. The model includes the bacteria's growth, division, and dispersal processes. The model is spatially explicit; this aspect is crucial since empirical research shows that the localized growth of bacteria significantly increases their resistance to phages, in contrast to bacteria growing in a well-mixed medium. Through simulations, we demonstrate the importance of the phage-bacteria interaction network topology and, on the other hand, the choice of phage strategy, invoking 'kill the winner' or 'arms-race' strategies among others.

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CP7

Persistence and Consistence in Chemical Reaction Networks with Distributed Time Delays

One of the most important properties of the dynamics of chemical reaction networks (CRNs) is persistence. This property means that initially present chemical species will never tend toward extinction. In particular, chemical reaction network theory provides various conditions for determining persistence in a CRN without time delays. On the other hand, since some reactions in many CRNs often consist of stepwise reactions, the time delays in the reactions cannot be ignored for analyzing the dynamics of the systems. In the previous work, we have given a sufficient condition for a CRN with discrete time delays to be persistent, that is, any positive solution to the delay differential equation (DDE) describing the time evolution of concentrations of species in the system does not approach the boundary of the positive orthant. We also have proven that persistence implies consistence for a CRN with time delays. Recently, a CRN model with distributed time delays has been proposed by G.Liptk et al. (2019). Although a distributed time delay gives the more realistic model than a discrete one, any condition of persistence given in the CRNT has not been generalized to the case of distributed time delays as long as we know. In the presentation, by characterizing the positivity of states in the omega limit set of the distributed DDE as a subset of the functional space, we try to extend the two results proven in the case of discrete time delays to the case of distributed one.

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CP7

Model of Quarantine Implementation in an Animal Shelter for Canine Distemper Outbreak

Canine distemper virus (CDV), similar to the human measles virus, is an extremely contagious virus that can cause outbreaks in dense canine populations such as shelters. Previous models of CDV in animal shelters have shown that by euthanizing animals at a high rate and testing the population swiftly shelters can prevent or reduce outbreaks. The current study was motivated by previous models to show that quarantining dogs, implementing a foster system, and euthanizing, when necessary, can also reduce outbreaks in animal shelters. Previous models incorporated euthanasia but have not addressed the vital impact of quarantining and optimization on population safety and virus control. The spread of CDV was modeled by a system of ordinary differential equations through S (susceptible), V (vaccinated), E (exposed), I (infected), Q (quarantined), and R (recovered) classes. We use optimal control theory, based on Pontryagin's principle, and numerical simulations to study the impact of quarantining to reduce euthanizing and the spread of disease within shelters.

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CP7

Network Based Analysis Identifies Tp53m-Brca1/2wt-Homologous Recombination Proficient (hrp) Population with Enhanced Susceptibility to Vigil Immunotherapy

Thus far immunotherapy has had limited impact on ovarian cancer. Vigil (a novel DNA-based multifunctional immune-therapeutic) has shown clinical benefit to prolong relapse-free survival and overall survival in the BRCA wild type and HRP populations. We further analyzed molecular signals related to sensitivity of Vigil treatment. Tissue from patients enrolled in the randomized double-blind trial of Vigil vs. placebo as maintenance in frontline management of advanced resectable ovarian cancer underwent DNA polymorphism analysis. Data was generated from a 981 gene panel to determine the tumor mutation burden and classify variants using Ingenuity Variant Analysis software or NIH ClinVar. STRING application was used to create a protein-protein interaction network. Topological distance and probability of co-mutation were used to calculate the C-score and cumulative C-score. KaplanMeier analysis was used to determine the relationship between gene pairs with a high cumC-score and clinical parameters. Improved relapse free survival in Vigil treated patients was found for the TP53m-BRCAwt-HRP group compared to placebo. Results suggest a subset of ovarian cancer patients with enhanced susceptibility to Vigil immunotherapy. The hypothesis-generating data presented invites a validation study of Vigil in target identified populations and supports clinical consideration of STRING-generated network application to biomarker characterization with other cancer patients targeted with Vigil.

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CP8

Dynamics of Large Flocks of Birds

Flocking birds exhibit complex dynamic behavior such as wave propagation, coordinated turns, and consistent geometric patterns of tens of thousands of individuals. Understanding this behavior may inform diverse topics such as microscopic biological systems that display similar behavior and self-organization of autonomous robots. However, the properties required for individual birds to create such group dynamics are still not well understood. To understand how complex flocking behaviors like murmuration can develop, we utilize several original and extended flocking models in a simulation of thousands of birds that runs and renders in real time with interactive parameter tuning. We discuss our results as well as the suitability of various metrics for quantifying flocking dynamics like murmuration.

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CP8

Differential-Geometric Controllability and Extremum Seeking is Linked to the Albatross Flying Physics

The albatross is one of the most efficient travelers in the animal world. One species, the wandering albatross, can fly nearly 500 miles in a single day, with just an occasional flap of its wings and minimal food/energy consumption. The flying phenomenon performed by the albatross, if conducted ideally, can lead to an energy neutral flight cycle: the Dynamic Soaring (DS) phenomenon/cycle. This phenomenon basically is about how soaring birds, such as, but not limited to albatross, can utilize wind shear to fly almost for free. In this presentation, we show that differential-geometric control theory can reveal, and in fact, characterizes the flight physics of the DS flight physics along with novel characterization with extremum seeking phenomenon. This mathematical effort in formulation and nonlinear control analysis can advance the possibility of bio-mimicking of efficient bird flights by unmanned systems.

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CP8

Allee Effects Plus Noise Induce Population Dynamics Resembling Binary Markov Highs and Lows

We show that the combination of Allee effects and noise can produce a stochastic process with alternating sudden decline to a low population phase, followed, after a random time, by abrupt increase in population density. We introduce a new, flexible, deterministic model of attenuated Allee effects, which interpolates between the logistic and a usual Allee model. Into this model we incorporate environmental and demographic noise. The solution of the resulting Kolmogorov forward equation shows a dichotomous distribution of residence times with heavy occupation of high, near saturation, and low population states. Investigation of simulated sample paths reveals that indeed attenuated Allee effects and noise, acting together, produce alternating, sustained, low and high population levels. We find that the transition times between the two types of states are approximately exponentially distributed, with different parameters, rendering the embedded hi-low process approximately Markov.

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CP8

Nonspreading Solutions and Patch Formation in An Integro-Difference Model with a Strong Allee Effect and Overcompensation

Previous work involving integro-difference equations of a single species in a homogenous environment has emphasized spreading behaviour in unbounded habitats. We show that under suitable conditions, a simple scalar integro-difference equation incorporating a strong Allee effect and overcompensation can produce solutions where the population persists in an essentially bounded domain without spread despite the homogeneity of the environment. These solutions are robust in that they occupy a region of full measure in the parameter space. We develop orbit diagrams showing various patterns of nonspreading solutions from stable equilibria, period two, to chaos. We show that from a relatively uniform initial density with small stochastic perturbations a population consisting of multiple isolated patches can emerge. In ecological terms this work suggests a novel endogenous mechanism for the creation of patch boundaries.

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CP8

Winning Strategies in Differential Games

Plenty of researches have been devoted to pursuit-evasion games, namely [Leon A. Petrosyan, Differential Pursuit Games, Izdat. Leningrad. Univ., Leningrad, 1977], [Mehdi Salimi, Massimiliano Ferrara (2019): Differential game of optimal pursuit of one evader by many pursuers, International Journal of Game Theory, 48 (2), 481-490]. In this research study, first we investigate a pursuit-evasion differential game with one evader and infinite number of pursuers in Hilbert space. The control functions of players are subjected to the geometric and integral constraint. Evader can scape from pursuers if there exists a strategy of the evader such that geometric point of evader and pursuers are different at any time for any admissible controls of the pursuers. We make a strategy for the evader that ensures scaping it from all pursuers. In the second part of the research, we introduce a winning strategy for pursuers.

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CP8

The Interplay Between Costly Reproduction and Unpredictable Environments Shapes the Dynamics and Stability of Cooperative Breeding

All sexually reproducing organisms are faced with a fundamental decision: to invest valuable resources and energy in reproduction or in their own survival. This trade-off between reproduction and survival represents the 'cost of reproduction' and occurs across a diverse range of organisms. It is widely assumed that cooperative breeding behavior in vertebrates when individuals care for young who are not their own results in part from costly parental care. When caring for young is too costly, parents need help from related or unrelated individuals to successfully raise their offspring. Cooperatively breeding birds and mammals are also more commonly found in unpredictable environments than non-cooperative species, suggesting that decisions about when to breed or help may represent complex yet critical choices that depend on the energy individuals have available to dedicate to reproduction given the harshness of the current environment. Here, we introduce a novel, socially-tiered model of a cooperatively breeding species that incorporates the influence environmental stochasticity. Through numerical and analytical methods, we use this model to show that costly reproduction and environmental variability are compounding factors in the evolution and maintenance of cooperation.

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CP9

A Mathematical Model of Coinfection of Influenza and Pneumonia

The interaction between respiratory diseases of influenza, and pneumonia is vital to understanding how coinfection might affect the transmission of pneumonia. We formulate an ordinary differential equation based model to analyze the qualitative behavior of influenza and pneumonia coinfection. We determine the effective reproduction number and show that in the absence of coinfection, disease-free, boundary, and endemic equilibria are locally and globally stable. Further, the model undergoes a backward bifurcation in the presence of the coinfection. Epidemiologically, this means that in order to eliminate the disease it may no be sufficient to bring R_0 below one. We then present numerical simulations to support the analytical results.

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CP9

A Toxicokinetic/Toxicodynamic (TK/TD) Model of Mortality for Sarin Inhalation in Rats

We describe a novel toxicokinetic/toxicodynamic (TK/TD) model of the probability of mortality due to the inhalation of the nerve agent sarin (GB) in rats. The model describes uptake, clearance, and the dynamics of GB and acetylcholinesterase with a set of 4 coupled ordinary differential equations. The model parameters were determined by using recent data on lethal dosage values for rats and mice obtained using modern techniques. This simple model accurately reproduces results from historical data sets and can predict the probability of mortality for GB for exposures with arbitrary concentration/time histories. The model was run using concentration/time

history data from Large Eddy Simulation to provide a realistic exposure scenario with high levels of intermittency. The results of the TK/TD model were compared with a calculation done using a Lagrangian transport code and a toxic load model under identical atmospheric conditions. The results from the two models differ significantly at both long and short exposure times, and we explain this difference in terms of the limitations of the toxic load model in these cases. This TK/TD model represents a first step in providing human injury and fatality calculation tools for the next generation of hazard prediction codes. A physiologically based TK/TD model is a well-founded alternative for predicting effects over the large range of exposure times and concentration histories likely in realistic exposure scenarios.

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CP9

Estimates of the Virus-Mediated Cell Fusion Rate of Sars-CoV-2

Many viruses, including SARS-CoV-2, have the ability to cause neighboring cells to fuse into multi-nucleated cells called syncytia. Much is still unknown about how syncytia affect the course of viral infection, including the time scale over which they form. Using data from a recent study of virus-mediated cell fusion, we use mathematical modeling to estimate the fusion rate of SARS-CoV-2 in the presence and absence of furin. We find that the presence of furin increases the fusion rate.

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CP9

Age-Dependent Ventilator-Induced Lung Injury

Patients with illnesses or infections that affect the respiratory system are commonly treated with mechanical ventilation (MV) in severe cases. While MV is often a life-saving intervention, it can induce further lung damage called ventilator-induced lung injury (VILI). Experimental data has indicated an increased risk for VILI in elderly patients. This information along with the increased demand for MV caused by the novel coronavirus SARS-CoV-2 emphasizes the need for further research on the age-dependent aspects of VILI. This paper expands upon a previous ordinary differential equation model for MV (Minucci *et al.*, JTB 2021) by including more biologically realistic dynamics for cell and cytokine diffusion into the alveolar lung space following epithelial damage. Additionally, we utilize *in vivo* mouse data to create plausible parameter estimates associated with both the young and old mice experiments. Parameter sets are then analyzed using various statistical methods, including random forest and other classification methods, to determine the important factors associated with severe or moderate responses to MV for both the young and old experimental groups. We also identify representative parameter sets that best depict the average transient behavior for each response group. Using the representative sets we identify significant parameters and simulate potential interventions to improve the response to MV.

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CP9

Optimal Antibiotic Dosing in the Presence of Resistant Bacteria

Misuse and over use of antibiotics has led to bacteria developing resistance to antibiotics. This has resulted in complications in treatment and treatment failures and is now a major public health challenge. Mathematical models can be very useful in determining efficient and successful antibiotic dosing regimens. In this study we consider the problem of determining optimal antibiotic dosing, in particular we look at the case where bacteria that are resistant to the antibiotics are present in addition to susceptible bacteria. We look at two different models of resistance acquisition, which have been identified as primary mechanisms for invivo drug resistance, both involve horizontal transfer of resistant genes from a resistant to a susceptible bacterium. We use a numerical optimization algorithm to determine the 'best' antibiotic dosing strategy, which is successful in eliminating bacteria while keeping the total antibiotic usage low at the same time. We first consider the case where a resistance is acquired via conjugation and then the case where resistance acquisition occurs via transference. We note that constant periodic dosing and dose tapering may not always succeed in eradicating the bacterial populations, while the optimal dosing protocol is successful.

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CP9

Modeling the Risk of Drug-Induced Liver Injury with Adverse Outcome Pathways and Bayesian Networks

The development of high throughput in vitro assays has had profound impact on toxicological assessment. It has the potential to lead to more efficient, accurate, and less animal-intensive testing. However, it is challenging to take advantage of the numerous in vitro tests in the actual risk assessment process. On the other hand, the adverse outcome pathway (AOP) framework has emerged as a rich source for mechanistic knowledge and as a potential tool to select and structure in vitro assays in predictive models for toxicity. In this study, we utilize knowledge encoded in AOPs to build a predictive model for drug-induced liver injury (DILI) using a Bayesian network approach. We reviewed AOPwiki and related literature to construct a comprehensive AOP network regarding DILI, which represents our current knowledge for molecular events that lead to liver injury by drugs and other chemicals. This constitutes a graphical guide to develop in vitro assays to detect liver injury. As the basic structure of AOP networks are directed acyclic graphs, they provide a natural opportunity to construct models with Bayesian networks. We present a Bayesian network model based on DILI AOP networks using L1000 and Tox21 data for gene expression and nuclear receptor binding. Due to the incorporation of significant expert knowledge in the form of AOP, the Bayesian network model has the advantage of being parsimonious and requires only a small number of assays to predict the risk of toxicity.

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CP10

Neuronal Mechanisms for Sequential Activation of Memory Items and Dynamic Branching

An important function of the brain is to adapt behavior by selecting between different predictions of sequences of stimuli likely to occur in the environment. First, we present a biologically inspired network model of activation of memory items in a sequence. We show that synaptic depression and noise drive the transitions from one memory item to the next and neuronal gain controls the switching between regular and irregular (random) activation. Then, we study the branching behavior of the model, both analytically and through numerically. Results show how synaptic efficacy, retroactive inhibition and short-term synaptic depression determine the dynamics of choices between different predictions of sequences having different probabilities. Further results show that changes in the probability of the different predictions depend on variations of neuronal gain. Such variations allow the network to optimize the probability of its predictions to changing probabilities of the sequences without changing synaptic efficacy.

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CP10

Using Phase Reduction Techniques to Control Nonpairwise Connections in Arbitrary Oscillatory Networks

Phase reduction techniques have been used to make complex oscillatory systems tractable by approximating them with systems of pairwise coupled (one-dimensional) phase oscillators [Pietras, Daffertshofer (2019)]. Recent advances show that three- and fourway interactions naturally appear in phase reductions of coupled oscillatory systems [Ashwin, Rodrigues (2016)]. Networks of coupled oscillators can exhibit undesired collective behaviour such as (partial) synchronisation. Methods to control the collective behaviour of oscillatory networks are usually limited to controlling pairwise phase interactions. We generalised pairwise synchronisation engineering [Kiss, Rusin, Kori, Hudson (2007)] to account for the higher order interactions. We design a time-delayed feedback and use gain and delay parameters to match the phase reduction of a network of arbitrary oscillators to a phase model that has the desired behaviour. Examples of applications could be controlling neuronal oscillators in the treatment of Parkinsons disease and epileptic seizures.

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CP10

Asymptotics of Calcium Puff Frequency

Calcium signaling is organized in a hierarchical manner. At the lowest (most microscopic) level, stochastic release of Ca^{2+} through a single IP3 receptor results in a small localized increase in cytoplasmic Ca^{2+} concentration. The IP3 receptors are typically tightly clustered, which means that a Ca^{2+} blip can stimulate the release of additional Ca^{2+} through neighboring receptors, so that the entire cluster emits a localized 'puff'. There is considerable evidence that calcium puffs are nonlinear stochastic phenomena: it has been observed for instance that IP3 channels can be highly active even when the average open probability is less than half its maximum. In this talk we use the theory of Large Deviations to determine accurate estimates for the frequency of calcium puffs in both excitable and-

nonexcitable cells.

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CP10

A Dynamical Mechanism for Generation of Early Afterdepolarization Patterns

Early Afterdepolarizations (EADs), which are voltage oscillations in cardiac action potential during the repolarization phase, are linked to the appearance of cardiac arrhythmias and other heart conditions. In this presentation we analyze the dynamical mechanisms underlying the formation of arrhythmogenic early afterdepolarizations (EADs) in two mathematical models of cardiac cellular electrophysiology: a biophysically detailed model of a ventricular myocyte with a large number of state variables (which allow a more faithful reproduction of experimental observations) and a low dimensional model, more suitable for theoretical analysis. Based on a comparison of the two models, with detailed bifurcation analysis using continuation techniques in the simple model and numerical explorations in the complex model, we propose a conjectured scheme involving a hysteresis mechanism with the creation of alternans and EADs in the unstable branch. This theoretical scheme fits well with electrophysiological experimental data on EAD generation and hysteresis phenomena.

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CP10

Bifurcation Structure and Classification of Spike-Adding Processes: the Hindmarsh-Rose Model

Bursting behavior is exhibited by a plethora of biological systems, such as neurons and pancreatic beta cells. The creation of new fast spikes on a bursting system is a relevant phenomenon, as it increases the duty cycle of the system. We investigate the dynamics underlying different spike-adding processes by studying the Hindmarsh-Rose neuron model, a prototype model for square-wave (or fold/hom) bursting that also exhibits tapered (or fold/Hopf) bursting. The connection between the spike-adding processes and the bifurcation structure of the system is detailed, and we propose a global scheme that locates each spike-adding process found in the model with respect to the bifurcation diagram. This global scheme provides a theoretical explanation to the different interspike-interval bifurcation diagrams (IBD) that have appeared in the literature for different models. We also explain the transitions between different spike-adding processes, a crucial point not previously studied.

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CP10

Control of Coupled Neural Oscillations Using Near-Periodic Inputs

Deep brain stimulation (DBS) is a commonly used treatment for medication resistant Parkinson's disease and is an emerging treatment for other neurological disorders. More recently, phase-specific adaptive DBS (aDBS), whereby the application of stimulation is locked to a particular phase of tremor, has been proposed as a strategy to improve therapeutic efficacy and decrease side effects. In this work, in the context of these phase-specific aDBS strategies, we investigate the dynamical behavior of large populations of coupled neurons in response to near-periodic stimulation, namely, stimulation that is periodic except for a slowly changing amplitude and phase offset that can be used to coordinate the timing of applied input with a specified phase of model oscillations. Using an adaptive phase-amplitude reduction strategy, we illustrate that for a large population of oscillatory neurons, the temporal evolution of the associated phase distribution in response to near-periodic forcing can be captured using a reduced order model with four state variables. Subsequently, we devise and validate a closed-loop control strategy to disrupt synchronization caused by coupling. Additionally, we identify strategies for implementing the proposed control strategy in situations where underlying model equations are unavailable by estimating the necessary terms of the reduced order equations in real-time from observables.

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CP11

Data-Driven Inference of Isostable-Coordinate Based Model Dynamics Using Neural Networks

The Koopman operator paradigm can be leveraged to infer a general, non-linear dynamical models and obtain its

input-to-output relations using an asymptotic expansion in the isostable coordinate basis. These isostable coordinates capture the dynamics associated with the slowest decaying Koopman eigenmodes. However, direct calculation of these input-to-output relations using this strategy requires knowledge of the underlying model equations. In this presentation, a strategy is considered to compute these isostable-coordinate-based models in a data-driven manner using neural networks whose layers are based on the asymptotically expanded input-to-output isostable coordinate relationships. A set of perturbations is applied to the dynamical system and these inputs along with the corresponding outputs are fed to the neural networks for supervised training to obtain the resulting model. For complex valued isostable coordinates, a transformation is derived that relies on complex conjugacy to ensure that the neural network weights remain real. This strategy is implemented and illustrated to capture dynamical behaviors associated with a population of coupled neural oscillators.

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CP11

A High-Throughput Deep Learning Pipeline for Data Analysis of Sector-Like Formations in Yeast Colonies

Prion proteins are commonly associated with fatal neurodegenerative diseases in mammals, but are also responsible for a number of harmless heritable phenotypes in *S. cerevisiae* (yeast). In normal conditions, yeast colonies grow in circular shapes, displaying a uniform white or pink color (prion phenotype) related to the fraction of normal (non-prion) protein. While in mammals prion phenotypes are irreversible, in yeast mild experimental manipulations destabilize prion phenotypes, introduce changes in the intracellular prion aggregation dynamics, and cause colonies to exhibit sectors showing both prion (white or pink) and non-prion (red) phenotypes. The precise mechanism of this destabilization and forces influencing the emergence of mixed colony phenotypes are unknown. As such, experimental colonies provide a rich dataset to uncover relationships between colony-level phenotypic transitions, molecular processes, and individual cell behaviors. Here, I present ongoing work on an automated deep-learning pipeline to extract detailed information about sector-like structure formations in images of yeast colonies. The pipeline uses a convolutional neural network and the circle Hough transform to quantify the shape, size, and frequency of sectors in experimental data. This approach will streamline quantification and annotation of yeast colonies grown under experimental conditions and offer additional insights into mechanisms driving colony-level phenotypic transitions.

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CP11

Parameter Identifiability and Subset Selection Techniques for Data-Driven Model Reduction with Applications to Biological Soft Tissues

The ability to accurately estimate and interpret parameters in mechanistic mathematical models is strongly tied to the quantities of interest (QoIs) for which data is available, the scope of such data, and the structure of the model with respect to its parameters. During calibration, models with more than a few parameters and limited data can exhibit several unidentifiable parameters. This talk presents strategies for combining local parameter sensitivity and identifiability techniques with the numerical solution of inverse problems via optimization to aid in robust parameter estimation and model reduction. Techniques used are based on an eigendecomposition or singular value decomposition involving the sensitivity matrix for QoIs tied to the data. Applications are illustrated for two problems in the mathematical modeling of biological soft tissues. The first application, in biomechanics, considers structural remodeling of the vessel wall in hypoxia-induced pulmonary hypertension using a two-layer nonlinear, hyperelastic, anisotropic Holzapfel-Gasser-Ogden (HGO) model. The second application, in wound healing, studies in vitro enzyme-mediated polymerization of fibrinogen into an insoluble fibrin matrix using an enzyme kinetics model with several internal complexes. In both cases, the overall approach is tailored to the application and the capabilities to preserve or enhance objective cost in the optimization while also identifying reduced models is demonstrated.

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CP11

Systematic Inference Identifies a Major Source of Heterogeneity in Non-Markovian Cell Signaling Dynamics: the Rate-Limiting Step Number

Identifying the sources of cell-to-cell variability in signaling dynamics is essential to understand drug response variability and develop more effective therapeutics. However, it is challenging because many signaling intermediate reactions are experimentally unobservable. This can be overcome by replacing them with a single random time delay, but the resulting process is non-Markovian, making it difficult to infer cell-to-cell heterogeneity in reaction rates and time delays. In this talk, we present an efficient and scalable moment-based Bayesian method that infers cell-to-cell heterogeneity in the non-Markovian signaling process. We apply this method to single-cell expression profiles from promoters responding to various antibiotics and discovered a major source of cell-to-cell variability in antibiotic stress-signal response: the number of rate-limiting steps in signaling cascades. This knowledge can help identify more effective therapies that destroy all pathogenic or cancer

cells.

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CP11

Inferring Dynamics of Biological Systems

Biological networks are complex and constructing dynamics for large systems can prove difficult. We will explore utilizing data-driven techniques to uncover the dynamics of a biological network from data provided. Several sparse identification algorithms will be presented and discussed. We will discuss applying these methods to data obtained for the Mitogen-Activated Protein Kinase (MAPK) pathway. The MAPK pathway is of particular interest in studying cancer mutations.

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CP11

Kernel Mean Embedding As a Unifying Theory for Distributional Data

Many problems in the life sciences involve distributions over some metric space. Kernel mean embedding (KME) is an elegant framework to process such data: the distribution is represented as an average of the sample embeddings mapped to a reproducing kernel Hilbert space. Starting from this embedding, we can suggest a kernel-based toolkit to predict, compare, visualize, optimize and learn from such distributions. We present a case study on how KME can be applied to pharmaceutical processes. Current methods only use the first two order statistics (i.e., mean and variance) to represent the particle size distributions, losing a lot of information. The KME framework allows us to efficiently represent and manipulate all the characteristics of the distributions of interest. In the end, we will reflect on how KME can further be used in the broader life sciences.

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CP12

Viral Master-Equation: Connecting Previous and Current Computational Virology Research Methods

The most common mathematical model in computational virology is a system of ordinary differential equations. This type of model is used for both in-host models and population level models. Due to an ordinary differential equation model treating the system as a well-mixed system, spatial heterogeneity is not captured in these models. For this reason, agent-based models have grown in popularity because they account for spatial effects. Previous work has shown that ordinary differential equation models and agent-based models can capture the dynamics of the same system, but the parameters from the two separate models are not comparable. This work aims to show how the two sets of parameters can be linked to each other by modeling a system first with a master-equation and then deriving the ordinary differential equation model and agent-based model from the master-equation.

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CP12

A Mathematical Model of Innate and Adaptive Immune Responses Initiated by Burn Injury

The World Health organization, American Burn Association, and Centers for Disease Control and Prevention, collectively, estimate 1.1 million people in the United States suffer from burn injuries annually. Understanding the collective effects of burns is fundamental for gauging injury severity and predicting healing outcomes. To repair tissue damage, an overlapping, coordinated sequence of phases (hemostasis, inflammation, proliferation, and remodeling) occurs. Pathological inflammation during this process impairs wound healing, increasing the likelihood of adverse individual outcomes. Here, we introduce an immunophysiological model of local dermal wound healing following burn injury. The model consists of a system of nonlinear ordinary differential equations that describe dynamics between various innate (neutrophils, macrophages) and adaptive (T lymphocytes) immune cells as well as fibroblast activity at the site of injury. A representative parameter set was identified from published literature to establish baseline values. Using the time series predictions for the baseline values as the comparator, numerical simulations were performed, allowing us to further verify the biological plausibility of its behaviors. We then utilize the model to first explore the effect of different inflammatory profiles in promoting timely tissue healing and preventing secondary infection for thermal burn injury.

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CP12

Computational Model of Drug Dissolution in the Stomach: Effects of Posture and Gastroparesis on Drug Bioavailability

The oral route is used most frequently for drug administration in human due to its safety, reduced cost, and high degree of patient compliance, but it is also the most complex way for an active pharmaceutical ingredient to enter the body. This complexity is because drug absorption via the gastrointestinal tract depends not only on factors related to the drug and its formulation, but also the contents and motility of the stomach. Also, the dynamic physiological environment of the stomach generates complex pill trajectories and non-uniform rate of dissolution and emptying of the drug into the duodenum, which potentially affects drug bioavailability. These issues pose several challenges to the design of drug delivery systems from RD, clinical, and regulatory perspectives. These are particularly relevant for disease conditions that are associated with alterations in the anatomy and/or physiology of the stomach as current clinical approaches to assess the efficacy of oral drugs are limited in their ability to elucidate the relationship between bioavailability and altered stomach. We employ StomachSim, a CFD model of human stomach, to investigate the effect of body posture and stomach motility on drug bioavailability and understand the fluid-dynamic mechanisms of drug dissolution.

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CP12

Effect of Cross-Immunity in a Multi-Strain Cholera Model

Observed in recent cholera outbreaks is the presence of two serotypes, strains of the cholera bacteria that mainly differ in their induced host immunity. Each serotype induces both self-immunity and a degree of cross-immunity to the other strain for some duration. We combine and extend previously studied SIRP and multi-strain models to consider the strain diversity of cholera. We explore various ways of incorporating host immunity into this deterministic multi-strain model, characterizing the dynamics and long-term behavior, particularly in the case of serotype coexistence.

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CP12

A Mathematical Framework to Augment the Q-Marsh Score in the Diagnosis of Celiac Disease

Celiac disease is a hereditary autoimmune disease that affects approximately 1 in 133 Americans. It is caused by a reaction to the protein gluten found in wheat, rye, and barley. After ingesting gluten, a patient with celiac disease may experience a range of unpleasant symptoms while small intestinal villi, essential to nutrient absorption, are destroyed in an immune-mediated process. The only known treatment for this disease is a lifelong gluten-free diet and there is currently no drug treatment. This work provides a mathematical model to better understand the effects of immune activation on gut health using a system of ordinary differential equations to track changes in small intestinal cell densities and relates them to the Q-MARSH score, a criterion used in the diagnosis of celiac disease. The model can be used to investigate and analyze the immune response and various theories behind the progression of this disease by focusing on understanding the dynamics of the small intestine in situations mirroring healthy function and celiac disease. By doing so, we can assist in further quantifying and augmenting diagnostic measures and investigate potential therapies to mitigate the negative effects of celiac disease.

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CP12

The Vaginal Microbiota and Its Association with Chlamydia Infection

Chlamydia trachomatics (C. trachomatics) is a major cause of bacterial sexually transmitted disease in the United States and is associated with adverse outcomes in the upper genital tract of women. It is unclear why some women are more likely to develop asymptomatic infection, have severe infection, or stay uninfected after exposure to *C. trachomatics*. Prior studies have shown a relationship between vaginal microbial composition and susceptibility to sexually transmitted infections including Chlamydia. However, little is known about the microbiome dynamics, especially in the upper genital tract, and its association with Chlamydia infection. We use mice as a model organism, seek to elucidate the association of genital tract microbiome dynamics with Chlamydia infection, and determining whether the time of infection affects the genital tract microbiome over time via analyzing the data collected before and over the course of infection.

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MS1

RNA Modeling with Limited Data

Ribonucleic acid (RNA) molecules play spectacularly versatile roles in living cells. Emerging biomedical advances such as precision medicine and synthetic biology point to RNA as the central regulator and information carrier. We are interested in predicting RNA structure, stability, and kinetics from the nucleotide sequence, and the design of molecules for therapeutic applications. For example, given the limited availability of crystal/NMR structures, how to build the native fold from the sequence? For a given RNA target, how to predict RNA-small molecule interaction and identify small molecules as potential drugs? Using physical and chemical principles, we recently developed IsRNA for RNA 3D structure prediction and RLDock for RNA-small molecule interactions. I will describe these new approaches and the proof of principles in RNA 3D structure prediction and in predicting RNA-small molecule binding.

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MS1

Characterizing Biomedical Datasets for Machine Learning

Often times, biomedical datasets have lots of nearly redundant information, such as two very similar compounds having nearly the same binding energy. This can lead to inflated performance metrics and models that are not generalizable for novel predictions. It is useful to characterize these datasets to understand the potential for this happening and attempt to mitigate it. This talk discusses the redundancy in drug binding data repositories, methods to characterize the similarities within a dataset, and ways to diminish the biases from over and underrepresented data.

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MS1

What can Geometric Combinatorics say about RNA Folding Prediction?

The formation of base pairs within single-stranded RNA molecules, such as viral genomes, creates structure and affects function. Yet, reliable prediction of this important base pairing information remains an open problem in computational molecular biology. RNA folding prediction is typically approached as a discrete optimization under a thermodynamic objective function. When reformulated as a linear program, we can fully analyze all possible multiloop entropy parameters using techniques from geometric combinatorics. In this way, we find new branching parameters which significantly increase prediction accuracy on well-defined families. Moreover, these results also illuminate why the general problem is so difficult.

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MS1

Evolutionary Signatures at Protein Interaction Hotspots

Protein interaction hot spots contribute disproportionately to the binding free energy of a protein-protein complex. In this work, we demonstrate that evolutionary signatures at putative hot spots are a strong indictor of natively bound protein-protein interfaces. We also present a study of feature analysis for our KFC hot spot algorithm, highlighting how combinatorial study of machine learning features adds insight into the dominant physiochemical properties of hot spots.

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MS2

Cortical Networks, Waves, Avalanches and the Cortico-Hippocampal Dialogue

During sleep, brain structures engage in a dialogue which facilitates memory processes. However, besides "hub" areas such as medial prefrontal cortex and entorhinal cortex, how the whole cortex is dynamically coupled to the hippocampus is unknown. We characterized cortical resting state activity with voltage-sensitive imaging and electrocorticography, together with electrophysiological potentials from the hippocampus. Cortical resting state activity is characterized by transient events, whose size distribution is be well approximated by a power law distribution, as in critical systems, but stratifying transients by magnitude reveals different modes of transient activity. While small transients have a limited number of co-activation modes, larger transients propagate as waves spanning a substantial portion of the cortical surface and can be classified based on their origin: one family is preceded by Retrosplenial cortex activation, the other by Somatosensory Cortex. Interestingly, hippocampal gamma power is proportional to the size of the cortical transients and preferentially associated with retrosplenial-led transients. We also found a significant causal interaction from RS activation to hippocampal gamma amplitude. Ripple events appear instead to have a much looser association with cortical activity evolution. These results begin to characterize resting state network dynamics at a fast time scale and suggest updates to our current theories of memory processes.

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MS2

From Mice, to Machine, to Man: Modelling Clearance and Proteopathy in Alzheimers Disease

Every day, over 28,000 people are diagnosed with dementia, making it a leading cause of death and economic burden worldwide. The most common form of dementia is Alzheimer's disease (AD). Our best defence against AD has, until recently, been insights gathered from experi-

ments using mice and numerous such experiments have studied the fundamental importance of the brain's clearance mechanisms. Mathematical modelling has joined the fight against AD and allows for safe, ethical, and cost-effective in-silico experimentation in man. My research delivers the first theoretical model of coupled brain clearance and AD progression, and my data-driven computational approach simulates 40 years of AD progression in less than 14 seconds of computational time. In this talk, I will describe a new model of AD and its coupled relationship with brain clearance. The resulting high-dimensional, network diffusion-reaction dynamical system yields theoretical insights into the neurodegeneration process and its relationship with clearance. Computational results, on high-resolution brain graphs constructed from the data of 426 patients, demonstrate the connection between clearance and AD progression. A key finding is that the coupling between proteopathic spreading and regional brain clearance may not only alter the trajectory of AD but also provide a potential window into understanding AD subtypes. AD research is changing, and mathematics is providing the critical bridge from mice to machine to man.

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MS2

Partial Synchronization in Neural Networks

Synchronization of neurons is believed to play a crucial role in the brain under normal conditions, for instance, in the context of cognition and learning and under pathological conditions such as Parkinson disease or epileptic seizures. In the latter case, when synchronization represents an undesired state, understanding the mechanisms of desynchronization is of particular importance. In other words, the possible transitions from synchronized to desynchronized regimes and vice versa should be investigated. It is known that such dynamical transitions involve the formation of partial synchronization patterns, where only one part of the network is synchronized. In the present talk, we discuss the occurrence of peculiar partial synchronization patterns such as chimera states and solitary states in neural networks.

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MS2

Metastability in Mesoscopic Network Models of Spiking Neurons with Short-Term Plasticity

The neuronal mechanisms of various cognitive functions have been linked to metastable dynamics of recurrent neural networks. Metastability, such as population spikes or spontaneous transitions between up- and down-states, may result from slow fatigue processes (e.g., short-term depression of presynaptic synapses), from noisy fluctuations, or from an interplay of both. Previous modeling studies that consider either detailed spiking neuron networks, or heuristic firing rate models, have not provided satisfactory mechanistic insights how single neuron dynamics and finite-size fluctuations contribute to metastable population activity. In this talk, we will propose a mesoscopic description for networks of spiking neurons with short-term depression that is based on a rigorous reduction from microscopic neuron dynamics. With this novel mesoscopic model, we investigate typical examples of metastable network dynamics and also shed new light on hippocampal replay.

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MS3

Predicting Experimental Sepsis Survival with a Mathematical Model of Acute Inflammation

In sepsis, the inflammatory response drives organ dysfunction and often results in death. We used four ordinary differential equations (ODEs) to simulate the dynamics of bacteria, the pro- and anti-inflammatory responses, and tissue damage, which approximates organism health status. The model was calibrated to experimental data from E. coli infection in genetically identical rats and validated with mortality data for these animals. Typical outcomes included recovery, aseptic death (overwhelming inflammatory response), or septic death (overwhelming bacteria) for a simulated infection when the initial inoculum, pathogen growth rate, local immune response strength, and pro-inflammatory response activation rate were varied. The likelihood of a septic outcome increased with an increase in the initial inoculum of bacteria, an increased pathogen growth rate, or a decreased host immune response. Results suggested that small changes in parameter values, such as pathogen or immune response parameters, could explain variability in mortality rates seen in the experiments. A sensitivity analysis suggested primary roles for local immune- and bacteria-related terms and lesser roles for global immune response and damage-related terms. Despite successful predictions of mortality, simulated trajectories tended to be clustered closely, suggesting that uncertainty in initial conditions could lead to difficulty in predicting outcomes of sepsis solely using inflammation biomarker levels.

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MS4

Optimal Curvature in Long-Range Cell-Cell Communication

Cells in tissue can communicate short-range via direct contact, and long-range via diffusive signals. In addition, another class of cell-cell communication is by long, thin cellular protrusions that are 100 microns in length and 100 nanometers in width. These so-called non-canonical protrusions include cytonemes, nanotubes, and airinemes. But, before establishing communication, they must find their target cell. Here we demonstrate airinemes in zebrafish are consistent with a finite persistent random walk model. We study this model by stochastic simulation, and by numerically solving the survival probability equation using Strang splitting. The probability of contacting the target cell is maximized for a balance between ballistic search (straight) and diffusive (highly curved, random) search. We find that the curvature of airinemes in zebrafish, extracted from live cell microscopy, is approximately the same value as the optimum in the simple persistent random walk model. We also explore the ability of the target cell to infer direction of the airinemes source, finding the experimentally observed parameters to be at a Pareto optimum balancing directional sensing with contact initiation.

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MS4

Modeling Microtubule Dynamics and Polarity in Neurons

The polarity and stability of the microtubule cytoskeleton are critical in supporting long-range directed transport of cellular cargo and long-term survival of neurons. However, microtubules also need to be dynamic and reorganize in response to injury events. Multiple mechanisms that contribute to the primarily minus-end-out filament organization in Drosophila dendrites have been identified. However, we lack an understanding of how these complex mechanisms ensure both healthy function over long time periods and dramatic rearrangement in response to injury. I will discuss a spatially-explicit mathematical model of the dendritic microtubule system in Drosophila neurons. This framework suggests several hypotheses for the microtubule dynamics, which we test using a stochastic model and validate with fluorescence experiments. Pairing this modeling framework with biological experiments has the potential to provide insight into the impact of various parameters and control mechanisms on polarity and dynamics in Drosophila dendrites.

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MS4

A Hard Spheres Approach to Simulating Catalytic Reactions Between Diffusing Point Particles

The simulation of reaction-diffusion processes in biology is a multiple scale problem. This problem is at the core of the grand challenge of whole cell simulation. One of the most common approaches to simulation at mesoscopic scales of reaction-diffusion processes is to summarise each molecule as a Brownian point in space and each reaction as the events that occur when these points are sufficiently close (like collisions of hard spheres). As with all simulation algorithms at this scale, there are limitations to this model. An important limitation is that it only describes bimolecular reactions. In this work, we show how to generalise this framework so that it incorporates complex high-order and catalytic reactions where multiple time scales are important.

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MS4

Optimal Cytoskeletal Dynamics for Intracellular Transport

The transport of cargo within cells is typically carried out by a combination of active motor-driven motion on cytoskeletal filaments and diffusion in the cytoplasm. It is known that the morphology of the cytoskeletal network differs between cell types and plays a significant role in determining transport. However, the network is not static but can turnover on the same time scale as the transport of cargo on the network. Here, we study the transport of cargo carried by myosin motors on a dynamic actin network. We use a stochastic simulation model that accounts for both active transport along filaments as well as passive diffusion in the cytoplasm and incorporates the dynamics of the explicitly represented actin network. We show how filament treadmilling rates affect cargo transport along with filament lengths, densities and motor attachment/detachment rates. In particular, using simulations and simple analytics, we show that the turnover rates of the network can be optimized for fast transport and that the optimal dynamics regime is consistent with in vivo conditions. Additionally the optimal regime can be tuned by both cargo properties and filament densities and lengths suggesting new ways for cells to regulate transport.

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MS5

Impulsive Stochastic Differential Equations Applied to Plants, Fire and Rainfall

In this talk, I will illustrate a few applications of impulsive stochastic differential equations to ecological topics. In particular, I used them to study how plants respond to drought in drylands, and how wildfires will influence plant communities and their recovery. Both topics are of uttermost social and ecological relevance, given the severity of the effects climate change is predicted to have in global drylands. I represented both fires and rainfall as pulse (delta-like) perturbations to dynamical systems (ODEs). Rainfall is an intermittent input of water for the soil and plants. Plants are well adapted to the nonlinear input of water, which promotes survival and sustains biodiversity in drylands. Wildfires, in combination with climate change, can be shifting the recovery trajectory of Mediterranean forests to an alternative ecosystem state, namely an open shrubland, which is often an undesirable state from a human perspective.

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MS5

Uncertainty Quantification in Randomized Logistic Models with Harvesting

In this contributed talk, we study a class of randomized logistic models with harvesting using the so called Random Differential Equations approach. We propose a full randomization of this relevant ecological model by assuming that the per capita rate, the carrying capacity and the initial condition are random variables. In contrast, the harvesting intensity is assumed to be a parametric stochastic process representing different types of capture. We obtain semi-explicit expressions for the probability density function of the solution, which is a stochastic process. This finding is done under very general hypotheses that permit treating a wide range of probability distributions. This is a key issue from a practical standpoint since it provides more flexibility when applying Inverse Uncertainty Quantification Techniques to set adequate probability distributions to each model parameter so that the model's response can capture uncertainties in simple data. We finally illustrate all the theoretical results by means of a variety of numerical simulations and an application using real world data.

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MS5

Mathematical Modeling of the Effects of Fruit Harvesting with Application to Pentadesma Trees

The study of the synergetic effects of multiple interacting disturbances on the dynamical behavior of a biological system has received extensive attention. However, the interactions among disturbances are highly complex and the impacts are still not well understood. In this talk, we present a mathematical model based on ordinary differential equations to study the effects of exogenous pressures on the dynamics of tree ecosystems. Specifically, it incorporates the effects of non-lethal harvesting and habitat reduction. The resulting model allows the derivation of a general formula to determine the rational non-lethal harvesting level and habitat size to ensure the sustainability of the plant ecosystem. The model will be applied to fruit harvesting of pentadesma trees under different habitat sizes.

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MS5

Random and Delayed Effects on Degradation Risk in a Dryland Vegetation Model

Common dryland vegetation models exhibit bistability for a certain range of environmental conditions, with an unstable equilibrium separating the basins of attraction of the vegetated and desert states. Random perturbations may lead to irreversible degradation of locally stable vegetated states, either from sufficiently large punctual disturbances or as the result of the cumulated effect of sufficiently frequent repeated alterations. In this talk we consider a mean field vegetation model including common processes in dryland ecology, and investigate how the presence of delay effects might affect recovery and degradation risk after different scenarios of random perturbations.

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MS6

Rare Events Analysis in Bacterial Populations

Dynamical processes on high-dimensional spaces are often influenced by small random fluctuations, giving rise to rare events of interest. Such rare events, which may occur over long timescales, play a wide variety of functional roles in a number of applied settings, including evolutionary dynamics, climate change, genetic circuits, and pandemic modeling. The high dimensionality associated to these processes is often an unavoidable feature that must be considered in full. For instance, large bacterial populations consist of a large number g of cell types, called genotypes, and the genotypic composition of the population is described by a probability vector $H \in [0,1]^g$, which lives in the $(g-1)$-dimensional probability simplex. Random fluctuations over time lead to fluctuations in genotypic composition, which causes the probability vector to randomly vary over time in the $(g-1)$-dimensional probability simplex. Thus, quantifying rare events over long timescales in these high-dimensional regimes becomes a formidable theoretical and computational challenge. In this talk, we will present an explicit and efficient computational strategy for rare events analysis using a large deviations framework for a discrete-time Markov chain describing bacterial evolution of *E. coli* populations. We will particularly focus on rare events involving the frequency of some intermediate-strength genotype becoming unusually large.

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MS6

A Simple and Efficient Method for Characterizing Daily Physiology from Wearable Data

Non-invasive data collection in real-world settings with wearables provides a new opportunity for characterizing daily physiology. However, accurate and efficient characterization remains an open problem because the complex autoregressive noise of the data makes it challenging to use simple and efficient methods for inference of clock proxies (e.g., least squares method). In this talk, we will introduce a simple approximation that alters the noise structure and thus enables one to use the least squares method. We will show its usefulness for personalized inference of circadian phase of heart rate rhythms by testing the simple method on over 100,000 days of real-world data.

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MS6

Noisy Delay Denoises Biochemical Oscillators

Delay can dramatically affect the dynamics of deterministic and stochastic systems. It can stabilize metastable states for certain stochastic biochemical models that feature positive feedback, for instance. In general, delay interacts subtly with stochasticity. For genetic regulatory networks, delay results from the transcriptional, translational, and post-translational processes associated with the synthesis of regulator proteins. This protein production delay is distributed (random) and operates on the order of minutes. We know that distributed delay can accelerate signaling in feed-forward architectures. Its impact on oscillatory systems, however, remains to be assessed. Here, we show that distributed delay denoises a variety of genetic oscillators, including a degrade-and-fire oscillator, a dual-feedback oscillator, repressilators, and the Kim-Forger model. We identify the universal mechanisms that drive the denoising phenomenon and we use queueing theory to analyze them.

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MS6

Universally Valid Reduction of Oscillatory Biochemical Networks with Simple Non-eElementary Propensities

For a biochemical reaction network to generate oscillation, sufficient nonlinearity of the reactions is required. To simply generate such nonlinearity in deterministic biochemical models, non-elementary reaction functions, obtained by reducing elementary reactions, have been widely used.

Recently, the deterministically driven non-elementary reaction functions have been heuristically used for stochastic simulations with the Gillespie algorithm. While this approach has been one of the most popular methods for efficient stochastic simulations, its validity condition has remained poorly understood. In this presentation, we derive a complete condition under which this approach can accurately capture the stochastic dynamics of reversible binding between two molecules, such as protein-DNA, the basis for oscillatory biochemical networks. Furthermore, we suggest alternative simplified reaction functions for stochastic reversible binding. This provides a universally valid framework for simplifying stochastic oscillatory biochemical networks. To facilitate the framework, we provide a computational package, ASSISTER, that performs the present framework automatically.

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MS7

Why Reduced Models Work? Understanding Ionic Transport in Channels via Focusing on the Important Stuff

Biological ion channels and synthetic nanopores are responsible for controlled transport of ions through a membrane between two bulk phases. What makes these systems amenable to modeling with reduced models is that they can be viewed as devices. This means that they are tiny machines that provide a stable output signal (ionic currents) if they get a given input signal (voltage or concentration difference). The relation of the input and output parameters are called device functions. Reduced models focus on the physics that produces the device functions (i.e., the physics of how inputs become outputs) rather than the atomic details inside the pore. We present four rules of thumb for constructing good reduced models of ion channels and nanopores. They are about (1) the importance of the axial concentration profiles, (2) the importance of the pore charges, (3) choosing the right explicit degrees of freedom, and (4) creating the proper response functions that replace the implicit degrees of freedom. The art of creating a good reduced model is in distinguishing the important degrees of freedom from the unimportant degrees freedom and to model both domains properly. We show examples for both natural (calcium channels) and synthetic (bipolar) nanopores.

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MS7

Maxwell, Coupling and Mitochondria

Mitochondria convert electron flow to H^+ gradients, which in turn produce ATP that powers the chemistry of life. The chemical and structural detail of these processes is known in magnificent and overwhelming detail, but quantitative analysis has proven elusive. The structure concentrates on atoms, molecules and charge, but as any engineer knows, it is the currents that allow manageable analysis. There are too many atoms, more than 10^{18} and interactions, to compute or understand,. The Maxwell equations enforce exact conservation of total current, including the ethereal current $\epsilon_0 \partial E/\partial t$ in a trivial but necessary generalization of Kirchhoffs current law. Huaxiong Huang, Shixin Xu, Zilong Song, and I have combined Kirchhoffs law with a field theory of chemical reactions to model a key component of the mitochondrion, cytochrome c oxidase. Coupling occurs both on the atomic chemical scale and the macroscopic scale. The coupling depends on the macroscopic structure in which the transporter oxidase is embedded. Coupling is different in the mitochondrion and in voltage clamps because the boundary conditions are different. The Maxwell equations create a component of coupling independent of atomic detail, just as they can couple chemically independent currents through the sodium and potassium channels of the nerve action potential. This coupling is essentially invisible in a structural description that focuses on atoms and neglects current.

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MS7

Recent Advances in Two Types of Ion Flow: Reaction/Diffusion in the Excess Buffer Limit and Advection/Diffusion of Hard Sphere Ions

While different, ion fluxes from either reaction/diffusion or advection/diffusion are important in many fields. Here, we review a recent analytic solution to the reaction/diffusion equations and how to include finite-sized ions (vs. point ions) in a simple advection/diffusion system. The reaction/diffusion equations in the excess buffer limit were recently solved analytically for one-dimensional flow from a point source (e.g., flow in a plane or in 3D space from a point source). This is generalized a numerical algorithm for fast simulations of particle flows from many sources. For advection/diffusion, we consider nanofluidic slits where ions are driven by either pressure or voltage gradients. We add the size of ions by coupling classical density functional theory of charged hard sphere fluids in the transverse direction between the slit walls and computing ion flux with the 1D Navier-Stokes equations.

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MS7

IV Curve Prediction of KcsA Potassium Channel

KcsA is a K channel with four subunits symmetrically ar-

ranged around the channel axis. Each subunit has two transmembrane helixes separated by a reentrant Ploop and selectivity filter (SF). SF of KcsA, consisting of a sequence motif (TVGYG), is essential for permeation and selectivity. Four K ion-binding sites exist inside SF, designated S1-S4. In addition, K ion can bind at intracellular/extracellular vestibules of SF designated as S5 and S0 sites. SF is generally too narrow to accommodate a K ion with its hydration shell, and thus must be dehydrated to enter SF. IV curve simulated from classic PNP equations has a serious mismatch with experiment due to the ignorance of steric effect and dehydration. Bikerman-Born-PB model is then used to cure this problem, by which we found in SF K only occupies S0, S2, S3, and S5 leaving S1 and S4 to be void at equilibrium. This is also verified by our MD simulation. The voidness of K at S1 and S4 sites makes these two sites ion-depletion zones, which robustly persist even when voltage is applied, and render Bikerman-Born-PNP model failing to produce any current when voltage is applied. No occupancy at S1 and S4 implies that K ion would jump over these two sites during its permeation through SF, which is not suitable to be modeled by a continuum concept. A reaction rate model was constructed for it with rate constants estimated by all atoms MD energy profiles. The IV curve predicted by our reaction rate model agrees well with experiment.

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MS8

Dynamics of Flags over Wide Ranges of Mass and Bending Stiffness

There have been many studies of the instability of a flexible plate or flag to flapping motions, and of large-amplitude flapping. Here we use inviscid simulations and a linearized model to more generally study how key quantitiesmode number (or wave number), frequency, and amplitudedepend on the two dimensionless parameters: flag mass and bending stiffness. In the limit of small flag mass, flags perform traveling wave motions that move at nearly the speed of the oncoming flow. The flag mode number scales as the -1/4 power of bending stiffness. The flapping frequency has the same scaling, with an additional slight increase with flag mass in the small-mass regime. The flapping amplitude scales approximately as flag mass to the 1/2 power. For large flag mass, the dominant mode number is low (0 or 1), the flapping frequency tends to zero, and the amplitude saturates in the neighborhood of its upper limit (the flag length). In a linearized model, the fastest growing modes have somewhat different power law scalings for wave number and frequency. We discuss how the numerical scalings are consistent with a weakly nonlinear model.

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MS8

Dynamics of Tethered Membranes in Inviscid Flow

We study the dynamics of membranes (with stretching stiffness but zero bending stiffness) that shed vortex wakes in inviscid flows. Previous studies have focused on membranes with fixed ends, where only static deflection occurs. Here we consider instead membranes held by tethers with hinged ends, and find that a variety of unsteady large-amplitude motions, both periodic and chaotic, may occur. We characterize the dynamics over ranges of the key parameters: membrane mass density, stretching stiffness, pretension, and tether length. We find the region of instability and the small-amplitude behavior in a linearized model by solving a nonlinear eigenvalue problem. We also derive asymptotic scaling laws by considering a simplified model: an infinite periodic membrane. We find qualitative similarities among all three models in terms of the oscillation frequencies and membrane shapes at small and large values of the parameters.

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MS8

Propulsion by Flexible Appendages and Hydrodynamic Schooling

I will discuss propulsion by flexible appendages, as in swimming or flying. A small-amplitude flow model combined with an efficient Chebyshev PDE solver and conformal mapping techniques enables efficient numerical solutions. These solutions elucidate the performance benefits garnered by optimizing flexibility characteristics of appendages. The method also generalizes to multiple flapping bodies through the so-called prime function. New results shed light on flow-mediated collective behavior, such as schooling and flocking.

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MS8

Unsteady Aerodynamic Theory for Membrane Wing Fliers

Mammalian fliers, such as flying squirrels and bats, are known for their use of extensible membranes for gliding and flight. These membrane wings adapt their shape passively to unsteady flow conditions, enabling several aerodynamic advantages over rigid wings. In pursuit of a theoretical model for evaluating these benefits, a theoretical framework is developed to predict the response of a two-dimensional membrane wing to unsteady flow conditions. An extensible membrane model is applied, assuming small camber and constant tension along the membrane, and the aerodynamic load on the airfoil is obtained using unsteady thin airfoil theory, permitting the analysis of vertical gust encounters or prescribed flapping motions. The membrane structural and lift responses to arbitrary prescribed motions and vertical gusts enable the derivation of extensions to the classical Theodorsen, Wagner, Sears, and Küssner functions that represent the rigid airfoil lift response to unsteady flow. These extensions constitute the first known effort to include membrane fluid-structure interaction in the analytical expressions used to describe the unsteady lift response of a flexible airfoil.

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MS9

Gβ Mediated Diffusive Coupling Synchronizes Actin Oscillators in Cell Motility

At the cortex of Dictyostelium, the actin cytoskeleton localizes in discrete patches which have been shown to oscillate at different phases. Recent findings suggest that the spatial coordination of actin oscillators is regulated by the G protein subunit Gβ, which diffuses rapidly throughout the cell. Upon Gβ sequestration, the following phenomena are observed: (1) higher fraction of actin patches becomes oscillatory; (2) phase difference between different sectors becomes smaller. To understand these observations, we model each actin patch as a conditional oscillator, which is governed by an excitable activator-inhibitor model coupled by bulk diffusion of Gβ. Assuming that Gβ promotes the actin activator Arp2/3 in each actin patch, we find that actin oscillations can emerge when the Gβ concentration is low. We show that spatial heterogeneity of Gβ can lead to phase differences in actin oscillators. We consider how additional spatial coupling by Arp2/3 can influence spatial patterning in this system.

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MS9

Robust Organ Initiation Requires Robust Hormone Patterning Conferred by Proper Ribosomal Function

Robustness, the invariant development of organs despite environmental influence and stochastic fluctuation, is crucial to organ function and organismal fitness. An Arabidopsis flower robustly develops four sepals that are of constant size, shape, and position. This enables the sepals to tightly close and protect the inner reproductive organs during their development. We previously found that the development related myb-like1 (drmy1) mutant develops sepals of variable size and shape, correlating with variable hormone patterning. But it remained unknown how the DRMY1 gene makes hormonal patterns and sepal development robust. In this work, we found that the drmy1 mutant has defective ribosomal function which is sufficient to disrupt robust hormone patterning. Using hormone mutants and treatments, we found that the change in hormone patterning is necessary and sufficient for variable sepal development. In addition, we propose that these hormone changes act to alleviate ribosome defects in this mutant and causes developmental variability as a side effect. Our results show that robust organ development needs robust hormone patterning, which in turn needs proper ribosomal function. Our work further suggests that ribosomes, an essential part of every cell, can have specific influences on how groups of cells are coordinated to grow into organs of robust size and arrangement.

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MS9

Turing Pattern Formation with Concentration-Dependent Domain Evolution

Pattern formation in reaction-diffusion systems has been extensively studied in the context of growing domains, with domain evolution implicated in pattern robustness and selection, with evolving domains also being a natural modelling framework for developmental scenarios. However, the majority of work to date has considered prescribed domain changes, rather than the more realistic prospect of concentration-dependent growth. In this talk, we develop a framework to model reaction-diffusion systems on manifolds that evolve in a concentration-dependent way. In particular, we pose a general form of one-dimensional domain growth, and extend this to n-dimensional manifolds under mild constitutive assumptions in the absence of more sophisticated mechanical considerations. Via linear stability analysis, using a comparison principle for non-autonomous evolving systems, we explore the impact of concentration-dependent growth on the initiation of pattern formation, showing that it can be reduced to the analysis of a particular prescribed growth model. We then numerically demonstrate a variety of dynamical regimes in one dimension, before presenting a variety of examples in planar geometries, which each give rise to a variety of new phenomena due to the coupling of reactions, diffusion, and growth. The dynamics we observe raise important questions in the modelling and analysis of biological systems, in addition to further mathematical analysis.

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MS9

Homeostasis in Input-Output Networks, with Applications to Biological Systems

Homeostasis refers to an important phenomenon in biology whereby the output x_o of a system is approximately constant on variation of an input I. We classify different homeostasis types in input-output networks networks with an input node and a different output node. We assume that only the input node depends explicitly on the input and that the output is the node value $x_o(I)$. We study infinitesimal homeostasis: points I_0 where $(dx_o/dI)(I_0) = 0$. We prove that the homeostasis types correspond to a set of irreducible blocks each associated with a subnetwork and these subnetworks divide into two classes: structural and appendage. Moreover, we discover an algorithm for determining the homeostasis subnetwork without performing numerical simulations on model equations. Applications to biochemical networks will be discussed.

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MS10

The Workflow of ML/DL Based Drug Discovery: from Lead Generation to Potency, ADMET, and Side-Effect Screening

Traditional drug design takes 2.6 billion dollars and 10-15 years to put an average new drug on the market. ML/DL and computational chemistry show a great potential to revolutionize drug discovery. My series of innovative ML/DL and computational chemistry models form a whole workflow of in silico drug discovery from lead generation, potency prediction, ADMET, and side-effect screening to binding simulations, which can largely replace traditional lab tests. These models outperform the published state-of-the-art methods in numerous standard benchmarks. More importantly, our models are the largest winner in D3R Grand Challenges (Drug Design Data Resource Blinded Community Prediction Challenges).

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MS10

Bayesian Topological Learning for Classifying the Structure of Biological Networks

Actin cytoskeleton networks generate local topological signatures due to the natural variations in the number, size, and shape of holes of the networks. Persistent homology is a method that explores these topological properties of data and summarizes them as persistence diagrams. In this work, we analyze and classify these filament networks by transforming them into persistence diagrams whose variability is quantified via a Bayesian framework on the space of persistence diagrams. The proposed generalized Bayesian framework adopts an independent and identically distributed cluster point process characterization of persistence diagrams and relies on a substitution likelihood argument. This framework provides the flexibility to estimate the posterior cardinality distribution of points in a persistence diagram and the posterior spatial distribution simultaneously. We present a closed form of the posteriors under the assumption of Gaussian mixtures and binomials for prior intensity and cardinality respectively. Using this posterior calculation, we implement a Bayes factor algorithm to classify the actin filament networks and benchmark it against several state-of-the-art classification methods.

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MS10

Generative Ai Drug Discovery

Machine learning algorithms have given us new tools to computational drug design. Here, I discuss our use of machine learning in optimizing binding affinity predictions and generating novel molecules for COVID-19 drug discovery. The methods we are using are based on deep neural networks, genetic algorithms, and a new data representation for molecules called SELFIES. Our drug binding predictions are comparable to state-of-the-art free energy calculations but a small fraction of the computational cost. Our generative chemistry algorithms are able to invent new molecules with high predicted activity with minimal input from a human user.

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MS10

Neighborhood-Complex Based Machine Learning (NCML) Models for Drug Design

The importance of drug design cannot be overemphasized. Recently, artificial intelligence (AI) based drug design has begun to gain momentum due to the great advancement in experimental data, computational power and learning models. However, a major issue remains for all AI-based learning models is efficient molecular representations. Here we propose Neighborhood complex (NC) based molecular featurization (or feature engineering), for the first time. In particular, we reveal deep connections between NC and Dowker complex (DC) for molecular interaction based bipartite graphs, for the first time. Further, NC-based persistent spectral models are developed and the associated persistent attributes are used as molecular descriptors or fingerprints. To test our models, we consider protein-ligand binding affinity prediction. Our NC based machine learning (NCML) models, in particular, NC-based gradient boosting tree (NC-GBT), are tested on three most-commonly used datasets, i.e., including PDBbind-v2007, PDBbind-v2013 and PDBbindv2016, and extensively compared with other existing state-of-the-art models. It has been found that our NCML models can achieve state of-the-art results.

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MS11

Extracting Intrinsic Neural Features of Bistable Perception with the Extended Dynamic Mode Decomposition

Perceptual bistability refers to an observers susceptibility

to admit two interpretations of an unchanging stimulus. Neurophysiological studies of bistable perception typically partition neural measurements into stimulus-based epochs where differences are assessed based on subject perceptual reports. Computational studies of bistable perception incorporate hypothesized mechanisms into models that replicate established behavioral principles of perception. To bridge the two approaches, we integrated techniques from data-driven dynamical systems and dimensionality reduction to derive intrinsic neural features from electrocorticography recordings in primary auditory cortex from humans performing an auditory bistable task. Within the derived features, we identified an ensemble of oscillators that exhibited phase-shifts entrained to a slowly-drifting variable aligned with subject-reported changes in perception. Projecting the neural data onto the drifting oscillators revealed low-dimensional dynamics along manifolds with discernible attracting states. By examining the neural data on timescales consistent with those used in computational models, we provide neural evidence supporting the biological plausibility of attractor-based computational principles. The feature extraction techniques used here generalize across recording modalities and are appropriate for instances when hypothesized low-dimensional dynamics characterize an underlying neural system.

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MS13

Modeling Asymmetries in Centrosome Protein Recruitment in the Early C. Elegans Embryo

Centrosomes are small nucleus-associated organelles that serve as the nucleation site for microtubule arrays. These microtubule arrays interact with motor proteins such as dynein at the periphery of the cell and position the nucleus prior to division. Proper positioning is especially important in asymmetric cell division, where daughter cells inherit unequal amounts of specific factors. In polarized cells, where specific factors are segregated to opposite ends of the cell as seen in early embryos of the nematode worm C. elegans, asymmetric cell division occurs as a result of dynein-mediated centrosome positioning along the polarity axis. Using a combination of stochastic and continuum models with experimental validation, we show that centrosome asymmetry is critical for centrosome positioning in the early C. elegans embryo, and that this asymmetry arises from differential recruitment of proteins to centrosomes during their maturation process.

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MS13

Learning Mechanisms of Chromosomal Movement During Mitosis

For cells to divide, they must undergo the process of mitosis: the spatial organization of their copied genetic material to precise locations. This task is done with surprising speed and accuracy, but the underlying microscopic molecular mechanisms are difficult to observe or disentangle. Instead, we take a data-driven approach by using macroscopic trajectory data to statistically learn dynamical interactions that drive the underlying motion. To explain these emergent interactions, we consider mechanistic models of the mitotic spindle describing various microtubule geometries and forces from molecular motors. By learning models directly from the data, we deduce possible microscopic mechanisms of how chromosomes are gathered to the spindle from their macroscopic movement. This work is in collaboration with Alex Mogilner (NYU) and the lab of Alexey Khodjakov (Wadsworth Center, NY State Dept of Health).

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MS13

Meandering through Networks: Protein Dispersion and Accumulation in the Endoplasmic Reticulum

The endoplasmic reticulum (ER) is a dynamic, membranous network of tubules and sheets stretching from the nuclear envelope to the cell periphery. Its crucial roles include facilitating the diffusive spread of proteins, lipids and ions throughout the cell, but the specific effects of network structure on these processes are not well understood. In prior work we developed fast, agent-based simulations of particles diffusing on tubular networks, using pre-computed propagators to enable particles to step efficiently from node to node. We leverage this method, together with analytic results for search times on a network, to explore the effects of heterogeneous network morphology on particle encounter kinetics. Our results are compared to dynamic in vivo measurements of photoactivated membrane proteins spreading through the ER, as well as accumulation of proteins at ER exit sites. In particular, we show that dynamic network rearrangements increase the spatial variability of protein spreading from an initial bolus. Our results highlight key structure-function relationships for the ER, linking its network architecture with its role as an intracellular transport system.

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MS13

The Influence of the Endothelial Surface Layer on the Motion of Red Blood Cells

The endothelial lining of blood vessels presents a large surface area for exchanging materials between blood and tissues. The endothelial surface layer (ESL) plays a critical

role in regulating vascular permeability, hindering leukocyte adhesion as well as inhibiting coagulation during inflammation. Once the ESL is pathologically altered, the changes in its topography are believed to cause vascular hyperpermeability and induce thrombus formation during sepsis. The occurrence of these biological phenomena requires Red Blood Cells (RBCs) stay within close proximity to the ESL, initiating RBC-layer interaction. To investigate the influence of various physical properties of the ESL on the motion of RBCs, we construct two models to represent the ESL combined with the immersed boundary method. In particular, we focus on analyzing how lift force and drag force change over time when a RBC is placed close to the ESL as the width, roughness, and permeability of the ESL vary. Our results suggest that increase in the ESL thickness has a dominant effect in slowing down the motion of RBCs for all physically-relevant permeability values, hindering the migration of RBCs from the layer; whereas effect of the roughness is minimal.

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MS14

Stochasticity Incorporated into Modeling Epidemiological Dynamics

In outbreaks, studying host heterogeneity based on demographic and/or environmental factors is critical to understanding the spread of infectious diseases. We will explore a base ordinary differential equation model, then incorporate heterogeneity through stochastic models formulated as a time-nonhomogeneous stochastic process (NHP) model with discrete random variables and a stochastic differential equation (SDE) model with continuous random variables.

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MS14

Generalized Stressors on Social Bee Colonies

Social bees play an integral role in enhancing agricultural sustainability and ecosystem preservation. The recent decline of social bee colonies highlights the value in understanding possible causes. Environmental stressors that interfere with social bee behavior and efficiency have been identified through mathematical models and empirical experiments as a potential cause for colony collapse. We model impairment due to stressors through a traditional disease modeling framework, building on existing mathematical models by stratifying the colony by impairment and caste. Further, we generalize the attributes of stressors such as their transmissibility, impairment level, lethality, and temporal-occurrence. Our model underscores the importance of further investigation into the various attributes of sublethal stressors as a cause for colony collapse.

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MS14

Modeling Immunity to Malaria with an Age-Structured PDE Framework

Individuals acquire protection from malaria through repeated exposure, and this immunity plays a crucial role in the dynamics of malaria spread. We develop and analyze an age-structured PDE model, which couples vector-host epidemiological dynamics with immunity dynamics. Our model tracks the acquisition and loss of anti-disease immunity during transmission and its corresponding nonlinear feedback onto the transmission parameters. We derive the basic reproduction number ($\mathcal{R}_0$) as the threshold condition for the stability of disease-free equilibrium and interpret $\mathcal{R}_0$ probabilistically as a weighted sum of cases generated by infected individuals at different infectious stages and ages. Numerical bifurcation analysis demonstrates the existence of an endemic equilibrium that spawns through a forward bifurcation in $\mathcal{R}_0$ (in the absence of disease-induced mortality) and we study the structure of this equilibrium as a function of system parameters. Our model reproduces the heterogeneity in the age distributions of immunity profiles and infection status created by frequent exposure. Motivated by the recently approved RTS,S vaccine, we also study the impact of vaccination; our results show a reduction in severe disease among young children but a small increase in severe malaria among older children due to lower acquired immunity from delayed exposure.

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MS14

Optimal Control Techniques in Addiction Modeling

Substance use disorders are often viewed mathematically as a social disease, where addictive behaviors are assumed to spread through social contact between individuals. Treating substance use disorders strictly as an infectious disease excludes those who develop this condition in isolation. In this talk, we extend SIS and SIR disease models to the context of substance use disorders by including both contact and non-contact routes into addiction. With the inclusion of non-contact, linear addiction rates, the dynamics of the model fundamentally change so that the addiction-free equilibrium (AFE) and the basic reproductive number no longer exist. To analyze these models, we instead employ techniques from optimal control to determine strategies which minimize substance use disorder in a population where the AFE does not exist.

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MS15

Synchronization of Oscillations in Pancreatic Islets

Insulin is secreted in pulses by beta-cells located in micro-organs within the pancreas called islets of Langerhans. Somehow the pulsatility is synchronized across the islet population, which consists of hundreds of thousands of islets, even though there is no physical contact among islets. The insulin secreted by beta-cells acts on liver hepatocyte cells to uptake glucose from the blood and the subsequent drop in glucose concentration reduces insulin secretion from beta-cells. One hypothesis is that this closed-loop system is responsible for islet synchronization. In this presentation, we describe our investigation of this synchronization mechanism, combining mathematical modeling with microfluidic experiments. A major focus is the delay between the time that liver cells act to uptake glucose and the time the reduction in glucose concentration is sensed by islets in the pancreas. How does this time delay affect islet synchronization? Can it contribute to the slow ultradian oscillations often observed in measurements of insulin from humans and other mammals?

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MS15

A Model of Non-Modular Biochemical Oscillator and Switch

Periodic gene expression dynamics are key to cell and organism physiology. Studies of oscillatory expression have focused on networks with intuitive regulatory negative feedback loops, leaving unknown whether other common biochemical reactions can produce oscillations. Oscillation and noise have been proposed to support the capacity of mammalian progenitor cells to restore heterogenous, multimodal expression from extreme subpopulations, but underlying networks and specific roles of noise remained elusive. We use mass-action-based models to show that regulated RNA degradation involving as few as two RNAs, applicable to nearly half of human protein-coding genes, can generate sustained oscillations without imposed feedback. Diverging oscillation periods synergize with noise to robustly restore cell bimodal gene expression in cell populations. The global bifurcation organizing this divergence relies on an oscillator and bistable switch which cannot be decomposed into two structural modules. Our work reveals surprisingly rich dynamics of post-transcriptional reactions and a potentially widespread mechanism useful for development and regeneration.

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MS15

Spiral Waves in Oscillatory Media with Nonlocal Coupling

Biological and physical systems that can be classified as oscillatory media give rise to interesting phenomena like target patterns and spiral waves. The existence of these structures has been proven in the case of systems with local diffusive interactions. In this talk the more general case of oscillatory media with nonlocal coupling is considered. We model these systems using evolution equations where the nonlocal interactions are expressed via a diffusive convolution kernel, and explore the existence of rotating wave solutions for these systems.

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MS15

Combined Multiple Transcriptional Repression Mechanisms Generate Ultrasensitivity and Oscillations

Transcriptional repression can occur via various mechanisms, such as blocking, sequestration, and displacement. For instance, the repressors can hold the activators to prevent binding with DNA or can bind to the DNA-bound activators to block their transcriptional activity. Although the transcription can be completely suppressed with a single mechanism, multiple repression mechanisms are utilized together to inhibit transcriptional activators in many systems, such as circadian clocks and NF-?B oscillators. This

raises the question of what advantages arise if seemingly redundant repression mechanisms are combined. Here, by deriving equations describing the multiple repression mechanisms, we find that their combination can synergistically generate a sharply ultrasensitive transcription response and thus strong oscillations. This rationalizes why the multiple repression mechanisms are used together in various biological oscillators. The critical role of such combined transcriptional repression for strong oscillations is further supported by our analysis of formerly identified mutations disrupting the transcriptional repression of the mammalian circadian clock. The hitherto unrecognized source of the ultrasensitivity, the combined transcriptional repressions, can lead to robust synthetic oscillators with a previously unachievable simple design.

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MS16

Efficient Tetrahedral Mesh Generation Scheme for Ion Channel Simulation

A finite element solution of an ion channel dielectric continuum model such as Poisson-Boltzmann equation (PBE) and a system of Poisson-Nernst-Planck equations (PNP) requires tetrahedral meshes for an ion channel protein region, a membrane region, and an ionic solvent region as well as an interface fitted irregular tetrahedral mesh of a simulation box domain. However, generating these meshes is very difficult and highly technical due to the three related regions having very complex geometrical shapes. In this talk, we will introduce a new and efficient mesh generation package for finite element ion channel calculation. Then several applications are presented.

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MS16

An Efficient Method for Calculating Current-Voltage Curves from Fully Atomistic Simulations

In this talk, I will present an enhanced sampling scheme using the Weighted Ensemble framework aimed at computing current voltage curves from all-atom molecular simulations of narrow ion channels. We show that the method matches brute force simulation of a small, model nanopore. It also matches all-atom K+ currents computed from brute force simulations of KcsA under non-physiologically large voltages, while also efficiently computing currents over a the physiological voltage range. The method becomes more efficient as the flux becomes smaller as when examining selectivity for poorly permeant ions. We discuss how this method can be extended to other systems such as lipid flipping by scramblases and how it can be used to explore forcefield parameterization.

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MS16

An Inverse Averaging Finite Element Method for Solving Three-Dimensional Poisson-Nernst-Planck Equations in Nanopore System Simulations

The Poisson-Nernst-Planck (PNP) model plays an important role in simulating nanopore and ion channel systems. In nanopore simulations, the large-size nanopore system and convection-dominated Nernst-Planck (NP) equations will bring convergence difficulties. Therefore, we propose an improved finite element method (FEM) with an inverse averaging technique to solve the three-dimensional PNP model, named inverse averaging FEM (IAFEM). First, the Slotboom variables are introduced to transform the non-symmetric NP equations into self-adjoint 2nd-order elliptic equations with exponentially behaved coefficients. Then, these coefficients are approximated with their harmonic averages calculated with an inverse averaging technique on every tetrahedral element edge. Our scheme shows good convergence when simulating single or porous nanopore systems, and it is stable for convection-dominated NP equations. Our method also guarantees conservation of currents, which some other stabilization schemes do not possess. Our numerical experiments on benchmark problems verify the scheme's accuracy and robustness, and the method performs better than the standard FEM for convection-dominated problems. A simulation of realistic chemical experiments is presented to illustrate that the IAFEM is effective for three-dimensional interconnected nanopores, ion channel, and semiconductor devices.

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MS16

A New Finite Element Iterative Solver for a Nonuniform Size Modified Poisson-Boltzmann Ion Channel Model

Size modified Poisson-Boltzmann (SMPB) equations have been studied for more than thirty years. However, how to efficiently solve a nonuniform SMPB ion channel (nuSMPBIC) model remains a difficult research topic. In fact, a nuSMPBIC model is a complex nonlinear system that mixes n nonlinear algebraic equations with one Poisson boundary value problem when a solution contains n ionic species. It also involves two physical domains — a simulation box domain for potential functions and a solvent domain for ionic concentration functions, not to mention its strong singularities and nonlinearities. In this talk, I will present a new finite element iterative scheme for solving a nuSMPBIC model. The novelty of this scheme lays on a damped two-block iterative method and a modified Newton iterative scheme for solving each related nonlinear algebraic system. This scheme has been implemented as a program package for an ion channel protein with a three-dimensional molecular structure and a solution of n ionic species with distinct ion sizes. Numerical results for a voltage-dependent anion channel in a mixture of four ionic species will be reported in this talk to demonstrate a fast convergence rate of the damped two-block iterative method, the high performance of the software package, and the importance of considering nonuniform ion sizes. This work was partially supported by the Simons Foundation,

USA, through research award 711776.

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MS17
Fluid Inertia and the Scallop Theorem

In Stokes flow, Purcell's scallop theorem forbids objects with time-reversible (reciprocal) swimming strokes from moving. In the presence of inertia, this restriction is eased and reciprocally deforming bodies can swim. Recent work has investigated an asymmetric spherical dimer of oscillating length as a simple model swimmer. Analytical, numerical, and experimental studies have shown a dense (i.e. inertial) dimer swims in Stokes flow. Similarly, numerical study shows a dimer in fluid of intermediate Reynolds number (Re = 1-1000) swims in a direction that varies depending on the degree of fluid inertia. Here, we introduce a general model for the inertial flow produced by an oscillating dimer at small amplitudes. We apply the finite element method, using the PETSc library to solve a coupled pair of linear PDEs, to probe the dimer's swim speed with respect to the degree of fluid or solid inertia. The results are compared to asymptotic solutions obtained via the method of reflections. We find the model's predictions match those of the dense Stokes swimmers in the appropriate limit, and that the behavior in inertial fluid is consistent with previous numerical analysis.

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MS17
Dynamics of Membrane Growth and Form

The growth, form, and division of membrane-bound vesicles and organelles is a unifying motif across biology. Membranes form the boundaries of the nucleus and cell, organelles such as mitochondria and endoplasmic reticulum, and vesicles used to transport proteins and other biomolecules. Importantly, these membranes are out-of-equilibrium systems as their lipid constituents are in a state of continual turnover and exchange. Here, we build on a model [Ruiz-Herrero, Fai, and Mahadevan, Dynamics of growth and form in prebiotic vesicles, PRL (2019)] in which vesicle growth is driven purely by physicochemical processes of membrane growth, permeability, and elasticity. We use the immersed boundary method to explore the fluid-structure interaction of growing vesicles. By comparing our simulation results to experiments on fatty acid vesicles, we show how the model captures essential behaviors required of prebiotic vesicles, membraneous bags of fluid of varying components and shapes is hypothesized to have served as the substrate for the origin of life.

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MS17
Glider Soaring in Turbulent Flows

A glider moving in a turbulent flow will continuously lose energy via drag. To balance this loss in energy and soar, energy must be continuously extracted from the flow, either by localizing in stable ascending currents (thermal soaring) or in a stable shear region (dynamic soaring). Recent observations of soaring birds show convoluted trajectories distinct from characteristic patterns exhibited during thermal and dynamic soaring, raising the intriguing possibility that energy can be extracted purely from transient ascending currents or shear. In this work, we simulate gliders navigating in a turbulent flow, which use their past experience to infer a strongly fluctuating flow field and actively make decisions. We build the decision-making component using a Monte Carlo tree search (MCTS), which exploits an adaptive filtering and prediction system to consider many paths into the future and execute a trajectory that maximizes the energy gained. We demonstrate the ability of gliders to extract energy from the flow, and identify the significant factors necessary for effective turbulent navigation.

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MS17
The Loopy Fluid Dynamics of Bird Lungs

We here present the results of a combined experimental and theoretical investigation into the fluid flows induced by an oscillating piston in a network with two connected loops. This system is inspired by the loopy airways of bird lungs which, unlike the branched airways of mammalian lungs, exhibit directed flows throughout the breathing cycle. Such directed flows have intrigued biologists since their observation a century ago, but the underlying mechanism behind pumping without valves has remained elusive. In both experiments and numerical simulations, we find that the oscillatory flow generated by the piston in one segment of the network is transformed into a directed flow in the other segment. Our simulations reveal that flow separation and vortex shedding at network junctions serve the valuing function of directing flows with appropriate timing in the oscillation cycle. These findings suggest strategies for controlling inertial flows through network topology and junction connectivity.

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MS18
A Mechanistic Model of Cellular Morphological Response to Cyclic Stretch

Many cells in the body experience cyclic mechanical loading, which can impact cellular processes and morphology. In vitro studies often report that cells reorient in

response to cyclic stretch of their substrate. To explore cellular mechanisms involved in this reorientation, a computational model was developed by adapting a previously developed model of the actinmyosinintegrin motor-clutch system. The model predicts that under most conditions, actin bundles align perpendicular to the direction of applied cyclic stretch, but under specific conditions, such as low substrate stiffness, actin bundles align parallel to the direction of stretch. The model also predicts that stretch frequency impacts the rate of reorientation and that proper myosin function is critical in the reorientation response. These predictions are consistent with reports from the literature and new experimental results. The model suggests that the impact of different stretching conditions on the direction of cell alignment can largely be understood by considering their impact on cellsubstrate detachment events, specifically whether detachments preferentially occur during stretching or relaxing of the substrate.

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MS18

Topological Data Analysis Reveals Insights into Blood Vessel Development and Disease

Vascular networks deliver nutrients and remove waste from tissues and play a pivotal role in many biological processes, including development and homeostasis. As the structure of vascular networks determines their overall function, we develop and analyze several statistical and topological approaches to quantify morphological patterns observed from data. We highlight the success of these methods through two case studies. In the first, we show that a topological filtration can be used to stratify the parameter space from many simulations of an agent-based model of angiogenesis. In the second case study, we apply statistical and TDA methods to several public datasets of segmented vascular network images and find that both approaches can be used to accurately predict images disease status. The methodologies we consider are broadly applicable to biological data that may arise from cancer, wound healing, development, and plant biology.

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MS18

Optimizing Parameter Estimation through Experimental Design and Analysis of Model Trajectories in State Space

The metabolic pathways of bacteria can be used in the synthesis of chemical products. Bioengineers are exploring the use of Microcompartments (MCPs), protein structures native to the bacteria which spatially organize the metabolism, to optimize the production of desired products. The relative time scales set by the permeability of the cell membrane, the permeability of the MCP shell, and the reaction kinetics determine if encapsulation can be used to optimize the flux. Estimating the permeability values and kinetic rates is essential to effectively engineer the metabolic pathway. The system can be described by a set of coupled PDEs with Robin boundary conditions in which only the external boundary states can be measured and the Robin coefficients are the unknown permeabilities of the cell and MCP. Estimating the permeabilities requires solving a high dimensional optimization problem in which most state variables are unmeasured or hidden. We develop a method, informed by the mathematical model and experimental observations, to plot the model manifold in state space and determine which characteristics of the measured states are most sensitive to unknown parameters. The discovered regions of high sensitivity in progress space are used to inform experimental design. This insight is used to reduce the dimension of the observations in the parameter estimation problem, improving computational time for parameter estimation.

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MS18

Dissecting Transition Cells from Single-Cell Transcriptome Data Through Multiscale Stochastic Dynamics

Advances in single-cell technologies allow scrutinizing of heterogeneous cell states, however, detecting cell-state transitions from snap-shot single-cell transcriptome data remains challenging. To investigate cells with transient properties or mixed identities, we present MuTrans, a method based on multiscale reduction technique to identify the underlying stochastic dynamics that prescribes cell-fate transitions. By iteratively unifying transition dynamics across multiple scales, MuTrans constructs the cell-fate dynamical manifold that depicts progression of cell-state transitions, and distinguishes stable and transition cells. In addition, MuTrans quantifies the likelihood of all possible transition trajectories between cell states using coarse-grained transition path theory. Downstream analysis identifies distinct genes that mark the transient states or drive the transitions. The method is consistent with the well-established Langevin equation and transition rate theory. Applying MuTrans to datasets collected from different single-cell experimental platforms, we show its capability and scalability to robustly unravel complex cell fate dynamics induced by transition cells in systems such as tumor EMT, iPSC differentiation and blood cell differentiation. Overall, our method bridges data-driven and model-based approaches on cell-fate transitions at single-cell resolution.

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MS19

Evolutionary de Rham-Hodge Method

The de Rham-Hodge theory is a landmark of the 20^{th} Cen-

tury's mathematics and has had a great impact on mathematics, physics, computer science, and engineering. This work introduces an evolutionary de Rham-Hodge method to provide a unified paradigm for the multiscale geometric and topological analysis of evolving manifolds constructed from a filtration, which induces a family of evolutionary de Rham complexes. While the present method can be easily applied to close manifolds, the emphasis is given to more challenging compact manifolds with 2-manifold boundaries, which require appropriate analysis and treatment of boundary conditions on differential forms to maintain proper topological properties. Three sets of unique evolutionary Hodge Laplacians are proposed to generate three sets of topology-preserving singular spectra, for which the multiplicities of zero eigenvalues correspond to exactly the persistent Betti numbers of dimensions 0, 1, and 2. Additionally, three sets of non-zero eigenvalues further reveal both topological persistence and geometric progression during the manifold evolution. Extensive numerical experiments are carried out via the discrete exterior calculus to demonstrate the potential of the proposed paradigm for data representation and shape analysis. To demonstrate the utility of the proposed method, application is considered to the protein B-factor predictions of a few challenging cases for which other existing models do not work well.

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MS19

Omnibus and Robust Deconvolution Scheme for Bulk RNA Sequencing Data Integrating Multiple Single-cell Reference Sets and Prior Biological Knowledge

Cell-type deconvolution of bulk tissue RNA sequencing (RNA-seq) data is an important step towards understanding the variations in cell-type composition among disease conditions. Various deconvolution methods have been developed. However, the performance of existing methods heavily relies on the quality of information provided by external data sources, such as the selection of single-cell RNA-seq (scRNA-seq) data as a reference and prior biological information. We present the Integrated and Robust Deconvolution (InteRD) algorithm to infer cell-type proportions from target bulk RNA-seq data. Owing to the innovative use of penalized regression with a new evaluation criterion for deconvolution, InteRD has three primary advantages. First, it is able to effectively integrate deconvolution results from multiple scRNA-seq datasets. Second, InteRD calibrates estimates from reference-based deconvolution by taking into account extra biological information as priors. Third, the proposed algorithm is equipped with a data-driven mechanism of self-control designed to be robust to the introduction of inaccurate information in the deconvolution system. Benchmark evaluations show that InteRD outperforms state-of-the-art methods. We further applied InteRD to a human pancreatic islet dataset and a human dorsolateral prefrontal cortex dataset; the results from InteRD agreed well with known biological facts.

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MS19

Cell-Cell Communication Modeling and Analysis Using Single-Cell Sequencing Data

Recent advances of single-cell technologies, in particular single-cell RNA sequencing and spatial imaging, provide an unprecedented opportunity for probing underlying intercellular communications that often drive heterogeneity and cell state transitions in tissues. In this talk, I will show our recent efforts in modeling and analyzing cell-cell communication from the high-throughput sequencing data. We developed an integrated method CellChat for systematic inference and quantitative analysis of cell-cell communication by integrating scRNA-seq data and prior knowledge of the interactions between signaling molecules. I will show how we can quantitatively build and analyze cell-cell communication networks in an easily interpretable way by applying systems biology and machine learning approaches. Furthermore, by leveraging spatial information from spatial transcriptomics, we developed a computational approach for inferring niche programs that capture the underlying cell-cell communication patterns and reveal how cells and signals coordinates together for function.

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MS19

Persistent Function based Machine Learning Models for Drug Design

Effective molecular representations are of key importance to the success of machine learning models in biomolecular data analysis. The advent of TDA has brought about a series of TDA-based machine learning models in drug design. In this talk, we will introduce a series of new persistent functions, in particular, persistent Ollivier Ricci curvature, persistent Forman Ricci curvature and persistent spectral models. Each of these persistent functions when computed under a filtration-induced persistent process results in an array of feature vectors derived from topological or geometrical invariants such as spectral eigenvalues and Ricci curvatures. The features are then inputs to deep learning and ensemble learning models which comprises of gradient boosting trees and convolutional neural networks (CNN). Our persistent Ricci curvature based molecular representations have been extensively trained and tested on three most commonly-used datasets, including PDBbind-2007, PDBbind-2013 and PDBbind-2016.

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MS20

Principles of Motor Learning and Stability in the Songbird

How are patterns of motor activity maintained in neural encodings over time despite ongoing change such as aging, injury, and fluctuations in the brain? Here we address this question by focusing on an animal model for motor learning: the songbird. Our analysis of behavioral and neural data reveals mechanisms to maintain robust song behavior at multiple scales in the songbird system. We develop a Gaussian Process model to examine dopamine neurons relationship to natural song in singing, adult birds. Spontaneous dopamine activity correlates with natural variations in song in a manner consistent with song evaluation. We then explore a second form of song maintenance that progresses with minimal behavioral feedback. Type-selective perturbations to neurons within HVC, a motor cortical-like nucleus that contributes to sequence and timing in song production, result in the rapid degradation and recovery of song in adult birds. Remarkably, recovery advances even in the absence of practice. We characterize the behavioral and neural trajectory of this perturbation process and examine though a computational biophysical model of HVC how local, unsupervised mechanisms could restore HVC dynamics without reference to behavioral feedback. This work highlights the cooperation of multiple mechanisms of adaptation and maintenance in sustaining stable motor behaviors.

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MS21

Glucose-Insulin Dynamics in Adolescent Girls with Reactive Hypoglycemia

Reactive hypoglycemia (RH) occurs when blood glucose falls below basal levels following consumption of high-sugar foods, and it can present as postprandial episodes of excess sweating, nausea, and dizziness. RH triggers a counterregulatory response that attempts to restore glucose concentrations to normoglycemic levels and represents a distinct metabolic state involving increased hepatic glucose release, increased lipolysis, and decreased peripheral glucose utilization. Standard minimal models of metabolite (e.g., glucose, insulin, glycerol, and free fatty acids) dynamics may not accurately describe the dynamics of metabolites under both standard and RH conditions. Furthermore, RH may complicate interpretation of model parameters since a single parameter is estimated from data collected under two distinct metabolic states. To model the counterregulatory response in glycerol dynamics, we developed a function to describe glycerol production due to lipolysis that allows maximum lipolysis rates to increase above basal fasted lipolysis rates in the presence of RH. We applied this model to glycerol and insulin data from adolescent girls with obesity experiencing RH during an oral glucose tolerance test. This modeling approach allows more robust representation of glycerol and insulin data occurring in individuals with RH.

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MS21

Quantifying Beta-Cell Responsivity for Patients with Cystic Fibrosis

Cystic fibrosis-related diabetes (CFRD) is the most common comorbidity among patients with cystic fibrosis (CF) and is associated with increased mortality. In patients with CF, dysglycemia is driven primarily by beta-cell failure and insulin insufficiency due to CF-related disruption of normal pancreatic function. If an individuals insulin secretion rate (ISR) during an oral glucose tolerance test (OGTT) is known, the responsivity of beta cells to a metabolic stimulus can be quantified using an established modeling approach. However, ISR cannot be measured directly during an OGTT, so reliable methods for estimating ISR profiles are needed. Since insulin secretion and clearance act on multiple timescales, C-peptide is used as a surrogate for insulin secretion. We employ a differential model of C-peptide dynamics, wherein ISR acts as a forcing function, to infer the statistical distribution of continuous ISR profiles from an individuals discrete C-peptide data. Additionally, by modeling ISR as a Gaussian process, a closed-form approximation of the ISR profile is obtained from a small number of numerically estimated parameters. This approach provides a detailed characterization of beta-cell responsivity that is more computationally efficient compared to existing methods. We apply this approach to quantify beta-cell dysfunction in a cohort of adolescents with and without CF.

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MS21

Relative Beta-Cell Function Estimation Without Insulin Measurements During Continuous

The pathogenesis of type 2 diabetes (T2D) is characterized by a relative failure of insulin-secreting pancreatic beta-cells to increase insulin concentrations to maintain normal

blood glucose concentration. Estimation of the secretory capacity of beta-cells is crucial to prevent and intervene in the disease. Glucose challenge tests have been used to estimate beta-cell function and insulin sensitivity. The product of beta-cell function and insulin sensitivity, termed the disposition index (DI), is of great value because it measures beta-cell function relative to insulin requirements. We developed a model disposition index (mDI estimated without insulin, or mDI w/o I) that does not require insulin measurements during an oral glucose tolerance test (OGTT) (Ha et al., Diabetes 2021 (70) suppl. 1). To further increase access and refine the assessments of beta-cell function, we adapted our model to calculate a model disposition index using continuous glucose monitoring (CGM). CGM has been in the spotlight of diabetes management and has revolutionized the field of medicine as they are approved for glucose monitoring and clinical decision-making in patients with diabetes.

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MS21

A New Disposition Index for Screening and Treating Type 2 Diabetes

Type 2 diabetes is a complex disease, but the known phenomenology can be reduced to the balance between insulin sensitivity (SI) and insulin secretion (beta-cell function, or BCF). High BCF can overcome low SI, and low BCF is acceptable when SI is high. More generally, if the product SI*BCF, called the Disposition Index (DI) is constant, then steady-state glucose (essentially, fasting glucose) is constant. The DI concept, developed by Cobelli and Bergman 40 years ago, is the most fundamental principle in the diabetes field. Mathematically, the SI-BCF plane can be viewed as the slow phase plane of a fast-slow system in which a separatrix divides trajectories that remain nondiabetic or tend towards diabetes. Clinically, DI has the potential to provide a diagnostic marker to distinguish normal glucose tolerance, pre-diabetes and diabetes and track pathogenesis or remission over time. Other forms of DI from other models share some of these good features, but we describe here a new DI that is easy to estimate from an oral glucose tolerance test (OGTT). Both glucose and insulin are needed to estimate SI and BCF from an OGTT, but DI requires only glucose, which is much easier and less expensive to measure. The model also provides universal diagnostic cut points appropriate for all ethnicities, whether obese and insulin resistant, such as African Americans and Europeans, or lean and insulin sensitive, such as East Asians. We confirm this with a simple dimensional analysis.

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MS22

Dueling Pacemakers and the Curious Behavior of Tunicate Hearts

"Sea squirts", such as the tunicate *Ciona savignyi*, are marine invertebrates with valveless, tubular hearts. They are widely regarded as model organisms for studying the development of vertebrate chambered hearts. Sea squirts also exhibit a bizarre phenomenon: after every minute or two of unidirectional pumping of blood, they can *reverse* the direction of blood flow. What mechanisms might underlie this odd behavior? How can we model the reversals mathematically, and what insights might this offer regarding our own hearts? To address these questions, we idealize the tubular heart as a one-dimensional excitable fiber driven by multiple pacemakers, and use an impulsively forced reaction-diffusion system to model action potential (AP) propagation. Because the reversal phenomenon can be understood through careful tracking of APs, we use perturbation methods to reduce the reaction-diffusion equations to a fully kinematic model of AP propagation. The kinematic model facilitates parameter estimation from experimental data, as well as derivation of simple mathematical criteria for reversals to occur. The models can easily replicate experimentally observed reversals while offering some clues regarding the underlying mechanisms. We conclude by discussing planned future work, including the use of optical mapping and micro-particle image velocimetry experiments to inform models coupling electrophysiology, circulation, and muscle contraction.

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MS22

Dynamics of Wall Shear Stress in Aorticopulmonary Septum Development

Intracardiac fluid factors contribute to heart development, but their mechanosensory role remains poorly understood in aorticopulmonary (AP) septum development and defects. The AP septum divides the outflow tract into the aortic artery and pulmonary trunk. Ablating AP septum precursors alters blood flow and leads to outflow tract defects. In fact, shortly after precursor removal, hemodynamic changesprecedemajor defects. However, there are limited data of blood velocity, pressure, and wall shear stress (WSS) in the outflow tract under both normal and ablated conditions. Due to the constant pumping and small size of the embryonic heart, WSS can not always be measured *in vivo* and is often roughly approximated. I develop computational models of fluid-structure interaction (FSI) of the embryonic chick heart that reveal the precise spatial and temporal patterning of WSS in the outflow tract during AP septum development under various hemodynamic conditions. First, I manually elevate WSS in the embryonic chick by elevating hematocrit levels and construct the FSI model from the resulting morphology to observe WSS pat-

terns. In the second portion of this study, I compare WSS patterns in outflow tracts of chicks that had distinct subpopulations of AP septal precursors ablated. The goals of the study are to establish the first detailed hemodynamic profiles throughout both the embryonic heart and aortic arches under normal and altered blood flow that lead to AP septal defects.

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MS22

Electromechanical Pumping in Embryonic Heart Tubes

Recent advancements in computational fluid dynamics have enabled researchers to efficiently explore problems that involve moving elastic boundaries immersed in fluids for problems such as cardiac fluid dynamics and animal swimming. The work presented here focuses on the development and implementation of such methods and models for the pumping of the tubular hearts. In particular, we develop neuromechanical models that integrate feedback between the conduction of action potentials, the contraction of cardiac muscles, the movement of the heart wall, and the motion of the blood. The coupling between the elastic heart tube and the viscous blood is resolved using a 2D and 3D parallelized and adaptive implementation of the immersed boundary method, IBAMR. These models are then used to resolve proposed pumping mechanisms in tubular hearts, including peristalsis and dynamic suction pumping. In addition, the challenges of refilling the heart tube at low Reynolds numbers are considered. The relatively rigid pericardium and torsionally wound muscles are included in the model to study their role in refilling.

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MS23

Effect of Myeloid-Derived Suppressor Cells on Glioblastoma-Immune Dynamics

The highly immunosuppressive tumor microenvironment of Glioblastoma multiforme (GBM) leads researchers to consider immunotherapies in hopes of improving treatment outcomes. Monotherapy with anti-PD-1 has proved to be unsuccessful likely due to added layers of immunosuppression besides the PD-L1/PD-1 axis. Murine experiments show that CCR2+ myeloid-derived suppressor cells (MDSCs), which suppress T cells, are chemo-kinetically recruited by gliomas to the brain. Further, combination treatment with PD-1 and a CCR2 antagonist unmasked the immune checkpoint inhibitors ability to reduce tumor growth. To gain insight on glioma-immune dynamics with the goal of future extension to immunotherapy, we develop and analyze an ODE model which includes immunosuppression via the PD-L1/PD-1 axis and MDSCs. We conduct parameter sensitivity analysis in combination with the approximate Bayesian computation rejection method to identify the interaction between the two layers of immunosuppression.

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MS23

Exploring the Interactions of Oncolytic Viral Therapy and Immunotherapy of Anti-CTLA-4 for Malignant Melanoma Mice Model

In this talk, we introduce a mathematical model to discuss the interactions of combined therapy of oncolytic viruses and a checkpoint inhibitor, anti-CTLA-4. The model incorporates both the susceptible and infected tumor populations, virus population, tumor-specific immune populations, virus-specific immune populations, tumor suppressive cytokine IFN-γ, and the effect of immune checkpoint inhibitor CTLA-4. Specially, we distinct the tumor-specific immune abilities of $CD8^+$ T and $CD4^+$ T cells and describe the destructive ability of cytokine on tumor cells as well as the inhibitory capacity of CTLA-4 on various components. Our model confirms that the combined therapy is more effective than OVT alone. We also investigate various dosing strategies to provide effective therapies on improving treatment outcomes. Our study reveals that the tumor killing rate by immune cells plays an important role in both the OVT monotherapy and the joint therapy. Moreover, parameters related to $CD8^+$ T cells have a large impact on treatment outcome with OVT alone whereas parameters associated with IFN-γ strongly influence treatment response for the combined therapy. This study indicates that it is the activation of host anti-tumor immune system responses rather than its direct destruction of the tumor cells play a major biological function of the combined therapy.

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MS23

An Agent-Based Model of Combination Oncolytic Viral Therapy and Anti-PD-1 Immunotherapy Reveals the Importance of Spatial Location When Treating Glioblastoma

A combination of oncolytic viral therapy and immunotherapy provides an alternative option to the standard of care for treating the lethal brain tumor glioblastoma (GBM). Although this combination therapy shows promise, there are many unknown questions regarding how the tumor landscape and spatial dosing strategies impact the effectiveness of the treatment. We aim to shed light on these questions using a novel spatially explicit computational model of GBM response to treatment. Our results suggest that oncolytic viral dosing in the location of highest tumor cell density leads to substantial tumor size reduction over viral dosing in the center of the tumor. These results can help to inform future clinical trials and more effective treatment strategies for oncolytic viral therapy in GBM patients.

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Using ODEs to Improve Cancer Treatments: Simplicity and Balance

Mathematical models of cancer growth and treatment are used to hypothesize answers to open questions, including what individual characteristics may lead to non-uniform patient responses to treatments, and how to optimize and personalize therapy strategies. Mathematical models can help to provide insights into the mechanisms that influence patient responses, and can occasionally lead to surprising outcomes. When multiple and sometimes conflicting goals are in play (such as aiming to kill as many tumor cells as possible while keeping the immune response as strong as possible), mathematical modeling can help to determine how to find balance in treatment approaches. In this talk, we will present a sample of simple mathematical models created to answer questions about chemotherapy, immunotherapy, combination therapy, and oncolytic virus therapy. These models are used to simulate disease dynamics with treatment interventions, and to look for the balance in treatment approaches that may slow, or even stop, disease progression.

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MS24

Control-Based Continuation Methods for Investigating Dynamical Transitions in Neurons

Neurons communicate through action potentials – rapid spike-shaped oscillations in their membrane potential. Stimulation results in transitions between spiking and quiescent behaviours. These occur in a systematic fashion, resulting in neuronal computation. Major insights have been gained from nonlinear dynamics, which explains the mechanisms between spiking-quiescent transitions in terms of bifurcation theory and slow-fast dynamics. This is used to explain the computational properties of a cell, in terms of its dynamical structure. Despite its wide-ranging success, bifurcation theory can only be directly applied to models, and not real cells. Here, I will discuss control-based continuation and its applications to single-cell dynamics. Control-based continuation (CBC) applies numerical continuation to experiments, to perform model-free bifurcation analyses of physical systems. I will discuss theoretical results of CBC experiments for neuronal systems, highlight similarities between CBC and conventional experimental methods, and propose future research directions involving hybrid CBC-dynamic clamp studies.

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MS24

Understanding Cell State Transitions Using Catastrophe Theory

During the development of an organism, cells specialize by transitioning between a limited set of discrete cell fates, defined by distinct gene expression profiles. These transitions occur in a characteristic sequence and are controlled by cues in the environment, such as morphogens. While quantitative models that describe signaling pathways and gene regulatory networks in great detail have been used to investigate cell differentiation, these suffer from having too many parameters to constrain with available data. Besides, their complexity makes it difficult to gain intuitive understanding. A popular and intuitive metaphor for the process of cell differentiation is the Waddington landscape, in which a differentiating cell is represented as a marble rolling down a landscape of hills and valleys, encountering decision points between different lineages, eventually settling in a valley that defines its cell fate. In this talk, I will show that this metaphor can be mathematically formalized using Catastrophe Theory, where the landscape is defined by a potential function and the different cell states correspond to attractors in the landscape. The signals the cell receives alter the landscape and control the bifurcations that destroy or create attractors. By combining this approach with approximate Bayesian computation, we show that we can quantitatively fit these models to large amounts of biological data and make novel predictions.

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MS24

The Effect of Coupling on Transitions of Interacting Neural Populations

Dynamical models consisting of networks of neural masses commonly assume that the interactions between neural populations are via additive or diffusive coupling. When using the additive coupling, a population's activity is affected by the sum of the activities of neighbouring populations. In contrast, when using the diffusive coupling a neural population is affected by the sum of the differences between its activity and the activity of its neighbours. These two coupling functions have been used interchangeably for similar applications. In this study, we show that the choice of coupling can lead to strikingly different brain network dynamics. We focus on a phenomenological model of seizure transitions that has been used both with additive and diffusive coupling in the literature. We consider small networks with two and three nodes, as well as large random and scale-free networks with 64 nodes. We further assess resting-state functional networks inferred from magnetoencephalography (MEG) from people with juvenile myoclonic epilepsy (JME) and healthy controls. To characterize the seizure dynamics on these networks, we use the escape time, the brain network ictogenicity and the node ictogenicity, which are measures of the network's global and local ability to generate seizure activity.

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MS24

Rate-Induced Tipping of the Compost Bomb: Sizzling Summers, Heteroclinic Canards and Metastable Zombie Fires

The Arctic is the fastest warming region on Earth. Understanding how a rapidly changing climate change im-

pacts Arctic systems is therefore an important challenge. This is the basis of the 'Compost-Bomb' instability, a theorized runaway heating of northern latitude peat soils when atmospheric temperature rises faster than some critical rate, first proposed in [Luke Cox, European Journal of Soil Science (2011), 62.1] and analysed in [Wieczorek et al, Proceedings of the Royal Society A (2011), 467.2129]. The Compost Bomb instability was one of the first examples of what is known as Rate-induced tipping or R-tipping. The key trigger for the compost bomb instability is heat produced by microbial respiration. Here, the original soil carbon and temperature model of Luke Cox is augmented with a non-monotone microbial respiration function, for a more realistic representation of the process. This gives rise to a meta-stable state, reproducing the results of [Khvorostyanov et al, Tellus (2008), 60B] where a complex PDE model is used. Two non-autonomous climate forcings are examined: (i) a rise in mean air temperature over decades (ii) a short-lived extreme weather event, with the rate-induced compost bomb observed in each. Using techniques of compactification, singular perturbation theory and desingularisation, we reduce the R-tipping problem to one of heteroclinic orbits, uncovering the tipping mechanism for each climate change scenario.

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MS25

Ticks, Fire, and Land: Modeling the Effects of Prescribed Fire on Tick-Borne Disease

Tick-borne illnesses are trending upward and are an increasing source of risks to peoples health in the United States. Hence, it is important to find a practical way of managing tick populations. Prescribed burns are a common form of land management, it can be cost efficient if properly managed and can be applied across large amounts of land. In this seminar, I will present a spatial stage-structured tick-host model with impulsive differential equations to investigate the effect of prescribed fire intensity, and the duration between burns on tick population and disease prevalence. Results indicate that fire intensity has a larger impact in reducing tick population than frequency between burns. Furthermore, burning at high intensity is preferable to burning at low intensity whenever possible. Exploring the use of prescribed burns in preventing the establishment of ticks into new areas shows that fewer burns are ineffective at preventing their establishment because ticks can recover relatively quickly following a burn. While frequent, long-term prescribed burns slows the propagation of ticks, their possibly establishment is inevitable and the additional use of other tick population management strategies is necessary to prevent their establishment.

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MS25

Modeling the Uncertainty of Antibiotic Resistance Evolution in a Population Using Agent-Based Models

One of the emerging challenges in medicine nowadays is the antimicrobial resistance (AMR). Some pathogens such as Gram-negative bacteria are particularly alarming due to their rapid adaptation to antibiotic treatments. In the face of this public health threat, mathematical models are essential for predicting the evolution of AMR and adopting better public health policies. In this work, we propose an agent-based computational model to describe the infection dynamics of the Acinetobacter baumannii Gram-negative bacterium and its resistance against the colistin antibiotic in the Valencia city hospitals. The model has been constructed by generating a synthetic population from the demographic information from the city, and a set of probability-based behavioral rules that model the interaction between individuals and the pathogen infection process. The model has been calibrated with real epidemiological data and simulations and predictions for the coming years have been carried out. The predictions suggest that the colistin-resistant A. baumannii has reached a stable situation in the Valencia city, but that its evolution has especially affected older age groups.

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MS25

General Stochastic Differential Equation Models of Animal Growth with Application to Optimization in Cattle Raising

The effect of environmental random fluctuations on the growth dynamics of individual animals is not captured by regression models, which commonly used mean growth curves X(t) (animal size at age t) satisfy the ODE dY(t)=b(a-Y(t))dt, where Y(t)=h(X(t)) is a transformed size by a model specific strictly increasing C^1 function h. To account for fluctuations, we use the stochastic differential equation models dY(t)=b(a-Y(t))dt+sdW(t), where W(t) is a Wiener process. These more realistic models can help farmers optimize the profit obtained by raising and selling an animal. To that end, we obtain the profit probability distribution, mean, standard deviation, and other quantities of interest under the more general and realistic market situation where the selling price per kg

paid to farmers depends on the animal's age and weight category. We apply results to real weight data of Mertolengo breed cattle males and conclude that farmers are selling the animals before the optimal age, resulting in a lower mean profit. Sensitivity analysis for small changes on model parameter estimates shows that they have a small effect on the optimal expected profit and a negligible effect on the optimal selling age. Acknowledgements. The authors work at the research center CIMA, supported by FCT (Fundao para a Cincia e a Tecnologia), project UID/04674/2020, within Operational Group PDR2020-1.0.1-FEADER-031130 - GoBovMais, funded by PDR 2020

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MS25

Uncertainty Analysis for the COVID-19 Pandemic

In this talk we will use several mathematical tools that allow us to investigate uncertainty in epidemics. We show how these tools can be used to study uncertainty for the COVID-19 pandemic. Mathematical models are based on multiple assumptions and the real-world changes constantly and especially during a pandemic. Some parameters' values vary over the time due to multiple factors including non-pharmaceutical interventions. Forecasting the COVID-19 pandemic has been a very complex problem. We design and analyze a mathematical model based on a system of stochastic differential equations, to get deeper insight about the complexity of COVID-19 pandemic forecasting. The results provide useful information regarding the difficulties that many studies have faced to forecast the dynamics of the COVID-19 pandemic. We find the basic reproduction number for the stochastic model that is a crucial threshold parameter to understand the dynamics of the COVID-19 pandemic and provide some ideas regarding the modeling of uncertainty in a pandemic.

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MS26

Beyond the Limits of Circadian Entrainment: Non-24-Hour Sleep-Wake Disorder, Shift Work, and Social Jet Lag

While the vast majority of humans are able to entrain their circadian rhythm to the 24-hour light-dark cycle, there are numerous individuals who are not able to do so due to disease or societal reasons. In this talk, we will use computational and mathematical methods to analyze a well-established model of human circadian rhythms to address cases where individuals do not entrain to the 24-hour light-dark cycle, leading to misalignment of their circadian phase. For each case, we provide a mathematically justified strategy for how to minimize circadian misalignment. In the case of non-24-hour sleep-wake disorder, we show why appropriately timed bright light therapy induces entrainment. With regard to shift work, we explain why reentrainment times following transitions between day and night shifts are asymmetric, and how higher light intensity enables unusually rapid reentrainment after certain transitions. Finally, with regard to teenagers who engage in compensatory catch-up sleep on weekends, we propose a rule of thumb for sleep and wake onset times that minimizes circadian misalignment due to this type of social jet lag. In all cases, the primary mathematical approach involves understanding the dynamics of entrainment maps that measure the phase of the entrained rhythm with respect to the daily onset of lights.

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MS26

Machine Learning for Wearable Data the Good, the Bad and the Ugly

The ability to accurately forecast the dynamics of a complex oscillating systems is fundamental to the study of many physical and biological systems. This is especially important for understanding and predicting the bodies natural 24 hour oscillations in physiology and behavior known as circadian rhythms. This talk with explore the limitations and strengths of machine learning techniques applied to circadian rhythm forecasting. The fundamental data used in training these models is the response of oscillators to external perturbations which can be traced out into phase response curves for data collected across the period of the oscillator. In this work, we study the application of machine learning techniques to complex nonlinear oscillator systems using phase response training data. Using simulated data we examine how well these techniques perform when the perturbations are generalized from the training data. Finally, we discuss the application of these techniques to the study of circadian rhythms and discuss some preliminary results for using wearable data (apple watch, fitbit) to build personalized models of circadian rhythms.

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MS26

Mathematical Modeling of the Human Circadian Rhythms Through Wearable Devices

Circadian rhythms are fundamental to all aspects of physiology and behavior, ranging from cellular dynamics to work performance. Measuring circadian phase has mostly been achieved in carefully controlled laboratory conditions. The

development and ubiquitous presence of smartphones and wearable devices have made it possible to passively detect and collect information of user behavior and health. Here, we discuss different methods developed to measure circadian phase from wearable devices in the real life settings. First, we present mathematical models of the human circadian clock, with different types of data collected from both research-grade and consumer-grade wearable devices. We then discuss using activity, which is recorded in almost every wearable device, to predict circadian phase in the real life settings. Finally, we present an application and extension of models of the circadian clock. Coupled with optimal control theory, these models can be used to provide optimal schedules to adjust the human circadian clock in daily life.

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MS26

Inferring the Impact of Melatonin on the Circadian Pacemaker Using a Macroscopic Model for Human Circadian Rhythms

The hormone melatonin, which is cyclically produced in the pineal gland, promotes sleep propensity and interacts bidirectionally with the circadian pacemaker in the suprachiasmatic nucleus (SCN). Melatonin supplements are regularly used to induce sleep and shift individuals circadian phase. To understand the phase shifting impact of exogenous melatonin we have developed a combined model of the SCN network and melatonin pharmacokinetics. This work builds off a prior mathematical model that explains how the large-scale oscillatory phenomenon of the pacemaker arises from the connections of many oscillators within the SCN. Pharmacokinetic interactions modeled in other work have been adapted to this network model. The parameters corresponding to the melatonin phase response curve (PRC) of individual cells within the SCN were estimated by fitting data from experiments measuring the phase response to 3.0 mg and 0.5 mg exogenous doses of melatonin. Thus, the model describes the direct impact of blood plasma melatonin on clock regulation. This generalizes to other melatonin dosing schemes and predicts the associated phase shifts. This framework can also be applied to investigate the interaction between the acute sleep promoting and phase shifting properties of melatonin.

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MS27

Multi-Scale Modeling of Myocardial Oxygen Supply and Demand in the Beating Heart

Over a three to four-fold range of oxygen demand, the human left-ventricular myocardium extracts roughly 80% of the oxygen delivered via the coronary blood supply. Thus, to maintain adequate oxygenation, myocardial blood flow must vary in proportion to changes in oxygen demand that occur, for example, during exercise. We have constructed multi-scale models of myocardial mitochondrial energy metabolism, myofibril cross-bridge kinetics and myocyte mechanics, whole-heart pumping mechanics, ventricular-vascular interactions governing myocardial perfusion, and whole-body cardiopulmonary blood flow accounting for autonomic control of vascular tone and cardiac inotropy and chronotropy. Integrating these model components together, we are able to simulate the in vivo relationships between myocardial power output, ATP demand, oxygen consumption, blood flow, and transmural regional perfusion in exercise. The integrated whole-body model is validated based on its ability to predict emergent features, such as maximum heart rate, maximal cardiac power output, and the oxygen cost of stroke work. The validated model is used to analyze an interpret data on in vivo myocardial perfusion in a large-animal model of heart failure and to identify and refine hypothesized mechanisms underlying microvascular dysfunction in this model.

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MS27

Modeling the Effects of Blood Flow Regulation on Oxygenation in the Retinal Microcirculation

Impairments in retinal blood flow and oxygenation have been implicated as contributing to the progression of glaucoma. Here, an established theoretical hybrid model of a retinal microvascular network is extended to include the effects on oxygenation of local blood flow regulation. A heterogeneous representation of the arterioles based on confocal microscopy images is combined with a compartmental description of the capillaries and venules downstream. A Green's function method is used to simulate oxygen transport in the arterioles, and a Krogh cylinder model is used in the capillary and venule compartments. Acute blood flow regulation is simulated in response to changes in pressure, shear stress, and metabolism. When blood flow regulation mechanisms are inhibited, model results predict a decrease in tissue oxygenation, as well as a greater spread in tissue oxygen levels throughout the vascular network. These results demonstrate that the oxygenation of the retina can be negatively impacted by impairments in blood flow regulation. The results also highlight the importance of using a spatially heterogeneous vascular network representation, as localized regions of poor oxygenation can be predicted that would not be identified using averaged oxygen measurements. This model framework will allow for comparisons to sectorial-specific clinical data, to help assess the potential role of impaired blood flow regulation in glaucoma.

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MS27

Mathematical Modeling of Cerebral Capillary Blood Flow Heterogeneity and Its Effect on Brain Tissue Oxygen Levels

Previous computational models of brain capillary networks have predicted that heterogeneous cerebral capillary flow patterns result in lower brain tissue partial oxygen pressures. However, these models have often considered simple capillary networks in terms of their geometric properties. Here, we describe computational models of brain capillary networks that have been used to determine how perturbations of network properties impact tissue oxygen levels. The models include variabilities in both their geometric (segment lengths and diameters) and three-dimensional, topological structure. The main result is that for a general class of networks, random perturbations of either segment diameters or conductances will always, on average, decrease the average tissue oxygen levels. This result is supported through both simulations of the models and mathematical analysis.

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MS27

Modeling Acute and Chronic Vascular Responses to a Major Arterial Occlusion

Peripheral arterial disease (PAD) is a serious illness in which major arteries become occluded, causing reduced blood flow to peripheral tissues. Developing improved treatment strategies for PAD requires a more complete understanding of the vascular changes that occur both proximal and distal to the site of occlusion. Mathematical modeling provides a useful tool to predict the role of collateral arteries in flow compensation following occlusion. In this work, a vascular wall mechanics model is used to simulate acute and chronic vascular adaptations in the collateral arteries and collateral-dependent arterioles of the rat hindlimb. On an acute timeframe, the vascular tone of collateral arteries and distal arterioles is determined by responses to pressure, shear stress, and metabolic demand. On a chronic timeframe, arteriogenesis (outward vessel remodeling) is modeled by increased passive vessel diameter, and angiogenesis (growth of new capillaries) is assumed to depend on venous oxygen saturation levels. The model predicts that acute responses only restore post-occlusion flow to 24% of non-occluded blood flow, while the addition of chronic responses (structural adaptation) yields blood flow that is 84% of the non-occluded level. Ultimately, the model predictions indicate that interventions which enhance collateral arteriogenesis would have the greatest potential for restoring blood flow to healthy levels.

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MS28

Sharp-Interface Immersed Boundary Methods for Biomedical Fluid-Structure Interaction

This talk will describe ongoing work that aims to create numerical methods for fluid-structure interaction (FSI) that integrate partitioned and immersed approaches to FSI. Like conventional partitioned methods for FSI, our approach uses separate governing equations for the fluid and structure that are coupled only along the fluid-structure interface. However, our fluid-solid coupling strategy is based on the immersed interface method, which allows us to avoid using body-conforming discretizations and simplifies models involving very large structural displacements and deformations. Further, numerical tests suggest that even a simple Dirichlet-Neumann coupling strategy yields a stable numerical method across a very broad range of mass density ratios, without needing subcycling or implicit coupling between the fluid and solid degrees of freedom. We demonstrate that further improvements in performance can be achieved through multirate time stepping that uses different step sizes for the fluid and structure variables. The talk will also present detailed benchmarking studies along with biomedical applications of this methodology, including to models of clot capturing in inferior vena cava filters.

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MS28

Emergent Asymmetries in the Metachronal Motion of Marine Worms Using Computational FSI Models

Metachronal waves are ubiquitous in propulsive and fluid transport systems across many different scales and morphologies in the biological world. Tomopterids are a soft-bodied, holopelagic worm that use metachrony with their flexible, gelatinous parapodia to deftly navigate the mid-water ocean column that they inhabit. In the following study, we develop a three-dimensional, fluidstructure interaction model of a tomopterid parapodium to explore the emergent metachronal waves formed from the interplay of passive body elasticity, active muscular tension, and hydrodynamic forces. After introducing our model, we examine the effects that varying material properties have on the stroke of an individual parapodium. We then explore the temporal dynamics when multiple parapodia are placed sequentially and how differences in the phase can alter the collective kinematics and resulting flow field.

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MS28

Eulerian Simulation of Complex Suspensions and

Biolocomotion

We present a numerical method specifically designed for simulating three-dimensional fluid–structure interaction (FSI) problems based on the reference map technique (RMT). The RMT is a fully Eulerian FSI numerical method that allows fluids and large-deformation elastic solids to be represented on a single fixed computational grid. This eliminates the need for meshing complex geometries typical in other FSI approaches, and greatly simplifies the coupling between fluid and solids. We develop a three-dimensional implementation of the RMT, parallelized using the distributed memory paradigm, to simulate incompressible FSI with neo-Hookean solids. As part of our method, we develop a field extrapolation scheme that works efficiently in parallel. Through representative examples, we demonstrate the method's suitability in investigating many-body and active systems, as well as its accuracy and convergence. The examples include settling of a mixture of heavy and buoyant soft ellipsoids, lid-driven cavity flow containing a soft sphere, and swimmers actuated via active stress. We also discuss extensions to the method to simulate poroelastic media.

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MS28

Lattice Boltzmann Reference Map Technique for Eulerian Simulation of FluidStructure Interaction

We present a fully Eulerian numerical method to simulate the interactions of deformable solids in fluids. With the reference map technique (RMT), we model finite-strain solids undergoing large deformation on one fixed grid. Fluids are coupled to the same grid and simulated using the lattice Boltzmann (LB) method. Our hybrid approach (LBRMT) provides a new implementation to model moving deformable boundary conditions in the LB method, and a simple and unified coupling of solids and fluids. It also inherits the improved computational performance from the LB method to simulate quasi-incompressible fluids in a parallelized fashion. The LBRMT is apt at simulating multibody contact of complex geometries since it uses one global velocity field for both phases. We demonstrate the convergence and applicability of the LBRMT in fluidstructure interaction (FSI) through examples of lid-driven cavity with deformable solids, sedimentation and floatation of soft bodies, bending and twisting of flexible rotors, and collective motion of actuated microswimmers.

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MS29

Thermodynamic Irreversibility of Learning

Adaptive systemssuch as a biological organism gaining survival advantage or a motor protein transporting intracellular nutrientsmust somehow capture predictable structure and identify irrelevant noise in their environment. This is the thermodynamic principle of Requisite Complexity: thermodynamic agents must match the complexity of their environment in order to maximize the production of useful work. Work production is the most relevant performance measure for an adaptive physical agent, and so maximizing work production corresponds to thermodynamic learning, drawing a direct parallel to the maximum-likelihood principle that guides machine learning. However, reckless pursuit of maximum work in the training phase easily leads to overfitting, which has dire energetic consequences. Irreversible entropy production diverges when thermodynamic agents are unconstrained in their pursuit of energetic advantage. This suggests that functional thermodynamic learning must include physical mechanisms for generalization.

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MS29

An Entropy-Based Method for Quantifying Asymmetry in Biological Systems

Symmetry often seems visually apparent in real biological systems. However, these systems are rarely exactly invariant under the associated transformation. It can therefore be challenging to apply the mathematical definition of symmetry to biology in meaningful ways. We propose a flexible, entropy-based method for quantifying the asymmetry of approximate symmetries that requires very little user input. We demonstrate its usefulness in simulated and real biological systems, and explore dynamics of approximate symmetries on both developmental and evolutionary timescales.

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MS30

Inferring the Causal Flow of Cell-Cell Communication from Single-Cell Transcriptomics

Cell-cell communication governs cell fate and decision-making in biology, primarily in the form of biochemical signaling, Understanding what forms of cell-cell communication are present in health and consequently perturbed in disease is crucial to fully understanding the functionality of biological systems. The recent explosion of single-cell RNA-sequencing has led to the development of cell-cell communication inference methods from gene expression data, enabling new studies on cell-cell communica-

tion at unprecedented depth and breadth. These methods reveal possible, simultaneous networks of relationships between cell types that are mediated by cell signaling. In this talk, we present work that builds on cell-cell communication inference output by inferring possible causal relations between signals. That is, does the presence of one signaling interaction cause a subsequent interaction, leading to a flow of information? We show how cell-cell communication and single-cell RNA-sequencing data can be framed in the language of causality and thus draw from existing tools developed for causal structure learning. We present some preliminary results of our method that have been applied to synthetic data generated by PDE modeling and suitable single-cell datasets.

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MS30

Mapping Cell-Cell Communications in Spatial Transcriptomics Data with Optimal Transport

The recent development of high-resolution omics level technologies has reshaped modern biological research. These high-dimensional and noisy datasets are accumulating at a fast pace. Efficient and biologically meaningful algorithms are needed to extract biological insights from these raw datasets. In this talk, I will discuss using optimal transport, a powerful geometric data analysis method, to integrate multimodal omics datasets and to infer cell-cell communications, a crucial process that drives the correct developments and functions of biological systems. I will also talk about a new formulation of optimal transport called supervised optimal transport inspired by these biological applications.

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MS30

Topological Data Analysis and Multiscale Modeling in Data-Driven Biology

Recent technological breakthroughs have enabled gathering data on large-scale and single-cell levels. Artificial intelligence (AI) has been widely applied to biological data in inferring the functions and dynamics of complex biological systems. However, the black-box AIs are insufficient for comprehensive understanding and interpreting the multiscale biological processes from complex, heterogeneous, and noisy data. Characterizing and modeling the biological processes demands novel computational tools. In this talk, we will present our works in building mathematics-driven AI models for multiple biological systems. We will discuss our topological data analysis (TDA)-driven machine learning models in learning protein mutational effects and guiding protein evolution. Moreover, we will discuss cellular dynamics from molecular and genomic scales using multiscale and data-driven modeling to uncover new insights in development and regeneration.

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MS30

Persistent Spectral Graphs and COVID-19 Related Research

The surge of COVID-19 infections has been fueled by new SARS-CoV-2 variants. The molecular mechanism underlying such surge is elusive due to the existence of more than 4500 non-degenerate mutations on the S protein. Understanding the molecular mechanism of SARS-CoV-2 transmission and evolution is a prerequisite to foresee the trend of emerging vaccine-breakthrough variants and the design of mutation-proof vaccines and mABs. We integrate the genotyping of more than 3.3 million SARS-CoV-2 genomes, a library of 185 human antibodies, tens of thousands of mutational data, topological data analysis, and deep learning to reveal SARS-CoV-2 evolution mechanism and forecast emerging vaccine-breakthrough and antibody-resistant variants. We demonstrate that vaccine-breakthrough and antibody-resistant mutations are the primary mechanism of viral evolution. We show that infectivity-strengthening and antibody-disruptive co-mutations on the S RBD can quantitatively explain the infectivity and virulence of all prevailing variants. We analyze emerging vaccine-breakthrough co-mutations in highly vaccinated countries and identify sets of co-mutations that have a high likelihood of massive growth. In addition, we found a antibody-resistant mutation Y449S has reduced infectivity compared to the original SARS-CoV-2 but can disrupt existing antibodies that neutralize the virus.

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MS31

Applications of Mathematical Models in the Development of SGLT2 Inhibitors

Sodium-glucose cotransporter 2 (SGLT2) inhibitors are a class of drugs initially approved to treat type 2 diabetes that have subsequently been approved for the prevention of cardiovascular events, renal outcomes, and heart failure. SGLT2 is the main transporter involved in renal glucose reabsorption whereas SGLT1 plays a primary role in intestinal glucose absorption and a lesser role in renal glucose reabsorption. Inhibiting SGLT2 reduces renal glucose reabsorption, increasing urinary glucose excretion (UGE), which in turn reduces plasma glucose concentrations and provides negative energy balance. Mathematical modeling was applied throughout the discovery and development programs to help characterize many of the effects of SGLT2 inhibitors (and combined SGLT1/2 inhibitors), including effects on renal glucose reabsorption, plasma glucose and HbA1c levels, intestinal glucose absorption, beta-cell function, fluid balance and hemodynamics, and body weight regulation. This talk will focus on two of these topics: (1) characterizing the rate of UGE as a function of both plasma glucose and drug concentrations and the development and application of a practical model-based method for estimating the renal threshold for glucose excretion (2) characterizing the impact of SGLT2 inhibition on body weight regulation and subsequent insights into how food intake changes in response to weight loss.

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MS31

Stochastic Modeling for Glycemic Management in the ICU

Glycemic management (GM) in ICU is a hard job and requires lots of attention from clinicians. Although non-diabetic, most ICU patients need exogenous insulin to control their blood glucose (BG) levels. Currently, clinicians follow a flow chart to adjust the exogenous intravenous (IV) insulin rates. Using mechanistic modeling-based control approaches for GM as a clinical decision support tool would enhance the GM results by reducing the burden on clinicians. The glucose-insulin system of ICU patients is highly non-stationary because of their health conditions and interventions. Also, BG measurements are routinely collected every 1-3 hours, providing at most 15 measurements per day. Moreover, insulin, a central system component besides BG, is rarely measured. These constraints lead us to build a model as simple as possible, still capturing the physiologic behavior of the system and useful for BG forecasting and control in the ICU. For this purpose, we developed a stochastic model consisting of two parts: the deterministic component modeling the mean behavior of BG levels and the stochastic component accounting for the variation in BG levels due to unresolvable dynamics with the deterministic part. The model output is a stochastic process providing the mean behavior and its uncertainty; the possible lowest and highest BG levels. We use this model to estimate the optimal IV insulin rate to keep BG levels in the target range with a linear quadratic Gaussian controller.

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MS33

From Fitting the Average to Fitting the Individual: A Cautionary Tale for Mathematical Modelers

An outstanding challenge in the clinical care of cancer is moving from a one-size-fits-all approach that relies on population-level statistics towards personalized therapeutic design. Mathematical modeling is a powerful tool in treatment personalization, as it allows for the incorporation of patient-specific data so that treatment can be tailor-designed to the individual. In this talk, we present a mathematical model of murine cancer immunotherapy that has been previously-validated against the average of an experimental dataset. We then ask: what happens if we try to use this same model to perform personalized fits, and therefore make individualized treatment recommendations? We find that if we approach this task by choosing a single cost function and a single fitting methodology, the personalized predictions made by the model may be of limited value. Using our modeling framework, we are able to identify what additional data would be needed, and/or what experimental conditions need to be met, in order to improve confidence in personalized model predictions.

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MS33

Early Prediction of Patient Response to Immunotherapy

Immunotherapies don't work for most cancer patients; but when they do work, they can work extremely well. Because there are often other treatment options to choose from, it is important to figure out as early as possible if a patient will be a "responder" or a "non-responder". I will present a method based on tumor size data, a simple equation and, machine learning to provide an early prediction of who will or will not respond [Gonzlez-Garca et al. (2021) CPT Pharmacometrics Syst. Pharmacol., 10: 230-240. https://doi.org/10.1002/psp4.12594].

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MS33

Development of Mathematical Biomarkers for Predicting Cancer Immunotherapy Outcome

Immunotherapy has emerged as a promising therapy for multiple cancers, but to date only a minority of patients have been reported to receive clinical benefit from immunotherapy. This is, in part, because biomarkers for prediction of immunotherapy efficacy remain outstanding, and thus clinicians lack the information needed to identify the optimal treatment strategy for each patient early in the treatment process. To address this challenge, we have developed a mechanistic mathematical model of cancer immunotherapy made up of a set of mathematical biomarkers (MBs) that accurately predicts tumor response and survival following immunotherapy as a function of physical and biological changes reflecting immune responses. Each MB is a model-derived parameter with functional relationships that link it to a set of clinically measurable surrogates. Using only tumor imaging data already collected as standard-of-care from 124 patients, we found that the MBs were able to sort patient response with accuracy across all cancer-drug combinations examined. We then validated the MBs with data from 177 additional patients that received either anti-CTLA4 or anti-PD1/PDL1 monotherapies. These results outperform the biomarkers used in current clinical practice in terms of prediction accuracy. This indicates that this readily-translatable predictive tool for personalized oncology may be broadly applicable to many additional cancer and immunotherapy combinations.

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MS34

The Effect of Non-Uniform Spatial Distribution of Heterogeneous Nodes in Pancreatic Beta-Cell Networks

Over the recent years, high-speed multi-cellular recordings from beta-cell networks within pancreatic islets has allowed

for the study of diffusive coupling and coordination in heterogeneous networks of order 103 bursting cells. To this end, we have developed a mathematical model for studying the effects of spatial distribution of excitability on the global dynamics of a diffusively-coupled network embedded in a three-dimensional space. In this work, we focus on two subpopulations of oscillators, one intrinsically-active and the other inactive. I will first discuss the development of measures for spatial sortedness as well as procedures to iteratively adapt this sortedness in the network. I will then discuss the implications of the resulting spatial nonuniformity on propensity of the network to exhibit globally coordinated oscillations. The goal of this work is to better understand how heterogeneity across several dimensions (coupling, excitability, and spatial distribution) can influence dynamic coordination in diffusively coupled oscillator networks. In the future, we will use this framework to study other networks structures, for example directed networks, networks with excitatory and inhibitory links, and networks with heterogeneous structural connectivity (e.g. scale-free networks).

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MS34

The Influence of a Transport Process on the Epidemic Threshold

In today's interconnected world, it is of paramount importance to take transport processes induced by human mobility into account when considering the spreading of an epidemic. The global airline or the local public transport network alike provide room for people to meet in oftentimes small and poorly ventilated spaces, facilitating the spreading of a contagion. Importantly, these transient encounters are not restricted to each individual's immediate social environment. In this talk, we will introduce a network model of epidemic dynamics in a population in the presence of a transport process. We will discuss the derivation of the corresponding mean-field equations and quantify the influence of the transport process on the epidemic threshold.

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MS34

Motifs and Synchrony-Asynchrony Transitions in Neuronal Networks

The study of motifs can help researchers uncover links between the structure and function of networks in biology, sociology, economics, and many other areas. Empirical studies of networks have identified feedback loops, feedforward loops, and several other small structures as motifs that occur frequently in real-world networks and may contribute by various mechanisms to important functions in these systems. However, these mechanisms are unknown for many of these motifs. In previous work, we have demonstrated that one can identify function-relevant process motifs (i.e., structured sets of walks) in a network, and that these process motifs can improve our understanding of mechanisms underlying emergent properties of dynamics on networks. In the current work, we study the relationship between network structure and synchronization in neuronal networks. Using coherence as a measure of synchrony, we identify the contributions of process motifs to synchrony, and we investigate how changes in a network's structure can affect these process-motif contributions and synchrony.

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MS34

From the Amazon Rainforest to Climate Tipping Elements: Network Interactions in Nonlinear Earth System Components

With progressing global warming, there is an increased risk that one or several climate tipping elements might cross a critical threshold, resulting in severe consequences for the global climate, for ecosystems and for human societies. However, it is known that the different climate components cannot be viewed as individual entities, but they interact across scales in space and time. Therefore, we assess the risk for the emergence of tipping cascades in two different interacting climate systems by using the recently developed python package PyCascades: (i) We investigate the role of local forest adaptations in the Amazon rainforest with respect to potential cascading forest transitions in response to future droughts. (ii) We analyze tipping risks in a small subset of four interacting tipping elements (Greenland Ice Sheet, West Antarctic Ice Sheet, Atlantic Meridional Overturning Circulation and Amazon rainforest) in response to temperature overshoots trajectories. In the latter example, we will also separate safe from unsafe overshoot scenarios

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MS35

Elements of Disease in a Changing World: Modelling Feedbacks Between Infectious Disease and Ecosystems

An overlooked effect of ecosystem eutrophication is the potential to alter disease dynamics in primary producers, inducing disease-mediated feedbacks that alter net primary productivity and elemental recycling. Models in disease ecology rarely track organisms past death, yet death from infection can alter important ecosystem processes including elemental recycling rates and nutrient supply to living hosts. In contrast, models in ecosystem ecology rarely track disease dynamics, yet elemental nutrient pools (e.g. nitrogen, phosphorus) can regulate important disease processes including pathogen reproduction and transmission. Thus, both disease and ecosystem ecology stand to grow as fields by exploring questions that arise at their intersection. However, we currently lack a framework explicitly linking these disciplines. We developed a stoichiometric model using elemental currencies to track primary producer biomass (carbon) in vegetation and soil pools, and to track prevalence and the basic reproduction number (R0) of a directly transmitted pathogen. This model, parameterized for a deciduous forest, demonstrates that anthropogenic nutrient supply can interact with disease to qualitatively alter both ecosystem and disease dynamics. Using this element-focused approach, we identify knowledge gaps and gener-

ate predictions about the impact of anthropogenic nutrient supply rates on infectious disease and feedbacks to ecosystem carbon and nutrient cycling.

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MS35

A Vaccination Model for Covid-19 in South Africa

The rate at which COVID-19 spread through South Africa varied over time as individuals responded to the ongoing pandemic and changing government policies. In this project we model the outbreak in the province of Gauteng assuming that several parameters vary over time. We first determine the approximate dates of parameter changes and relate them to government policies. Unknown parameters are then estimated from available data and used to analyze the impact of each policy. We conclude by considering the implementation of two different vaccines at varying times. Our results quantify the impact of different government policies and demonstrate how vaccinations can alter infection dynamics.

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MS35

Data-Driven Modeling of Covid-19 Transmission Through Interactions Within Communities of Nepal

The impact of the COVID-19 pandemic appears to be quite variable depending on the network of interaction adapting in the communities. In this regard, the data from Nepal provides a unique opportunity to get insights into COVID-19 transmission because of the existing complex interaction network within Nepalese communities due to the open-border of some communities with India, one of the most COVID-19 impacted countries in the world, and heterogeneity in contact patterns among communities. In this talk, I will present data-driven models to describe COVID-19 transmission through Interactions within Communities of Nepal. I will demonstrate how our models can provide vital information for developing control strategies and vaccination programs to manage healthcare facilities in Nepal.

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MS35

Implications of Disease Spread Due to Variability in Body Mass from Larval Stages in Aedes Aegypti

Zika is a virus which is generally mild in expression. However, many cases of severe birth defects from pregnant women infected with Zika have occurred. The virus is primarily spread by mosquitoes, and control of mosquitoes can help decrease the spread of Zika and other pathogens. The success of many control measures is highly dependent upon ecological, physiological, and life history traits of mosquito species. One trait of interest is mosquito body mass, which depends upon many factors associated with the environment in which juvenile mosquitoes develop. Our experiments examined the impact of larval density on the body mass of *Aedes aegypti* mosquitoes, which are important vectors of Zika. To investigate the interactions between the larval environment and mosquito body mass, we built a discrete time mathematical model that incorporates body mass, larval density, and food availability and fit the model to our experimental data. From the larval model, we build an adult model that considers gonotrophic cycle stages as well as disease spread with a simple SEIR model for humans. The dynamics are not straight forward as some traits of large mosquitoes increase the likelihood of Zika epidemic, while others diminish transmission. We consider how mosquito body mass affects a potential Zika outbreak using our mathematical model.

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MS36

Bifurcations of Sleep Patterns under Homeostatic and Circadian Variation

The timing of human sleep is strongly modulated by the 24 h circadian rhythm and the homeostatic sleep drive, the need for sleep that depends on the history of prior awakening. The homeostatic time constants may vary with development or interindividual characteristics and have been identified as important parameters for generating the transition from polyphasic to monophasic sleep. Features of the mean firing rate of the neurons in the suprachiasmatic nucleus (SCN), the central pacemaker in humans, may differ with age or seasonality. We employ a physiologically-based flip-flop sleep-wake model to study the bifurcation sequences governing the transitions from polyphasic to monophasic sleep patterns as we vary the homeostatic time constants and temporal profile of the SCN firing rate. In particular, we modulate the rate at which the SCN firing rate transitions from low to high levels of activity, as well as the duration of its peak activity. We reduce the dynamics of the sleep-wake model to a one-dimensional circle map that captures the circadian phase of sleep onsets on successive days. Analysis of the structure and bifurcations in the map reveals changes in the average number of sleep episodes per circadian day caused by the separate or combined effects of the circadian waveform and faster accumulation/dissipation of sleep pressure.

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MS36

Analysis of Data from Consumer-Grade Wearables to Examine Circadian Rhythms Across Populations and Light Schedules

With the rise of wearable technology in recent years, large-scale collections of physiological and behavioral data have

become readily available for analysis. Mathematical models can effectively process these increasingly accessible signals, such as heart rate and activity, into information about the circadian rhythm of an individual. One subset of these models predicts circadian phase (often via a limit-cycle oscillator framework) based on the light and/or activity pattern of an individual, while another recently developed model instead extracts heart rate phase and other information by accounting for circadian variation, the impact of activity, and effects due to other physiological processes. The intersection of these frameworks has the potential to allow for a multifaceted and detailed understanding of an individuals circadian rhythm, based on data collected from consumer-grade wearables. In this talk, we adapt these modeling approaches to examine circadian features across populations, including students, cancer patients, and individuals with COVID-19. We discuss large-scale differences across populations and implications of the models for tracking disease progression, using a combination of synthetic and real data in order to test algorithm performance in terms of phase extraction and anomaly detection. Finally, we explore parameter differences across populations and the effects of parameter perturbations on the models.

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MS36

Modeling the Effects of Napping and Non-Napping Light Schedules on the Human Circadian Oscillator

A major developmental milestone during early childhood is the consolidation of sleep from a biphasic sleep-wake pattern (afternoon nap and nighttime sleep episodes) to a single monophasic nighttime sleep episode. An advance in the timing of the circadian system is associated with reduced napping behavior, but it is unknown if this advance is a feature of the developing circadian system or altered patterns of light exposure. Using a validated mathematical model of the human circadian pacemaker, we investigated potential mechanisms for producing the circadian phases associated with napping and non-napping light schedules. Extant physiological and behavioral data from 20 children (34.22.0 months) were used in this analysis. We found that the model predicted different circadian phases for each pattern of light exposure: both the decrease in afternoon light during the nap and the later bedtimes associated with napping toddlers contributed to the observed differences in circadian phase. In addition, we systematically quantified the effects on phase shifting due to nap duration, timing, and light intensity. We found larger phase delays occurred for longer and earlier naps. Therefore, napping status affects circadian timing due to altered patterns of light exposure. Furthermore, these findings suggest napping status may affect re-entrainment dynamics in toddlers experiencing circadian misalignment (e.g., jet lag).

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MS36

Circadian Interventions in Shift Workers: Coupling Math with User-Centric Design

Shift workers experience profound circadian disruption due to the nature of their work, which often has them on-the-clock at times when their internal clock is sending a strong, sleep-promoting signal. Mathematical models can be used to generate recommendations for shift workers that move their internal clock state to better align with their work schedules, promote overall sleep, promote alertness at key times, or achieve other desired outcomes. Yet for these schedules to have a positive effect in the real world, they need to be acceptable to the shift workers themselves. In this talk, I will survey the types of schedules a shift worker may be recommended by an algorithm, and how they can collide with the preferences of the real people being asked to follow them, and how math can be used to arrive at new schedules that take these human factors into account.

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MS37

Plant Mutualisms are Ubiquitous and Difficult to Model

Mathematical ecology has a long and successful history of modeling negative interactions between organisms, such as competition and predation. Modeling mutualisms, where members of different species provide benefits to each other, is much more difficult. Simple models based on differential equations have a tendency to be highly unstable, and fixing this requires looking more deeply into the mechanisms by which benefits are shared. I present a model of interactions between plants, pathogens, and fungal mutualists that builds on careful consideration of resource allocation. This mutualism, like most others, is context-dependent, meaning that interaction becomes negative in certain environments, and thus interacts with pathogens to shape plant diversity.

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MS37

Bifurcation Analysis of an Environmentally-Cued Gene Regulatory Network in Arabidopsis

Given a differential equation model, it is usually of interest to understand which dynamical system behaviors (such as bistable switch-like behavior) are possible as a function of the model parameters. Numerical bifurcation software, such as XPP, can help in this pursuit. However, such software cannot compute an analytic expression for a bifurcation curve of interest in terms of the model parameters. Recently, we have developed a method for finding analytic expressions of bifurcation curves using the resultant. In this talk, I will describe how to find a bifurcation curve from a model of a recently discovered Arabidopsis heat-sensitive epigenetic regulatory network using resultant analysis. A downside to the method is that the associated expression can include many terms and become unwieldy to use in practice. I will also discuss more recent work concern-

ing how to approximate these analytic expressions to find more interpretable expressions in different areas of parameter space.

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MS37

Mechanical Models of Plant Growth

Understanding the growth of plants is fundamental to current efforts in food security and bioenergy, as well as being an interesting biological question in its own right. Cellular level plant growth is driven by a high internal turgor pressure, causing viscous stretching of the cell wall which is combined with new material deposition, whilst growth and emergent morphology at the level of e.g. a root involves coordination across multiple cells and cell files. The cell wall itself is a complex material with a highly ordered microstructure, producing evolving non-linear anisotropic mechanical behaviour that can be manipulated under enzymatic control to alter growth rates at the cellular level, and hence drive macroscale geometric changes at the organ scale. We present a series of mathematical models across multiple spatial scales, from the cell wall microstructure to whole organ level, aiming to elucidate the mechanical mechanisms underpinning plant growth.

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MS37

Forecasting Flowering Time under Warming Climates by Modeling Epigenetic Memory in the Vernalization Pathway

There is an increasing potential to incorporate recent advances in our understanding of molecular-genetic pathways of flowering-time regulation to forecast shifts in flowering phenology in response to rising temperature. Recent studies developed models that integrate temperature and photoperiod signals into the network of floral regulatory genes, and predicted the shortening of flowering duration under warming based on the expression dynamics of major flowering-time genes in the perennial herb Arabidopsis halleri subsp. gemmifera. Nevertheless, empirical testing of the model prediction is still lacking. We performed temperature manipulation experiments and common garden experiments to test the model predictions using plants from two distant populations of A. halleri. We also quantified expression levels of two major flowering-time genes and compared the observed and predicted gene expression patterns. Our experiments in the laboratory and the field demonstrated that flowering duration of A. halleri was significantly shortened under warming conditions. Our results also revealed that the end of flowering was more sensitive to the climate warming than the onset of flowering in A. halleri. The approach that integrates phenology monitoring, gene expression analyses, and mathematical modeling that we employed in this study will be a powerful tool to predict how ecosystem respond to future climate change.

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MS38

Wall Shear Stress Characteristics in 3D RBC-Resolved Modeling of Blood Flow in Microvascular Networks

Blood flow through vessels results in shear stress exerted on the vessel walls, and this wall shear stress (WSS) is responsible for many important physiological processes. In the microcirculation WSS has been linked to regulating endothelial cell behavior driving both the creation of new vessels (angiogenesis) as well as changes to microvascular network topology (angioadaptation). Despite its importance, spatial characteristics of the WSS in realistic 3D microvascular networks arising due to both the presence of highly deformable red blood cells (RBCs) as well as the geometric complexity of the vasculature remain largely unknown. In the first part of this talk, I will discuss recent findings (Balogh & Bagchi 2019) using a high-fidelity, 3D computational model of blood flow in microvascular networks with RBCs fully resolved. Characteristics of the full 3D distribution of WSS and its gradient (WSSG) will be discussed as arising due to bifurcations, mergers, and vessel tortuosity. Furthermore, the specific influence of RBCs on such characteristics will be presented. In the second part of this talk I will discuss more recent work on WSS specifically in angiogenic microvascular networks which integrates in vivo data with both 1D and fully resolved 3D models. Findings and new insights into the actual WSS values observed in such networks, as well as the heterogeneity and spatial characteristics, will be presented.

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MS38

Modeling Transport in Microcirculation Using 2D Particulate Flow Simulations

Particulate flows are ubiquitous in various applications such as biological flows. Here we study mixing in vesicle suspensions. Vesicles, which resist bending and are locally inextensible, serve as an experimental and numerical proxy for red blood cells. The motivating application is the study of transport phenomena in microcirculation. We investigate transport specifically in a Couette apparatus, which is governed by an advection-diffusion equation, and we consider mixing in the absence and presence of vesicles using our boundary integral equation simulations in two dimensions. The advection-diffusion equation is discretized spectrally in space, and with a second-order L-stable Strang splitting in time. The mass transport equation is coupled with the vesicle suspension through the velocity field and the initial condition. To our knowledge, there are no universally accepted measures of mixing. Here, we study two measures: the mix-norm defined by a Sobolev norm of negative index and a standard moment fluctuation of the transported species. We define mixing efficiency in terms of mixing measure in the absence of vesicles relative to the measure in the presence of vesicles. We then study the correlation of mixing efficiency with the Peclet number, the volume fraction of the vesicle suspension, and the type of

initial conditions.

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MS38

The Effect of Porous Microvessel Linings on Red Blood Cell Behavior in Diverging Bifurcations

Oxygen transport depends on the heterogeneous distribution of red blood cells (RBCs) throughout the body. This distribution depends on how RBCs are divided or partitioned at diverging vessel branches (bifurcations) and by the presence of a flexible, porous endothelial surface layer (ESL; 1 micron thick) that coats the vessel walls. Here we consider a flexible, two-dimensional model of RBCs passing through a diverging, ESL-lined capillary bifurcation. The RBC is represented by interconnected viscoelastic elements suspended in fluid modeled by Stokes equations for viscous flow. The ESLs resistance to flow is modeled using the Brinkman approximation for porous media with a corresponding hydraulic resistivity and its resistance to compression is modeled using an osmotic pressure difference between the ESL and free flowing plasma. For isolated cell simulations, decreasing either of these ESL properties resulted in RBC partitioning nonuniformity increasing slightly, RBC deformation decreasing, RBC velocity relative to blood flow velocity decreasing and RBCs penetrating more deeply into the ESL. Decreased RBC deformation decreases release of vasodilators such as ATP and nitric oxide, affecting vascular regulation, and increased penetration has been correlated with more clotting. We will also share preliminary results using two RBCs that suggest that increased interaction increases partitioning nonuniformity, RBC deformation and RBC penetration into the ESL.

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MS38

On the Interplay Between Hemodynamic and Oxygenation of the Aneurysmatic Abdominal Aorta

The aim of this work is to develop an integrated fluidochemical framework able to simulate the complex flow fields and oxygen transport in patient-specific models of abdominal aortic aneurysm. The intraluminal thrombus plays a key chemo-mechanical role in the evolution of aneurysms, which is not fully understood. Therefore, we present a coupled fluidporous structureoxygen transport computational model that provides insight into the salient behavior of thrombi under flow in compliant arteries, as well as the effects of thrombi on hemodynamics and arterial wall oxygen starvation, since local changes in tissue oxygenation and perfusion is a critical metric of its functional state. The Reynolds-Averaged Navier-Stokes equations and Biots poroelasticity equations are used to model blood flow through the aorta and fluid-saturated thrombus respectively, while for oxygen transport due to the porous flow in the tissue, the convection-diffusionreaction equation has been applied. Using this multiphysics model, we investigate how thrombus properties, such as permeability and compressibility, affect the risk of oxygen deprivation within the aneurysmal wall. Our results have shown that thrombi are associated with lower oxygen levels within the aortic tissue, which may cause arterial wall degeneration. We have also performed a systematic sensitivity study to assess the relationship between morphological features of the thrombus and the transport of oxygen to the aortic wall.

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MS39

From Direct Measurements to Models of Collective Cell Migration

In a model organism, we use a combination of computational and experimental tools to tease apart the specific morphogenetic modules of the cardiopharyngeal progenitor cells responsible for forming the heart (and the pharynx). The heart progenitors provide one of the simplest examples of collective cell migration whereby just two cells migrate with defined leader-trailer polarity in between two tissues. The cells are also capable of moving individually, albeit by a shorter distance, with imperfect directionality, and with altered morphology. Thus, maintaining contact and the leader-trailer polarity is important for directed migration to the destination. However, it is unclear why a two-cell system is better at migration than an individual cell. Based on in-vivo fluorescence imaging of the embryo, we obtain morphological measurements of the cells. Borrowing on formulation of active droplet theory, we extract intracellular pressure and forces at the intersection of interfaces (e.g. cell-cell, cell-surface, cell-environment). The 2-cell system migrates persistently due to the difference in contact angle at the leading of the leader cell and trailing edge of the rear cell. We present our biophysical framework and compare the emergent force distributions and speed in the 2-cell system with different perturbations.

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MS39

Myosin-Independent Force Transmission for the Extracellular Matrix Stiffness Sensing

Cells transmit different levels of traction in response to the ECM stiffness, which is critical to induce different levels of signaling. One of the frequent destinations of signaling is non-muscle myosin II, which generates contractile force within F-actin cytoskeleton. To explain differential traction, a molecular clutch model, where dynamic clutches between myosin-based F-actin retrograde flow and adhesions result in the force transmission to the ECM, had been developed. However, as myosin II is both the cause and the result of mechanotransduction, myosin alone might not explain the initial difference in force transmission. In this study, using high-resolution traction microscopy and myosin inhibitor, we show that differential force transmission in response to stiffness is myosin-

independent. Inhibiting either of two actin nucleators, Arp2/3 and formin, in addition to myosin abrogated the increasing trend and induced biphasic force-stiffness trend by lowering the traction in high stiffness regime. We developed an actin polymerization-powered molecular clutch model where actin flows not only by myosin contractility but by actin polymerization. The model suggests that Arp2/3 inhibition should make adhesions slip more easily. Together, our data suggest that initial ECM stiffness sensing event by FAs is regulated by actin polymerization-based retrograde flow, synergistically mediated by Arp2/3 and formin.

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MS39

The Immersed Boundary Method for Excitability and Structural Plasticity of Dendritic Spines

Dendritic spines are biochemical and electrical compartments in the synapse to relay neuronal signals to transform their structural information to function. They are highly dynamic in cytoskeletal structure, even in the fully developed stages. The dynamics of the secondary messenger calcium and the holoenzyme CaMKII in dendritic spines is a basis for neuronal plasticity. The immersed boundary (IB) method is advanced for fluid-structure interaction in the context of advection-electrodiffusion of the mediating ions/molecules and synaptic excitability coupled to actin-based motility in dendritic spines. The electrodiffusion of each ionic species and its transport across ion channels is regulated by continuous chemical potentials around the membrane, recapitulating microscopic osmotic effects. Two-phase viscoelastic fluids/gels represent polymeric actin networks, and the associated IB method is formulated as a saddle-point problem. The inflow of calcium governed by electrodiffusion and actin/hydrodynamics experience the reactions to calmodulin and CaMKII. The transitions of chemical reactions-drift-diffusion are treated by a systems of master equations and Monte Carlo Gillespie method. We have model validation with 1) theoretical thermodynamics and voltage-current relationship with osmotic effects and active exchange transporters, 2) actin flow and CaMKII distribution and the associated volume changes by glutamate uncaging and depolarization with published experimental data.

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MS39

Modeling Collective Directed Migration of Astrocytes in a Wound Healing Assay

Astrocytes, a type of glial brain cell, are known to play an active role in almost all areas of embryonic development and homeostasis of the central nervous system. Experimental studies have shown that, postnatally, astrocytes behave similarly to epithelial cells: they establish individual spatial domains with limited overlap with their neighbors and they mechanically interact with their neighbors by adhering via their processes and repelling their cell bodies. To examine the distribution of forces in migrating astrocytes in a wound healing assay, we develop a vertex model that restricts traction force generation to the leading front and compare numerical simulations to experimental data.

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MS40

Multiscale Modeling of Prion Diseases

Prion proteins are responsible for a variety of fatal neurodegenerative diseases in mammals but are harmless to Baker's yeast (S. cerevisiae)- making it an ideal system for investigating the protein dynamics associated with prion diseases. Most mathematical frameworks for modeling prion aggregate dynamics either focus on protein dynamics in isolation, absent from a changing cellular environment, or modeling prion aggregate dynamics in a population of cells by considering the "average" behavior. However, such models are unable to reproduce in vivo properties of different yeast prion strains. In this talk, I will discuss results from recent cell-based model simulations where we study how factors across scales impact the emergence of population level phenotypes in growing yeast colonies. In particular, the rate of disease onset is related to both the replication and transmission kinetics of propagons, the infectious agents of prion diseases. In the model, each cell has their own configuration of prion aggregates governed by kinetic parameters previously estimated by our group for six different yeast prion strains. We use our model simulations to study how population level phenotypes are a natural consequence of the interplay between the cell cycle, budding cell division and prion aggregate dynamics. We then quantify how common experimentally observed outcomes depend on population heterogeneity.

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MS40

Development of a Quantitative Approach for Calibrating Agent-Based Models of Cancer Using Tumor Images

Agent-based models (ABMs) have made great advances in the study of tumor development and therapeutic response, allowing researchers to explore the spatiotemporal evolution of the tumor and its microenvironment. However, these models face serious drawbacks in the realm of parameterization parameters are typically set individually based on various data and literature sources, rather than through a rigorous parameter estimation approach. While ABMs could be fit to time-course data, that type of data loses the spatial information that is a defining feature of ABMs. On the other hand, tumor images, while providing spatial information, represent only a single time-point, and it is exceedingly difficult to compare tumor images to ABM simulations beyond a qualitative visual comparison. Without a quantitative method of comparing the similarity of tumor images to ABM simulations, a rigorous parameter fitting is not possible. Here, we present a novel approach that provides a quantitative comparison of tumor images and ABM simulations. We compute the similarity between ABM predictions and tumor images as a set of spatially-resolved datapoints, preserving the spatial layout of cells. This allows us to then minimize the difference between the two using standard parameter-fitting algorithms.

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MS40

A Computational Model of the Epidermis with the Deformable Dermis and Its Application in Skin Wound Healing

Following injury, skin activates a complex wound healing program. While cellular and signaling mechanisms of wound repair have been extensively studied, the principles of epidermal-dermal interactions and their effects on wound healing outcomes are only partially understood. We developed a multiscale, hybrid mathematical model of skin wound healing. The model takes into consideration interactions between epidermis and dermis across the basement membrane via diffusible signals, defined as activator and inhibitor. Simulations revealed that epidermal-dermal interactions are critical for proper extracellular matrix deposition in the dermis, suggesting these signals may influence how wound scars form. Our model predicts the important role of signaling across dermal-epidermal interface and the effect of fibrin clot density and wound geometry on scar formation.

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MS41

Data-Driven Methods for Model Identification in Biological Systems from Indirect Measurements

Inferring the structure and dynamical interactions of complex biological systems is critical to understanding and controlling their behavior. I am interested in discovering models, assuming I have time-series data of important state variables and knowledge of the possible types of interactions between state variables. The problem is then selecting which interactions, or model terms, are most likely responsible for the observed dynamics. Several challenges make model selection difficult including nonlinearities, varying parameters or equations, and unmeasured state variables. I will describe methods for reframing these problems so that sparse model selection is possible including sparsity-constrained variational annealing and methods to improve data informativity. I will discuss differences between methods designed for chaotic systems and those with non-chaotic attracting fixed points, as well as robustness issues.

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MS41

Topological Data Analysis of Organoid Data

Organoids are cell cultures that can be grown in a laboratory, mimicking certain functions of organ tissues in a mammalian body. By virtue of their similarity to mammalian organs, in terms of 3D tissue composition, organoids can be used to study organ development, disease progression and tissue responses to treatments in settings where 2D cell cultures fail to recapitulate what happens in vivo. It is known, for example, that both cancer and (successful) cancer treatment affect the subsequent development and composition of a tissue and, by extension, the shape of an organoid. In this talk, we present topological methods to study different data sets of videos of organoid experiments, including organoids derived from various organs of human and mouse GI tracts. We demonstrate how topological data analysis captures dynamic changes in the shape and size of these organoids. Based on these dynamic changes in shape and size over time, our analysis can discriminate between wild type and cancerous organoids and identify successful treatment effects.

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MS41

Predicting Single Cell Migration Data with Deep Learning

Mathematical modeling approaches to cell migration, such as ordinary or partial differential equations, require constant refinement, are laborious to develop, and are often inaccurate for single cells. On the other hand, machine learning approaches are quick, but may lack interpretability and the ability to predict. To validate mathematical models, large amounts of quantitative data are often required but are expensive to obtain. Here we present a novel machine learning algorithm to automatically hyper-accurately segment cells in microscopy images. The deep convolutional neural network mimics the human task of tracing objects in an image. Using these hyper-accurate cell segmentations, we investigate whether we can predict cell movement from cell morphology in chemotaxis assays.

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MS41

Top(bug)logical Data Analysis

From synchronized neurons to locust swarms, collective behaviors abound anywhere in nature that objects or agents interact. Investigators modeling collective behavior face a variety of challenges involving data from simulation and/or experiment. We present projects that use topological data analysis (TDA) to address two challenges, namely model selection and detection of dynamical of transitions, both in the context of collective behavior of insects. In the first project, we study motion tracking data from laboratory experiments on pea aphids and use TDA for model selection, determining whether the aphids' behavior is better described by a model that incorporates social interactions or by a control model that does not. In the second project, we study dynamical transitions related to a eusocial behavior in honeybees: food exchange, also known as trophallaxis. When applied to our experimental data, TDA detects distinct temporal regimes, namely, pre- and post- food distribution phases, separated by a food-exchange phase during which clusters of bees form. In both projects, the key approach is to characterize a system's dynamics via the time-evolution of topological invariants called Betti numbers, accounting for persistence of topological features across multiple scales.

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MS42

Olfactory Bulb Processing of Ortho Versus Retronasal Odors

Olfaction is a key sense for many cognitive and behavioral tasks and is particularly unique because odors can naturally enter the nasal cavity from the front or rear, i.e., ortho- and retro-nasal, respectively. Prior imaging studies have shown the brain responds differently to these two modes of stimulation even with identical odors. Yet little is known about the differences in how olfactory bulb (OB) cells process and subsequently transfer this odor information to higher brain. Based on our multi-electrode array recordings of mitral cells in rat OB, we find significant differences between ortho and retro stimulus in trail-averaged population spiking statistics. It is believed that these differences have large implications for how the OB and successive higher brain regions code these modes of stimulation, but our preliminary findings indicate that using trial-averaged population spiking statistics alone to understand coding may be misleading. Using GABA_A agonists and antagonists, we find too little or too much inhibition can reduce average coding accuracy of ortho vs retro odors in OB. Specifically, excess inhibition is found to increase the difference in ortho versus retro firing rate while also reducing coding accuracy. We are currently developing a computational rate model based on our MC data to better understand the inhibitory effects on coding accuracy.

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MS42

Interneuron Subtypes Shape Computations in the Visual and AuditoryCortices

Inhibitory neurons play a crucial role in many components of sensory processing, including modulating feature selectivity, mediating response suppression, and maintaining an asynchronous network state. Past mathematical models have successfully replicated and furthered our understanding of some of these processes by considering a recurrent network of excitatory and inhibitory neurons. However, experimental evidence has shown that significant diversity exists within this inhibitory population, with 80% of neurons falling into one of three major subtypes: parvalbumin (PV)-, somatostatin (SOM)-, and vasointestinal peptide (VIP)-expressing neurons. In this talk, I will construct spatial models of the visual and auditory cortices that incorporate this diversity and make use of tools such as linear response theory to investigate the connectivity properties of these circuits. I will use these models and techniques to show how a division of labor among these interneuron subtypes enables the cortex to 1) have neurons selectively respond to directional auditory sweeps and 2)

control gamma band synchronization during the presentation of visual stimuli.

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MS42

Sensory Input to Cortex Encoded on Low-Dimensional Periphery-Correlated Subspaces

As sensory signals make their way from the sensory periphery to central neural circuits, they become mixed with complex ongoing cortical activity. How do neural populations keep track of sensory information, separating signals from the noisy ongoing activity? Here we consider large neural populations simultaneously-recorded from primary sensory cortices and upstream sensory brain regions. We show that sensory signals are encoded more reliably and separated from noise in certain low-dimensional subspaces. We identified these coding subspaces based on correlations between cortex and upstream brain regions; the most correlated dimensions were best for decoding. Subspaces with approximately 5 dimensions were optimal for decoding although the neural populations we studied were much higher dimensional. We show that this principle generalizes across diverse sensory stimuli in the olfactory system and the visual system of awake mice. Our results suggest the cortex may multiplex different functions by executing them in different low dimensional subspaces.

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MS42

Dynamic Attention Coding in Sensory Cortical Populations

Shifts in attention are associated with changes in spontaneous and sensory-evoked activity in neural populations throughout the brain, including extrastriate visual and prefrontal areas. Although these neurophysiological attention correlates are dynamic, the computational roles of the dynamics themselves have been seldom studied. We recorded neural populations in visual and prefrontal cortical areas of monkeys performing spatial selective attention tasks, and analyzed the dynamics of attention signals at the level of individual neurons and of neural populations. First, we found that attention signals in sensory cortex were dynamic on faster timescales than attention signals in frontal cortex. This may indicate a division of labor across brain areas for computations that rely on different dynamic regimes. Second, we found that the time-course of attention effects was highly heterogenous across visual neurons, and this variation was related to other functional properties of neurons, such as whether they were inhibitory/excitatory, or the strength of their functional coupling to the broader population. This provides important clues about the circuit organization of dynamic attention processes. Third, we found that the strength of dynamic stability on a moment-by-moment basis was related to attentional lapses evident in behavior. Taken together, these findings advance our understanding of attention mechanisms in the context of the dynamic brain.

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MS43

Dynamic Properties of Pituitary Cell Networks

Pituitary hormones are secreted by five families of endocrine cells. These cells are electrically active, and hormone secretion occurs when the cells produce bursts of electrical impulses. Although most of what is known about pituitary cell biophysics comes from studies of dispersed cells, in the physiological environment cells of each type form networks, where gap junctions electrically couple one cell to its neighbors. Such structural networks give rise to functional networks in which cells whose activity is synchronized are considered to be neighbors. While the determination of structural networks of pituitary cells is technically very difficult, determination of functional networks is more tractable, using calcium fluorescence in pituitary slices. Such studies have demonstrated that the functional networks are scale-free, with a power-law degree distribu-

tion, characterized by a few high-degree hubs and many low-degree nodes. In this presentation, we use mathematical models of scale-free structural pituitary cell networks to determine what the functional network properties tell us about the structural network. We address several questions: Are the hubs of functional (structural) networks also hubs of the structural (functional) networks? To what extent is it possible to construct a structural network using data from a functional network? How does the giant component of synchronized cells decay as cells are systematically or randomly silenced or eliminated?

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MS43

How Do Asynchronous Brain Rhythms Mask the Dynamics of Synchronous Activity During Loss of Consciousness from Propofol

General anesthesia is characterized by changes in the EEG, primarily quantified using spectral analysis techniques, such as the spectrogram. EEG spectra display not only peaks that are indicative of the presence of neural rhythms, but also an overall trend of asynchronous activity that decays with frequency. Although EEG correlates of loss of consciousness (LOC) due to anesthetics such as propofol are often ascribed to changes in neural synchrony, mounting evidence suggests that some changes result from asynchronous neural activity. We have recently investigated how propofol alters the broadband (0.5-100 Hz) asynchronous properties of the EEG, and examined what implications this may have for interpreting changes in neural rhythms during LOC. We combined analysis of EEG recordings of humans undergoing propofol administration with biophysical modelling to decompose changes in the EEG during LOC into synchronous and asynchronous sources. Our results revealed that IPSP decay rate and mean spike rate shape asynchronous EEG features, that propofols effects on these parameters largely explain the changes in EEG spectra during LOC, and that traditional spectral EEG analysis likely conflates these effects with changes in rhythmic activity. We concluded that the propofol-induced alpha rhythm appears before LOC, and that the moment of LOC is uniquely correlated with the sudden appearance of a delta rhythm. I will provide a summary of these results in my talk.

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MS43

Are Oscillations Within Islets Governed by Pacemakers?

Beta cells within the pancreatic islet coordinate their secretion of insulin during elevated glucose levels. Electrical coupling between beta cells gives rise to a syncytium reminiscent of cardiac tissue. Recent experimental work has suggested that a small population of hub cells, defined by correlated functional connectivity of calcium traces, and further identified to have higher glucokinase activity, are important for islet coordination. In particular, silencing hub cells was able to greatly reduce the islet activity, leading to the hypothesis that a small set of pacemaker cells drive islet activity. Historically, theory and modeling studies have favored a more democratic interpretation of islet activity where there may be leader cells initiating activity but loss of any one cell at most delays the inevitable bursting activity. In this case the response curve to glucose has been shown both in experiment and in models to be sharpened by electrical coupling (ie. more cells must reach threshold to initiate activity, but then, across this threshold, more cells are recruited to activity as compared to uncoupled cells). In this talk we review some of the arguments against the likelihood that islets are governed by a cardiac-like pacemaker.

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MS43

Modelling the GnRH Pulse Generator Dynamics

The gonadotropin-releasing hormone (GnRH) pulse generator controls the pulsatile secretion of the gonadotropic hormones LH and FSH and is critical for fertility. The hypothalamic arcuate kisspeptin neurones (KNDy) are thought to represent the GnRH pulse generator, since their oscillatory activity is coincident with LH pulses in the blood; a proxy for GnRH pulses. However, the mechanisms underlying GnRH pulse generation and controlling its dynamics remain elusive. We developed a mathematical model of the kisspeptin neuronal network and confirmed its predictions experimentally, showing how LH secretion is frequency-modulated as we increase the basal activity of the arcuate kisspeptin neurones in vivo using continuous optogenetic stimulation. Furthermore, gonadal steroids regulate GnRH pulsatile dynamics across the ovarian cycle by altering KNDy neurones' signalling properties. To better understand these mechanisms, we again combine in vivo experiments with mathematical modelling. Our results reconcile previous puzzling findings regarding the estradiol-dependent effect that several neuromodulators have on the GnRH pulse generator dynamics. Therefore, we anticipate our model to be a cornerstone for a more quantitative understanding of the pathways via which gonadal steroids regulate GnRH pulse generator dynamics.

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MS44

Modeling 3D Interactive Cardiac Simulations in Real Time

Cardiac disease has been a leading cause of death in the US and globally for several years. Many attributes of electrophysiological arrhythmias are caused by the emergent phenomena in three-dimensional tissue. Numerical simulations can help provide mechanistic insight into the formation and termination of arrhythmias. However, numerical solution of the cardiac electrophysiological models in tissue has a high computational cost due to the small spatial resolution demanded by the small size of the cardiac myocytes. Furthermore, the time marching problem is further complicated by the small time-steps required by the steep upstroke of the cardiac action potential. General Purpose GPU (GPGPU) processing has been previously proposed to accelerate the solution of such problems. In this study, the cartesian grid alongside finite differences is proposed to facilitate GPGPU parallelization of 3D cardiac models on realistic structures using WebGL 2.0. We present a compression algorithm which can be used with the cartesian grid to avoid creating a mesh while accurately applying zero-flux boundary conditions. This method can provide higher acceleration compared to other GPGPU implementations. The result is a three-dimensional code that can run close to real-time on personal computers.

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MS44

Robust Automaticity and Emergent Tissue Heterogeneity in a Calcium Feedback Regulatory Model of the Sinoatrial Node

The sinoatrial node (SAN) is the primary pacemaker of the heart. SAN activity emerges at an early point in life and maintains a steady rhythm for most of the lifetime of the organism. The emergent activity and long-term stability imply the presence of dynamical feedback control of SAN cell activity. Recent work in the neuroscience field proposed a minimal regulatory model of neuronal ion channel conductance based on [Ca2+]-mediated feedback. This mechanism in brief works as follows: An individual cell tries to match a set intracellular Ca2+ (Cai) target through regulation of ion channel mRNA and subsequent membrane expression levels. If the Cai is below the target, ion channel expression increases, thus leading to higher average Cai. Here, we adapt this regulatory model to the SAN rabbit cell. Our results show that the SAN cell activity can emerge from low starting conductances. As conductances increase, the cell reaches its [Ca2+] target and ion channel conductances reach a steady state. Further, the cells can adapt their activity to different [Ca2+] targets, to outside stimuli such as increased pacing rates, or to ion channel perturbations. In a 2D tissue, combinations of cell-cell coupling and [Ca2+] target ranges lead to heterogeneous ion channel expression and Ca transients, similar to recently published experimental recordings. Thus, the proposed model explains experimental findings with a minimal description of Cai and ion channel regulatory network feedback.

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MS45

Surfactant Self-Assembly at Immiscible Liquid-Liquid Interfaces for 3D Printing Applications

Description: Multicomponent amphiphilic systems containing oil, water, and surfactants have been widely utilized in applications ranging from oil recovery and drug delivery to artificial cells and membranes. Here, surfactant self-assemblies at the water-oil interface have been used to develop a new liquid-in-liquid 3D printing technique to fabricate aqueous constructs by injecting the continuous tubules of aqueous solutions within a polar oil phase. The photopolymerization of these printed liquid constructs render them mechanically robust and lock in the shape of printed constructs. SAXS measurements confirm the presence of nanostructures (HEX and LAM morphology) within the cured printed constructs. Tensile tests revealed that printed constructs are mechanically robust and can be tuned by changing the composition of aqueous solutions. The work presented here has implications in a wide variety of complex fluid systems, including surfactant mixtures, polymer solutions, emulsions, and colloidal domains.

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MS45

Hydrodynamics of a Semipermeable Vesicle under Strong Confinement

Lipid bilayer membranes have a native permeability for water molecules. In the absence of osmolarity, the water flux is often assumed to be negligible. However, we demonstrate that semipermeability can cause large amounts of fluid exchange, even in the absence of osmolarity. We investigate the effects of semipermeability on the hydrodynamics of an inextensible vesicle under mechanical loads caused by an external flow and extreme confinement. Several comparisons are made between impermeable and semipermeable vesicles.

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MS45

Influence of Membrane Slip on General Vesicle Dynamics

Vesicles are multiphase fluid systems where a lipid bilayer separates the two fluids. They form model systems for more complicated biological cells and have been proposed for various biotechnologies such as drug delivery systems. Due to the complex nature of the membrane, an understanding of how the properties of said membrane is crucial to advancing the use of vesicles in modern technologies. One less investigated property of these membranes is the ability to slide past each other due to the layers being weakly coupled. From a macroscopic point-of-view, this appears as a jump in the tangential velocity of the surrounding fluid, with the magnitude of this discontinuity depending on membrane properties. Building upon prior works in modeling vesicles with fully coupled membranes, a numerical model is presented capable of modeling vesicles with interfacial slip in general flows. After a brief discussion of the numerical methods involved, including the composition of computational stencils, the model will then be used to explore the dynamics of vesicles in various types of flows as a function of the membrane slip coefficient.

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MS45

Microtubule-Mediated Deformation of Cell Nucleus with Permeability

The cellular nucleus is enclosed by a permeable membrane mechanically supported by a meshwork of lamin fibers. The morphology and integrity of the nucleus are essential for the cell's function. Recent experiments show that loss of the lamin network results in nuclear deformations and rupture. To understand the mechanistic basis of this phenomenon, we developed a mathematical model that accounts for, and couples, the fluid flows around and through the permeable membrane, and the pulling on the membrane by membrane-bound, but mobile, molecular motors attached to impinging microtubules. Here the microtubules are assumed to nucleate from a cellular centrosome. We found that this model predicts the formation of a sharp corner in the vicinity of the centrosome, rather reminiscent of the Taylor cone for a surfactant-laden drop in an elongational flow. We analyze the equilibrium shape of the membrane in terms of the total number of motors and their mobility in the nuclear membrane. Our model provides a more mechanistic understanding of nuclear deformation in cells and can give insights into the correspondence between motor forces and membrane deformation leading to nuclear rupture, which has been observed in some cancer cells.

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MS46

Impact of Data Structure, Availability and Noise Distribution on Practical and Structural Identifiability of an Seir Model

With the increasing practice of using biological data to assess and parameterize theoretical models, it is important to understand the conditions under which we can reliably recover model parameters from available data. This is particularly important in the context of epidemiological data, which may gradually become available alongside an emerging infection or may only be reported over large time intervals. In this work, we consider an SEIR infection model, with three unknown parameters. Our goal is to assess how different methods and resolutions of data collection determine parameter identifiability. We consider the impact of the frequency and duration of observations, for different types of observed data (infections, incidence, and cumulative incidence). We utilize both Monte Carlo simulations and correlation matrices to assess parameter identifiability under these conditions. We additionally present preliminary work connecting parameter identifiability to model specification, in the context of nested models.

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MS46

The Role of Infection on Shifts in Population Cycles in a Discrete-Time Epidemic Model

One-dimensional discrete-time population models, such as for logistic or Ricker growth, exhibit periodic and chaotic dynamics. Adding epidemiological interactions into the system increases its dimension and the resulting complexity of its behaviors. Previous work showed that while a discrete SIR model with Ricker growth exhibits qualitatively similar total population dynamics in the presence and absence of disease, a more complicated viral infection (SIV) system does not. Instead, infection in the SIV system shifts the periodic behavior of the system in a manner that distinguishes it from the corresponding disease-free system. Here, we examine a SI model with Ricker population growth and show that infection produces a distinctly different bifurcation structure than that of the underlying disease-free system. We use analytic and numerical bifurcation analysis to determine the influence of infection on the bifurcation structure of the system. In addition, we derive the basic reproductive number and determine the influence of population growth and decay parameters on. Our work shows that even in the SI model, infection dynamics can shift the location of period-doubling bifurcations as well as the onset of chaos.

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MS46

Asymptotic Profiles of the Steady States for an SIS

Epidemic Patch Model with Asymmetric Connectivity Matrix

The dynamics of an SIS epidemic patch model with asymmetric connectivity matrix is analyzed. It is shown that the basic reproduction number R_0 is strictly decreasing with respect to the dispersal rate of the infected individuals, and the model has a unique endemic equilibrium if $R_0 > 1$. The asymptotic profiles of the endemic equilibrium for small dispersal rates are characterized. In particular, it is shown that the endemic equilibrium converges to a limiting disease-free equilibrium as the dispersal rate of susceptible individuals tends to zero, and the limiting disease-free equilibrium has a positive number of susceptible individuals on each low-risk patch. Moreover a sufficient and necessary condition is found to guarantee that the limiting disease-free equilibrium has no positive number of susceptible individuals on each high-risk patch. Our results extend earlier results for symmetric connectivity matrix, and we also partially solve an open problem by Allen et al. (SIAM J. Appl. Math., 67: 1283-1309, 2007)

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MS46

Modelling the Effect of Travel-Related Policies on Disease Outbreaks in a Metapopulation Structure

Emerging infectious diseases (EIDs) often render a potential for global spread. This problem is likely exacerbated by the explosive growth of international transportation, especially air travel. Although their effectiveness is debatable, long-term travel restrictions can lead to enormous socio-economic burdens and likely mental health sequelae. Here, based on existing literature and gained knowledge during the COVID-19 pandemic, we develop a metapopulation model framework to evaluate the impact of travel policies between populations, involving testing and quarantine. Within this framework, we consider a leaky quarantine with a fixed duration, after which a fraction of the exposed or infectious travellers enter the population. We explore how the peak of incidence and the time of 0.1% prevalence respond to the dispersal rate, the true-positive rate of testing of the exposed and the infected individuals, and the duration of quarantine following travels.

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MS47

Stochastic Rotating Waves

Abstract: In this talk, we start with a short summary of several important mathematical results for stochastic travelling waves generated by monostable and bistable reaction-diffusion stochastic partial differential equations (SPDEs). The aim is to bridge different backgrounds and to identify the most important common principles and techniques currently applied to the analysis of stochastic travelling wave problems. Then we are going to explain a recent result on stochastic pattern formation going beyond travelling waves: stochastic rotating waves generated by SPDEs. We establish two different approaches for stochastic rotating waves, the variational phase and the approximated variational phase, which both help us to compute a stochastic ordinary differential equation (SODE), which describes the effect of noise on neutral spectral modes associated to the special Euclidean symmetry group of rotating waves. Furthermore, we prove transverse stability results for rotating waves showing that over certain time scales and for small noise, the stochastic rotating wave stays close to its deterministic counterpart. Joint work with J. MacLaurin and G. Zucal.

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MS47

Effects of Moderate Noise on a Limit Cycle Oscillator: Counterrotation and Bistability

The effects of noise on the dynamics of nonlinear systems is known to lead to many counterintuitive behaviors. Using simple planar limit cycle oscillators, we show that the addition of moderate noise leads to qualitatively different dynamics. In particular, the system can appear bistable, rotate in the opposite direction of the deterministic limit cycle, or cease oscillating altogether. Utilizing standard techniques from stochastic calculus and recently developed stochastic phase reduction methods, we elucidate the mechanisms underlying the different dynamics and verify our analysis with the use of numerical simulations. Last, we show that similar bistable behavior is found when moderate noise

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MS47

Balanced Neural Fields

We use statistical mechanics techniques to obtain population density equations for large sparse neural networks. The connectivity is that of 'balanced excitation and inhibition', meaning that the sum of the magnitudes of all typical inputs into any one neuron typically diverges with the system size, however the level of excitation typically balances the level of inhibition, thereby preventing the system from blowing up. The density of connection decays with distance, and in taking the large size limit one obtains a spatially-distributed neural-field equation. We finished by proving the existence of 'bump attractors' of locally-excited neural activity.

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MS47

Synchronization of Stochastic Oscillators Through Common Noise

In this work we study the level of synchronization in stochastic biochemical reaction networks that support stable mean-field limit cycles and are subject to common external switching noise. Synchronization in stochastic limit cycle oscillators due to common noise is usually demonstrated by applying Itos lemma to the logarithm of the phase difference. However, this argument cannot be straightforwardly extended to our case because of its discrete state space. Assuming the intrinsic and extrinsic noises operate at different time scales, we prove that the

average level of synchronization is of the order of the rate of the intrinsic noise (inversely proportional to the system volume) times the square of the switching rate of the external noise. Moreover, we show in numerical experiments the approximate asymptotic value of the synchronization level by applying this result to classical oscillators found in the literature.

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MS48

A Multiscale Cell-Resolved Computational Technique for Simulation of Hemolysis in Large Vessels

When red blood cells (RBCs) experience non-physiologically high stresses, e.g., in medical devices, they can rupture in a process called hemolysis. Directly simulating this process is computationally unaffordable given that the length scales of a medical device are several orders of magnitude larger than that of a RBC. To overcome this separation of scales, the present work introduces an affordable computational framework that accurately resolves the stress and deformation of a RBC in a spatially and temporally varying macroscale flow field such as those found in a typical medical device. The underlying idea of the present framework is to treat RBCs as one-way coupled tracers in the macroscale flow and resolve the fluid velocity in their immediate vicinity as well as the motion of the membrane by employing the boundary integral method coupled to a structural solver. The governing equations are discretized in space using spherical harmonics, yielding spectral integration accuracy. The predictions produced by this formulation are in good agreement with those obtained from simulations of spherical capsules in shear flows and optical tweezers experiments. The accuracy of the present method is evaluated using unbounded shear flow as a benchmark. Its computational cost grows proportional to p^5, where p is the degree of the spherical harmonic. It also exhibits a fast convergence rate that is approximately $O(p^6)$ for $p \leq 20$.

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MS48

High-Throughput Measurement of the Human Red Blood Cell Shear Modulus Distribution as a Function of PO2

One of the fundamental questions around the human circulatory system is to determine how blood flow can be distributed when and where it is needed. For example, J. Wan and his colleagues[1] very recently showed that cerebral functional hyperemia is initiated in the capillaries with RBCs acting as oxygen sensors to regulate cerebral blood flow. In this case, the interactions between deoxygenated hemoglobin (deoxyHb) and band 3 protein in the RBC membrane are the molecular switch that responds to local PO2 changes. RBC deformability is largely governed by the membrane shear modulus. State-of-the-art microfluidic platforms for high-throughput measurements of RBC mechanical properties have not enabled measurement of the shear modulus heretofore. These limitations challenge the development of diagnostic devices based on RBC shear modulus biomarkers. In this talk, we will review the development of our high-throughput microfluidic platform to address this significant gap in technology[2]. Our approach allows us to measure the shear modulus of individual RBCs and generate shear modulus distributions including measurements of thousands of cells in minutes. We will then discuss the modification of our platform to make similar measurements but at controlled PO2 saturation levels in the blood. [1] Zhou et al., Sci. Adv. 2019; 5 : eaaw4466 29 May 2019;[2] Saadat et al., Lab on a Chip , 20, pp. 2927-2936 (2020).

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MS49

Actin-Myosin Dynamics During Bleb Stabilization

Blebs are pressure driven spherical protrusions of the plasma membrane which form when a patch of cell membrane is detached from the cortex and expands under the influence of flowing cytosol. The stabilization of the membrane protrusion is characterized by a complete degradation of the old cortex (actin scar) and the formation of a new cortex beneath the protruded membrane, a process that takes about 20 seconds in *Dictyostelium discoideum* cells. The mechanism by which the cortex is degraded at the actin scar and simultaneously reformed at the developing bleb boundary is not fully understood. Our recent microscopy data reveals an accumulation of myosin II in the actin scar immediately following the detachment of the membrane and prior to a complete degradation of the actin scar. This accumulation is only present where the membrane is detached from the cortex. Simultaneously, myosin II is enriched at the new bleb boundary at a rate that lags behind the formation of the cortex by about 2 seconds. We hypothesize that myosin accumulation, potentially induced by membrane detachment, contributes to cortical degradation in the actin scar and is delayed in the new bleb boundary to allow the new cortex to stabilize. A mathematical model of actin-myosin dynamics in the actin scar is developed and analyzed to test our hypothesis.

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MS49

Mechanics of Cell Migration in Confinement

Migrating cells, such as metastatic cancer cells, move in complex tissue environments. In this talk I will discuss

work my group has done investigating how the velocity and shape of migrating cells is affected by the geometric and mechanical properties of the environment they are in. To capture some physical understanding, we develop simple theoretical models which we study using analytical calculations and numerical simulations. I will present our simple model of a cell as an active droplet and discuss our results on how the velocity, shape and migration mode of this model is affected by fluid and elastic environments. I will then consider constrictions and the conditions necessary for a model cell to successfully pass through a constriction. For the case of constrictions smaller than the cell nucleus, I will introduce our simple model of a nucleus. As well as analysis of experimental data, I will share ideas of what we think is necessary for a cell to force its nucleus through a small constriction.

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MS49

Simulating Filament Dynamics Unravels the Motility Mechanism of Spiroplasma

Spiroplasma is a unique, wall-less bacterium that swims by flipping the handedness of its helical shape at one end of the cell. This change in chirality moves outward from the end at constant speed, causing a kink in the cell shape to move down the length of the cell and also causing rotation of the cell body. The handedness of the cell eventually flips back to its original state at the end where the kink started, with this second kink also moving down the length of the cell until the entire cell is back its original state. An array of filaments has been found inside the cell and anchored to the cell membrane that are implicated in producing the cell shape, but how these filaments produce these traveling kinks remains mysterious. To address this question, we developed two models for creating helicity, one that involves bending and the other that involves twisting. We simulated the dynamics of Spiroplasma in the context of these two models using a new finite-volume filament dynamic algorithm that we developed. In this talk, I will describe this new algorithm and discuss how we used these simulations coupled with experimental measurements to determine whether Spiroplasma drives its motility through bend- or twist-driven mechanisms.

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MS49

Numerical Model for a Viscoelastic Cell Cortex

The cell cortex is a key regulator for the cell's shape and its functions, for instance during cell division. It shows elastic properties on short timescales and viscous properties on longer timescales. Hence to properly simulate it, a viscoelastic model covering the whole viscous to elastic spectrum is needed. Using the GENERIC framework we developed the surface equivalent of the upper convected Maxwell model. In this talk we present our numerical implementation of a viscoelastic surface embedded in a viscous fluid. We use this model to simulate the influence of active surface tension or other surface forces on the cell cortex. An example of which are the counter rotating flows observed during cytokinesis. We study the influence of these and how changing the viscoelastic parameters changes cell shape and the distribution of a surface bound molecule concentration. We observe that these counter rotating flows can promote a ring of high molecule concentration which could facilitate cell division.

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MS50

Applying Mechanistic Models to Understand Variable Responses of SIV to IL-15 Immunotherapy

Immunotherapy has potential for treating chronic infections such as human immunodeficiency virus. Effectiveness of therapy may depend on intrinsic host immune factors and on the state of the infection within the host. We employ a mechanistic model of simian immunodeficiency virus (SIV) infection and Interleukin-15 (IL-15) agonist therapy to identify factors influencing IL-15 efficacy in two non-human primate cohorts. One cohort previously controlled SIV without treatment (controllers), and IL-15 therapy temporarily restored this control. The other cohort had no history of control (non-controllers) and saw no consistent viral suppression with IL-15 therapy. The model is separately calibrated to each cohort using plasma viral load and peripheral blood CD8+ T cell data. Bayesian uncertainty quantification is used to compare parameter values and model predictions between the two cohorts. Notably, higher levels of pre-treatment CD8+ T cell activation in the non-controllers contribute to the reduced effectiveness of IL-15, as there is less potential for increased activation. This aspect is qualitatively validated by additional experimental data. The immune-dampening response to IL-15-induced inflammation is also distinct between the cohorts, as is the growth rate of the virus. Our mathematical model could inform which infection states and host conditions would most benefit from IL-15-based immunotherapies.

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MS50

Exploring Intracellular Dynamics and Underlying Mechanisms of Transport

Live cell imaging and single particle tracking techniques have become increasingly popular amongst the mathematical biology community. Lysosomes, known for endocytosis, phagocytic destruction, and autophagy, move about the cell along microtubules. Intracellular transport of lysosomes is carried out in membrane-bound vesicles through the use of motor proteins. Single particle tracking methods utilize stochastic models to simulate intracellular transport and give rise to rigorous analysis of the resulting proper-

ties, specifically related to transitioning between inactive to active states. We find confidence in our methodology and develop simulations to capture these properties at multiple frames rates. Determining an optimal frame rate for capturing live cell data is necessary in order to successfully infer properties or the underlying mechanisms. We rely on an optimal frame rate to extract properties about the microtubule network of the cell.

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MS50

Explainable-AI Predicts Flying Fox Food Shortages with Applications to Future Pandemics

Food availability is an important indicator of physiological stress and health in Australian flying fox populations, which in turn are hypothesized to be causal of increased viral shedding and thus increased infectious disease spillover risk. Here we present a machine learning model that classifies time periods of food shortage as a function of climatological and ecological covariates collected from 2005 to 2020 in eastern Australia. By leveraging techniques from explainable artificial intelligence, we identify a reduced set of input features that help explain the variance in the outputs to derive a reduced model with increased prediction accuracy and decreased complexity. We discuss how these results overlap with understanding of flying fox ecology, and how the model might be employed to anticipate periods of food availability and mitigate infectious disease spillover risk.

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MS50

Emergent Collective and Deterministic Behavior of Mitotic Spindle from Stochastic Chromosome Dynamics

Mitotic spindle is a remarkable molecular machine segregating chromosomes prior to cell division. The spindle self-assembles from centrosomes, microtubules and chromosomes very rapidly and accurately, so that in the end all chromosomes are bioriented (each chromosome is attached to the opposite spindle poles). For decades, the so-called search-and-capture model of this self-assembly was dominant. This model posited that the microtubules randomly probe the cell space until, by chance, all chromosomes connect to the microtubules. Recent data indicate that most chromosomes achieve biorientation at the same time in the same place, putting this model in doubt. I will show that both the data and stochastic computational model argue that a much more deterministic process of polarity sorting in a complex microtubule-motor system results from the rapid stochastic process and accounts for the rapid and accurate assembly of the spindle.

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MS51

Mean-Field Approximations for Kuramoto Networks with Neural Plasticity

Synaptic plasticity is considered the primary mechanism for learning and memory. Neurons with similar activity patterns strengthen their synaptic connections, while others connections may weaken. Synaptic plasticity is rarely examined at the mesoscopic level, as, typically, comparisons between spike times or firing rates of individual neurons are required to update the synaptic coupling strength. Assuming a network of coupled Kuramoto oscillators, we define spike time differences in terms of phase differences. We then update the coupling weights based on these phase differences. By approximating the coupling weight dynamics with the average coupling strength and applying the Ott-Antonsen ansatz, we arrive at a mean-field description of the network dynamics. This mean-field model allows us to examine the role of synaptic plasticity at the mesoscopic level and investigate the formation of cluster states in a tractable manner.

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MS51

Thalamo-Cortical Networks: Reduction, Analysis, and Modulation

The thalamus is a body of neural cells that relays impulses to the cerebral cortex from the sensory pathways. Feedback from the cortex gives rise to thalamo-cortical loops that generate emergent brain rhythms from the interplay of single cell ionic currents and network mechanisms. Here we discuss parsimonious models of cortex and thalamus using different types of nonlinear integrate-and-fire unit. The integrate-and-fire-or-burst model is a natural choice for building a model thalamus (from networks of relay and reticular cells) that can intrinsically oscillate via post-inhibitory rebound (mediated by a slow T-type calcium current) whilst the cortex can be more simply modelled using a network of quadratic integrate-and-fire neurons. In both cases we discuss the reduction to a lower dimensional mean-field model, utilising a separation of time-scales argument for slow synaptic interactions in the thalamus model, and the Ott-Antonsen ansatz for the cortical model. The resulting firing rate equations for both brain organs are coupled to form a thalamo-cortical loop model. The relevance of this model for understanding brain response to sensory drive is highlighted with a comparison to human neuroimaging data for median nerve stimulation.

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MS51

A Mean-Field Firing-Rate Model for the Suprachiasmatic Nucleus

We present a mean-field formalism for studying firing-rate statistics of brain regions whose neurons exhibit atypical firing patterns and heterogeneous electrophysiological properties. Indeed, while mean-field formalisms have successfully modeled signaling in many brain regions, the suprachiasmatic nucleus (SCN)the human circadian pacemakerpresents unique challenges. Namely, SCN neurons intrinsically exhibit depolarized low-amplitude membrane oscillations (DLAMOs), depolarization block (DB), and standard action potential firing, but at different times of day. Further, GABA reversal potential and molecular circadian phase of SCN neurons, among other properties, vary across the network or slowly over time. To address these challenges, our formalism consists of a system of integro-differential equations describing the time evolution of the mean and standard deviation of synaptic conductances across the network. Electrophysiological properties of SCN neurons are incorporated by computing responses to synaptic conductance inputs of a Hodgkin-Huxley-type SCN neuron model that exhibits DLAMOs and DB. Such responses are then averaged over distributions of relevant quantities and included in the differential equations. Results show that a large spread in circadian phases across SCN neurons reduces the size of oscillations in SCN network firing activity, identifying a mechanism by which systematic disruptions of neuron electrophysiology could contribute to circadian disorders.

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MS51

An E-I Rate Model for PING and ING

Rate models for describing the mean-field activities of neuronal ensembles can be used effectively to study network function and dynamics, including synchronization and rhythmicity of excitatory-inhibitory populations. However, traditional Wilson-Cowan-like models, being amenable to math analysis, are found unable to capture some dynamics such as inhibitory network gamma oscillations (ING) although use of an explicit delay can help. We resolve this issue by introducing a mean-voltage variable that considers the subthreshold integration of inputs and works as an effective delay in the negative feedback loop between firing rate and synaptic gating of inhibition. I will describe an r-s-v firing rate model for inhibitory networks which is biophysically interpretable and capable of generating ING-like oscillations. Linear stability analysis, numerical branch-tracking and simulations show that the rate model captures many of the common features of spiking network models for ING. We further extend the framework to excitatory-inhibitory networks. With our 6-variable r-s-v model, we describe the transition from PING to ING by increasing the external drive to the inhibitory population without adjusting synaptic weights. Having PING and ING available in a single network, without invoking synaptic blockers, is beneficial for explaining the emergence and transition of two different types of gamma oscillations.

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MS52

Reading the Flash Glucose Monitoring Trace in Diabetes: What Are the Metrics of Glucose Homeostasis?

The widespread usage of the "continuous (or flash) glucose monitoring (FGM)" is an exciting development in the field of glucose monitoring technology. The glucose time series, collected every 15 minutes for two weeks, represents a high resolution, high density source of information that can potentially be mined to characterize the physiology of a patient's glucose disposal in some detail. A consensus analysis recently developed by the ATTD (Danne et al., Diabetes Care, 2017) aims to standardize the metrics used to characterize an FGM; most of these, however, are morphological in nature. We argue that "classical" investigations, such as the OGTT, which aim to quantify glucose clearance ought to be possible to translate to the FGM. I will describe our attempts to develop (i) a proof-of-concept version of the OGTT for the FGM, and (ii) models of A1C determined from the FGM trace.

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MS52

Novel Closed-Form Approximations of Stationary Single-Channel Calcium Nanodomains

Ca^{2+} elevations in the vicinity of open Ca^{2+} channels (Ca^{2+} "nanodomains") trigger secretory vesicle exocytosis and other fundamental cell processes. Ca^{2+} nanodomains are shaped by the interplay between Ca^{2+} diffusion and binding to intracellular Ca^{2+} buffers, and can be estimated by approximating the stationary solution of the corresponding reaction-diffusion problem, in closed form. Such closed-form approximations help in the modeling of Ca^{2+}-dependent cell processes, without resorting to computationally expensive numerical simulations. However, previously developed approximants had been shown to represent asymptotic expansions restricted to specific regions of the relevant parameter space, and only apply the case case of buffers with a single Ca^{2+} binding site, whereas most biological buffers have more complex Ca^{2+}-binding stoichiometry. Here we describe a new closed-form approximation method based on interpolation between the short-range Taylor series of the Ca^{2+} or buffer concentration with the corresponding long-range asymptotic series expressed in inverse powers of distance from channel location. We show this this new method achieves reasonable accuracy for a wider range of buffering conditions, and can also be extended to the case of Ca^{2+} buffers with two Ca^{2+}-binding sites. Supported in part by NSF DMS-1517085 (V.M) and

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MS52

Estimating Incretin Effects from Modeling Oral Glucose Tolerance Tests

Incretin dependent insulin response has been shown to be impaired in type 2 diabetes (T2D). Incretin effects have been estimated experimentally by doing an Isoglycemic Intravenous Glucose Infusion Experiment (IIGI) where plasma glucose profiles are matched to that in the corresponding Oral Glucose Tolerance Test (OGTT) on the same patients. As this method requires two separate experiments to be conducted on the same patients, an alternative method of estimating the incretin effect from one experiment such as the OGTT would be useful. We developed an extended minimal model of glucose-insulin-glucagon dynamics where the effect of GLP-1 or GIP on insulin secretion in an OGTT was also investigated. This theoretical model offers an alternative method of estimating the incretin effect by fitting data from OGTT experiments where plasma incretin concentrations are monitored in addition to insulin and glucagon. A comparison of the incretin effect obtained from modeling the OGTT is made with that obtained experimentally from OGTT and the corresponding IIGI data. Such modeling also allows one to estimate the extent to which GLP-1 augmentation, for example, would increase insulin secretion in an individual with T2D who has some residual incretin effect.

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MS52

A Type-2 Diabetes Biomarker from Continuous Glucose Monitoring

The incidence of type-2 diabetes (T2D) in the USA has doubled over the past fifteen years and similarly concerning trends are observed around the world. In T2D patients, the body produces the regulatory hormones insulin and glucagon, but their effectiveness has waned to the point where blood glucose levels can get dangerously high. If diagnosed early, T2D can be reversed by changes in life style and diet, while more advanced cases can only be managed, not cured, by drugs like Metformin. Thus, early detection is quintessential. Currently used "gold standard" tests are both invasive (requiring blood samples, fasting or ingesting calibrated amounts of sugar) and inaccurate, threshold values varying from one health organisation to the next. We explore the feasibility of extracting a biomarker for T2D from Continuous Glucose Monitors (CGMs) that subjects can wear while going about their daily routine, effectively replacing few measurement taken under controlled conditions by many taken under normal circumstances. Based on a concise model of homeostatic control and data from various clinic trials, we present a novel biomarker and discuss its accuracy and sensitivity.

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MS53

Stiffness Determination for Umbilical Arteries by Parameter Fitting

The surgery using the decellularized human umbilical artery (UA) as a by-pass graft is employed to repair the occluded or narrowed coronary artery to restore normal blood flow. During the decellularization process, immunogenic cellular components in the UA are removed to minimize the immune cells biological activities on the extracellular matrix for the UAs adaptation to the patients coronary artery. To make the decellularization process more complete, the outer layer is removed, and only the inner layer is used for the bypass graft. The stiffness of the layer-reduced UA is different from the original UA, and is difficult to measure directly by lab experiments due to its tiny, cylindrical shape. This study aims at establishing proper biomechanical models and employing numerical techniques to obtain the stiffness of the layer-reduced UA. A strain-energy function for the isotropic elastic material and fibers in the tissue is set up to derive the Cauchy stress with prescribed internal pressure boundary conditions. The models consist of stiffness parameters for the shear modulus and fiber stiffness. Experimental data and theoretical results are used to set up the objective functions. We employ optimization techniques by MATLAB to obtain the stiffness parameters. The results are analyzed for its significant physiological effects used in the by-pass graft.

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MS53

Computational Modeling of Intimal Thickening Induced by Hemodynamical Shear Stresses with Fiber Fields in 2D Vessels

Atherosclerosis has been a primary cause of potentially fatal cardiac diseases, like coronary artery heart disease and

many more. It has been a subject of many investigations for decades. However, intimal growth due to fluid(blood)-structure(blood vessels) interaction is less studied. This lecture will focus on intimal growth in arteries, induced by hemodynamical shear stress. Growth is modeled using morphoelasticity theory, assuming endothelial cells release PDGF (platelet-derived growth factor) in a shear-dependent manner. Blood flow is highly idealized (it is unidirectional with a no-slip boundary condition at the endothelium; it remains constant as the vessel deforms; it is steady and non-turbulent). Each of the three layers of an artery has transversely helical collagen fibers associated with them. These transversely helical collagen fibers play an important role in determining the rate of growth of the intima. The fiber fields in the three arterial layers are simulated numerically using conformal maps. The optimal growth is found by minimizing a strain-energy function that consists of a neo-Hookean term, an exponential term that registers the anisotropy induced by the collagen fibers, a penalty term that penalizes large deformations, and an auxiliary term that ensures that the deformation in a stress-free configuration is zero. This model should be viewed as providing a framework for coupling more fully 3D hemodynamics simulations to disease progression.

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MS53

Personalized Pharmacological Treatment for Pulmonary Arterial Hypertension Based on Hemodynamic Response

Pulmonary arterial hypertension (PAH) is a disease associated with an elevated mean pulmonary arterial pressure. Sustained vasoconstriction is one of the hallmarks of PAH. Thus, the treatments of PAH include arterial vasodilators (such as PDE5 inhibitors) along with the inhalation of nitrous oxide (NO). To understand the mechanics and degree of effectiveness of these pharmacological treatments, it is necessary to quantitatively estimate the impact of various chemical pathways on the modulation of the active tone of vascular smooth muscle cells (VSMC). To do so, we aim to develop a biochemo-mechanical model that couples the NO-sGC-cGMP chemical pathway with a hemodynamics model.

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MS53

Tumor Grows to Lower Extracellular Matrix Conductivity Regions under Darcy's Law and Steady Morphology

We study a classic Darcys law model for tumor cell motion with inhomogeneous and isotropic conductivity. The tumor cells are assumed to be a constant density fluid flowing through porous extracellular matrix (ECM). The ECM is assumed to be rigid and motionless with constant porosity. One and two dimensional simulations show that the tumor mass grows from high to low conductivity regions when the tumor morphology is steady. In the one-dimensional case, we proved that when the tumor size is steady, the tumor grows towards lower conductivity regions. We conclude that this phenomenon is produced by the coupling of a special inward flow pattern in the steady tumor and Darcys law which gives faster flow speed in higher conductivity regions.

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MS54

Machine-Learning Approaches for Predicting Experimental Cardiac Voltage Time Series

Disruptions to the electrical behavior of the heart caused by cardiac arrhythmias can result in complex dynamics, including highly irregular or chaotic action potentials. Accurate forecasts of cardiac voltage behavior could allow new opportunities for intervention and control but would require efficient computational methods. In this talk we discuss our recent work using machine-learning approaches based in reservoir computing to forecast cardiac action potentials. We show that such methods can successfully and efficiently predict time series of synthetic and experimental datasets of cardiac voltage for multiple action potentials.

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MS54

Spiral Wave Teleportation as a Mechanism for Cardiac Defibrillation

We identify and demonstrate a universal mechanism for terminating spiral waves in excitable media using an established topological framework. This mechanism dictates whether high- or low-energy defibrillation shocks succeed or fail. Furthermore, this mechanism allows for the design of a single minimal stimulus capable of defibrillating, at any time, turbulent states driven by multiple spiral waves. We demonstrate this method in a variety of computational models of cardiac tissue ranging from simple to detailed human models. The theory described here shows how this mechanism underlies all successful defibrillation and can be used to further develop existing and future low-energy defibrillation strategies.

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MS54

Controllability of Voltage- and Calcium-Driven Cardiac Alternans in a Nonlinear Map Model

Ventricular fibrillation, a life-threatening cardiac arrhythmia, is sometimes preceded by electrical alternans, which is a beat-to-beat alternation in cellular action potential duration. Alternans may arise from instabilities in either voltage or intracellular calcium cycling. Although a number of techniques have been proposed to suppress alternans, most have focused on appropriately adding a new ionic current or adjusting the timing of pacing stimuli, rather than affecting intracellular calcium directly. In addition, most of the methods proposed to suppress alternans have been tested using models that do not include calcium-driven alternans. Therefore, it is important to establish a theoretical basis for understanding how control methods may perform when alternans is driven by instabilities in calcium cycling. In this study, we applied controllability analysis to a discrete map of alternans dynamics in a cardiac cell. In particular, we computed modal controllability measures to determine to what extent different control strategies can suppress alternans. The controllability measures indicated that perturbing action potential duration was the most effective strategy for suppressing both voltage- and calcium-driven alternans, although perturbing the sarcoplasmic reticulum calcium load was also a promising strategy for suppressing calcium-driven alternans. Our study provides insight into the feasibility of controlling alternans driven by different mechanisms.

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MS54

The Ability of Ephaptic Coupling to Produce Short Wavelength Patterns of Discordant Alternans

Computational models have struggled to explain the ability of cardiac tissue to, under some circumstances, exhibit small domains of in-phase alternations of action potential durations (APDs), known as discordant alternans, during rapid pacing. In our study, we demonstrate that, using an improved model of intercell coupling called "ephaptic" coupling, we can readily produce these short-wavelength domains while still maintaining normal wave propagation speeds. When wavefront propagation from one cell to the next occurs primarily through ephaptic coupling, conduction velocity can be normal, even if gap junction resistances are 100 times the value typically used in simulations. This higher gap junction resistance allows for much lower coupling on the trailing edges of propagating waves, which in turn makes variations in APD over short distances, and therefore short-wavelength discordant alternans, possible. We find that the gap junctions are still essential in this scenario, but play a supportive, rather than a primary, role. Our study suggests that ephaptic coupling may be more important than previously thought, both when discordant alternans is present, and possibly, during normal wave propagation as well.

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Nonnegative Solutions and Bilayers Governed by the Degenerate Functionalized Cahn-Hilliard Equation

The Functionalized CahnHilliard equation has been proposed as a model for the interfacial energy of phase-separated mixtures of amphiphilic molecules. We study the existence of a nonnegative weak solutions of a gradient flow of the Functionalized CahnHilliard equation subject to a degenerate mobility that is zero for u¡0. Assuming the initial data is positive, we construct a weak solution as the limit of solutions corresponding to non-degenerate mobilities and verify that it satisfies an energy dissipation inequality. Our approach is a combination of Galerkin approximation, energy estimates, and weak convergence methods. We will also discuss the corresponding geometric evolution of bilayers governed by the degenerate FCH equation.

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MS55

Hydrodynamics of Janus Particles Self-Assembled as Vesicles

Janus particles are widely used for self-assembly of mesoscopic structures with specific functions. We have constructed a model for self-assembly of Janus particles to form bilayer membranes under a hydrophobic potential (SIAM J. Multiscale Modeling, 2020). In the present work, we illustrate the hydrodynamics of a vesicle made of such bilayer membranes. We use boundary integral equations to examine the hydrodynamics under various conditions:

a quiescent flow, a planar shear flow, a linear elongation flow, and a Poiseuille flow. The simulation results show strong similarities to the vesicle hydrodynamics of a permeable lipid bilayer membrane and yield flowing conditions such as tank-treading motion, an asymmetric slipper, and membrane rupture. Moreover, the Janus-particle bilayers exhibit intermonolayer slip similar to that for two lipid monolayers and we calculate the friction coefficients.

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MS55

Compositional Evolution of Quasi-Bilayers in the Two-Component Functionalized Cahn-Hilliard Equation

Multicomponent mixtures in general support bilayers with a diversity of lipid compositions. We study a strong two-component FCH model with a ra- dial symmetric potential which admits a family of quasi-bilayers with various compositional ratios between amphiphile A and B. In the absence of pearling bifurcation, the compositional and geometric evolution of quasi-bilayers de- couples, in the sense that the former evolution takes place in the 1/e time scale when the normal velocity of the interface is still zero. More specifically, the composition ratio satisfies a nonlocal equation accommodating rich dynamics. Depending on the competition between the phase separation and the quenching of the background, the composition ratio evolves into, (1) a homogeneous profile; (2) a phase separation profile where the bilayer consists of pure A regions and pure B regions; or, (3) a quenched profile in a co-dim two manifold. In case (2) and (3), a rapid spatial variation of the composition ratio promotes surface diffusion terms from lower orders. While the evolution of phase separation profiles mimics Allen-Cahn type coarse graining, novel dynamics emerges from the evolution of rapid varying profiles in a neighborhood of the quenched manifold: the compositional pro- file stays nearby the quenching manifold and evolves into a periodic profile with a large period.

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MS55

Pathways Connecting Two Opposed Bilayers with a Fusion Pore: A Molecularly-Informed Phase Field Approach

A phase field model with two phase fields, representing the concentration and the headtail separation of amphiphilic molecules, respectively, has been constructed using an extension of the OhtaKawasaki model (Macromolecules, 1986, 19, 26212632). It is shown that this molecularly-informed phase field model is capable of producing various self-assembled amphiphilic aggregates, such as bilayers, vesicles and micelles. Furthermore, pathways connecting two opposed bilayers with a fusion pore are obtained by using a combination of the phase field model and the string method. Multiple fusion pathways, including a classical pathway and a leaky pathway, have been obtained depending on the initial separation of the two bilayers. The study shed light on the understanding of the membrane fusion pathways and, more importantly, laid a foundation for further investigation of more complex membrane morphologies and transitions.

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MS56

Optimal Control of the COVID-19 Pandemic: Age-Dependent Release Policies in Ecuador

Social distancing policies, such as extended school and workplace closures, have been widely used to control the spread of COVID-19. However, after an initial lockdown stage, societies are forced to find an equilibrium between the need to reduce contagion rates and reopen their economies. To estimate how the changes in population mixing have affected the diseases progression, we use an age-stratified SEIR model to reconstruct the dynamics of COVID-19 in Ecuador between February and August 2020 across four different periods defined by policy interventions. Then, we apply optimal control theory to maximize the number of people returning to normal activities and minimize the number of actively infected individuals with minimal economic costs. This work allows testing reopening scenarios after the lockdown and strict social distancing policies. Finally, we compare optimal reopening strategies with strategies that suggest releasing specific age groups to reduce risk and negatively impact the economy.

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MS56

Multistage Spatial Model for Informing Release of

Wolbachia-Infected Mosquitoes as Disease Control

Wolbachia is a natural bacterium that can infect Aedes mosquitoes and block the transmission of mosquito-borne diseases, including dengue fever, Zika, and chikungunya. Field trials have been conducted worldwide to suppress local epidemics. We present a new partial differential equation model for the spread of Wolbachia infection in mosquitoes. The model accounts for both the complex Wolbachia vertical transmission cycle and detailed life stages in the mosquitoes, and it also incorporates the spatial heterogeneity created by mosquito dispersion in the two-dimensional release domain. Field trials and previous modeling studies have shown that the fraction of infection among the mosquitoes must exceed a threshold level for the infection to persist. We identify a threshold condition for having a self-sustainable Wolbachia infection in the field. When above this threshold, we also show the model gives rise to a spatial wave of Wolbachia infection. We quantify how the threshold condition and invasion velocity depend on the diffusion coefficients and other model parameters, and we study different release scenarios to inform the efficient spatial design of the releases.

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MS56

The Impact of Structural Network Change on Infectious Disease Propagation

Throughout our daily lives, we establish connections with other individuals either by visiting a grocery store, attending a local social gathering, or meeting with family and friends. We can view these interactions as a persons general social network. Certain events such as a large-scale natural disaster can disrupt these networks by either reducing the number of connections or disconnecting certain connections. As observed in the recent pandemic, the localities that enacted strong health measures with regard to minimizing social interactions helped reduce the transmission of the disease. In this presentation, we will examine how changes in the network structure can impact the spread of an infectious disease.

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MS57

The Cancellation Effect at the Group Level

Group selection models combine selection pressure at the individual level with selection pressure at the group level. Cooperation can be costly for individuals, but beneficial for the group, and therefore, if individuals are sufficiently much assorted, and cooperators find themselves in groups with disproportionately many other cooperators, cooperation can evolve. The existing literature on group selection generally assumes that competition between groups takes place in a well-mixed population of groups, where any group competes with any other group equally intensely. Competition between groups however might very well occur locally; groups may compete more intensely with nearby than with far-away groups. We show that if competition between groups is indeed local, then the evolution of cooperation can be hindered significantly by the fact that groups with many cooperators will mostly compete against neighboring groups that are also highly cooperative, and therefore harder to outcompete. The existing empirical method for determining how conducive a group structured population is to the evolution of cooperation also implicitly assumes global between-group competition, and therefore gives (possibly very) biased estimates.

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MS57

Multi-Agent Reinforcement Learning Dynamics in Partially-Observable Stochastic Games

Collective learning and decision-making under various forms of uncertainty is important for animals, humans, and machines. The question ofan adequate theoretical foundation for multi-agent learning, however, remains open. I will present how to efficiently describe the emergent behavior of biologically plausible and parsimonious learning agents faced with partially-observable worlds through a dynamical systems approach, which is formally related to evolutionary game theory. The introduced learning dynamics illustrate that partially observant agents can learn better outcomes faster, in a more stable way, and even overcome social dilemmas. The method also allows the application of dynamical systems theory to partially observable multi-agent learning, as demonstrated by the emergence of catastrophic limit cycles, a critical slowing down of the learning processes, and the separation of the learning dynamics into fast and slow directions, all caused by partial observability. The presented approach has the potential to become a practical, lightweight, and robust tool for mathematical researchers working in the fields of biology, social sciences, and machine learning to create insights into collective learning in uncertain and changing environments.

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MS57

The Role of Loners in the Evolution of Cooperation in Group-Structured Populations

The evolution of cooperation has been studied in many systems, from bacterial communities to human populations. It is well known that population structure is crucial to a system's dynamics. In human populations, group memberships are fundamental. Humans meet and interact with each other based in large part upon their common group memberships. From a theoretical perspective, there exist network-based models to study human dynamics, but they generally do not allow for multiple group affiliations or incorporate barriers to group entry. In this work, we present a generalized framework, based on evolutionary set theory, in which individuals are distributed across groups. These individuals interact, through an evolutionary game, with those who share their groups. The system updates stochastically, with strategy and group memberships subject to evolutionary updating. We impose realistic group membership rules, including flexibility in the number of memberships and barriers to group entry. We find that with these rules, cooperation can emerge, but that it is most favored when we allow for the existence of "loners": a changing subset of individuals who spend a temporary "time-out" period not interacting with others. This work provides an analytical framework in which behavior in re-

alistic population structures can be studied, and adds to a growing body of literature that recognizes the existence of loners as vital parts of systems.

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MS57

Modeling the Public Health Impact of E-Cigarettes on Adolescents and Adults

Since the introduction of electronic cigarettes to the United States market in 2007, vaping prevalence has surged in both adult and adolescent populations. E-cigarettes are advertised as a safer alternative to traditional cigarettes and as a method of smoking cessation, but the U.S. government and health professionals are concerned that e-cigarettes attract young non-smokers. Here, we develop and analyze a dynamical systems model of competition between traditional and electronic cigarettes for users. With this model, we predict the change in smoking prevalence due to the introduction of vaping, and we determine the conditions under which e-cigarettes present a net public health benefit or harm to society.

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MS58

Synchronous Pulsed Flowering and Pattern Formation in Individual Flowers of Passiflora Incarnata

A careful observation of the number of flowers flowering in an individual plant of passion flower (*Passiflora incarnata*) revealed temporal oscillations with a period of approximately 30 days. A follow up study including four plants revealed synchronous pulsed flowering in the system. These oscillations do not seem to depend directly upon external factors like temperature, humidity, and sunlight. Therefore, it is concluded that they must be dependent on internal factors like flower inducing florigen and anti-florigen. A modified Lotka model is used to account for the observed oscillations in flowering in the system. A closer examination of individual flowers reveals interesting concentric circular patterns that are violet in color. Following the study of the onset of colors in individual fibrils, the pattern formation in these flowers is explained using an activator-inhibitor model of Gierer and Meinhardt that involves diffusion and autocatalytic and inhibitory steps. [S. Goyal, R. Reji, S. S. Tripathi and N. Sathyamurthy, Synchronous pulsed flowering in *Passiflora incarnata*, Current Science, 117, 1211 (2019); 1. A. P. Bhati, S. Goyal, R. Yadav and N. Sathyamurthy, Pattern formation in *Passiflora incarnata*: An activator-inhibitor model, J. Biosci. 46, 84 (2021)]

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MS58

Patterns of Intramolecular Anthocyanin Association

Red, blue, and purple colors in plants are typically due to plant pigments called anthocyanins. We augment previous models for spatial anthocyanin patterns to include intramolecular anthocyanin aggregation. We show that nonlinear effects due to aggregation combined with a spatially varying total concentration allow for a spatial pattern of colored and uncolored species.

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MS58

Mathematical Modelling of Anthocyanins: Rationalising Pigmentation in Flowers, Fruits, and Red Wines

Anthocyanins are polyphenolic compounds that make major contributions to red, purple and blue colours of flowers, fruit and young red wine. These pigments have potential industrial applications as alternatives to synthetic food colours and as pH-dependent indicators of product freshness and quality. The ability to accurately measure and predict anthocyanin behaviour across many scientific disciplines (e.g., plant physiology, pollination ecology, food and wine science) is therefore essential, but quantitative information for anthocyanin dynamics in biological and chemical systems is currently limited. We used predictive mathematical modelling and chemical analysis techniques to characterise complex reaction kinetics involving model anthocyanin, malvidin-3-glucoside (M3G). In particular, kinetic modelling was conducted to represent the process of intermolecular copigmentation, which contributes to anthocyanin colour stabilisation in plants and red wine. Fourier analysis techniques were also used to analyse empirical data for M3G, with the aim of enhancing data fidelity within laboratories and wineries. Overall, such predictive modelling may help optimise the use of raw materials (e.g., grape) within anthocyanin-containing systems while minimising the human and physical resources that are typically required for phenolic monitoring. Furthermore, the ability to mitigate undesirable colour loss could increase opportunities for commercial use of anthocyanin-based products.

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MS58

Development and Evolution of Self-Organizing Pigmentation Patterns in Monkeyflowers

The emergence of complex tissue patterns from seemingly uniform, undifferentiated cells during development is an essential feature of all multicellular organisms. One of the most prominent theoretical mechanisms often invoked to explain biological pattern formation is the reaction-diffusion (RD) model, which postulates that local activation of pattern differentiation factors combined with long-range inhibition of the activity of those factors can produce dynamic, self-organizing spatial patterns. Numerous empirical and simulation studies have suggested that the RD mechanism underlies a wide range of pattern formation processes. However, we still know very little about the actual genes encoding the hypothetical activation and inhibition factors in most empirical systems, even less about the biophysical properties of these factors where candidate genes have been identified, and virtually nothing about

how modulation of the properties of these activators and inhibitors affects pattern evolution in nature. Here I describe our work addressing these three fundamental questions by studying the development and evolution of anthocyanin pigment spots or stripes in monkeyflowers, with a suite of approaches including fluorescence imaging, genetic mapping, transgenic manipulation, and mathematical modeling.

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MS59

Efficient Calculation of Fully Resolved Electrostatics Around Large Biomolecules

We present a simple framework for calculating the electric potential by solving the nonlinear Poisson-Boltzmann equation and the free solvation energies of large biomolecules. We develop a novel solver capable of solving nonlinear elliptic equations, where the diffusion coefficient, the source term, the solution and its flux are discontinuous across the interface. We also develop a fast algorithm to construct the surfaces of large molecules. The interface is represented by the zero-level set of a signed distance function, empowering a natural and systematic approach to generate adaptive Cartesian grids, which drastically reduce the computational cost by focusing resources to regions near the surface of the molecules. The solver is implemented on a forest of Octree grids in parallel to enable fast computations over large molecules.

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MS59

Big, Small and Periodic: Increasing the Application-Space of Molecular Solvation Theory with Treecodes, Cutoffs and Ewald

3D-RISM is a powerful tool for calculating solvation properties of biological molecules at infinite dilution for use in molecular modeling, drug design, and molecular biology. However, 3D-RISM can be prohibitively slow for many applications while others are densely-packed environments with periodic boundary conditions. To address this, we have implemented a number of numerical methods - treecode summation, cut-offs and periodic boundaries - in the AmberTools molecular modeling suite. Using treecode summation, we improve the scaling of 3D-RISM scaling from $O(N_{\text{atom}}^2)$ to $O(N_{\text{atom}} \ln N_{\text{atom}})$, enabling calculations on a microtubule with over 1.2 million atoms. We also implemented analytically corrected cut-offs for the short-ranged Lennard-Jones potential, reducing the execution time on small, drug-like molecules by a factor of 10. To account for periodic boundaries, we used particle-mesh Ewald summation, allowing 3D-RISM to be used to improve X-ray crystal structure refinement. Together, these numerical methods expand the range of problems that 3D-RISM can be applied to.

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MS59

Data-Driven Coarse-Grained Modeling of Non-Equilibrium Systems

Modeling a high-dimensional Hamiltonian system in reduced dimensions with respect to coarse-grained (CG) variables can greatly reduce computational cost and enable efficient bottom-up prediction of main features of the system for many applications. However, it usually experiences significantly altered dynamics due to loss of degrees of freedom upon coarse-graining. To establish CG models that can faithfully preserve dynamics, previous efforts mainly focus on equilibrium systems. In contrast, various biological systems are known out of equilibrium. Therefore, this work concerns non-equilibrium systems and enables accurate and efficient CG modeling that preserves non-equilibrium dynamics and is generally applicable to any non-equilibrium process and any observable of interest. To this end, the dynamic equation of a CG variable is built in the form of the non-stationary generalized Langevin equation (nsGLE), where the two-time memory kernel is determined from the data of the auto-correlation function of the observable of interest. By embedding the nsGLE in an extended dynamics framework, the nsGLE can be solved efficiently to predict the non-equilibrium dynamics of the CG variable.

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MS59

Advances in Modeling Molecular Interactions

Accurate modeling of molecular interactions is essential for computational studies of biomolecular structure, dynamics, and interactions. To enable chemical accuracy in molecular simulations, we are developing the next-generation classical mechanics potential, AMOEBA+, and related high-performance computing platform. Traditionally classical force fields heavily rely on error cancellations and the separation between electrostatics and other interactions can be arbitrary. By contrast, the AMOEBA+ potential aims to provide not only accurate total interaction energy but also meaningful components of intermolecular forces. The AMOEBA+ potential is established based on systematic investigation of fundamental interatomic forces and ab initio energy decomposition through Symmetry Adapted Perturbation Theory (SAPT), as well as a wide range of experimental data. The intermolecular potential energy function includes permanent atomic multipole-based electrostatics, many-body polarization, repulsion, dispersion, charge penetration and transfer contributions. The local valence com-

ponents are modeled by polynomials or neural networks. All energy and force terms are implemented in the Tinker9 GPU molecular dynamics package. The improvements in AMOEBA+ are crucial for advancing the accuracy and transferability of classical potentials in modeling molecular interactions, realizing the full potential of molecular modeling and design in silico.

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MS60

Mechanisms Underlying Internal vs. External Fibrinolysis

Fibrinolysis, the enzymatic degradation of the fibrin mesh that stabilizes blood clots, is critical for preventing natural clots from becoming problematic. When "internal' lysis initiated naturally by the body's lytic enzymes is not working properly, dangerous blood clots can form and require "external' lysis initiated clinically by large doses of lytic enzyme. Clots can be contracted (with compressed volumes, denser fibrin networks, and a higher percentage of total fibrin on the exterior of the clot) or uncontracted (with bigger volumes, looser fibrin networks, and a more homogeneous distribution of clot components). Experimental data show that clot structure has a differential influence on internal vs. external lysis – for example, contracted clots are more resistant than uncontracted clots to external lysis but are faster to degrade via internal lysis – but the mechanisms responsible for these differences are unknown. We build a 3-dimensional, multiscale, stochastic model to investigate the mechanisms underlying internal and external lysis. The model includes detailed structural and biochemical features of clots and is used in conjunction with laboratory experimentation to identify conditions under which internal and external lysis are most effective. Results of this work have implications for improved clinical outcomes, as therapeutic strategies can be targeted to take advantage of (or avoid) mechanisms identified by the model.

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MS60

Multiphase Continuum Modeling of Blood Clot Formation in Aneurysms and Patient-Specific Left Atrial Appendages

Due to their shape, some aneurysms and left atrial appendages (LAA) represent a favorable environment for stagnant flow circulation and potential blood clotting. The factors contributing to clot formation in these areas remain poorly understood due to the complexity of the coagulation system and the lack of appropriate experimental models. To address this question, we develop a novel multiphase continuum framework that describes the interplay between platelet aggregation, blood biorheology, and plasma coagulation. After validating the model against known benchmarks, we conduct numerical simulations to elucidate the effects of morphology, flow intensity and red blood cells on the structure and size of the formed thrombi in aneurysms. We show that high-hematocrit, low neck size, and slower flow intensity are all important factors contributing to the pathogenesis of thrombi in aneurysms. After that, we adapt the same model to study clot formation in patient-specific geometries of the left atrial appendage during atrial fibrillation. We discuss how numerical simulations can be used to estimate the risk of clot formation in patients with atrial fibrillation.

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MS60

Computational Models of Platelet Deposition in Arterial Thrombosis

The formation of wall-adherent platelet aggregates is a critical process in arterial thrombosis. A growing aggregate experiences frictional drag forces exerted on it by fluid moving over or through the aggregate. The magnitudes of these forces are strongly influenced by the permeability of the developing aggregate; the permeability depends on the aggregates porosity. Aggregation is mediated by formation of ensembles of molecular bonds; each bond involves a plasma protein bridging the gap between specific receptors on the surfaces of two different platelets. The ability of the bonds existing at any time to sustain the drag forces on the aggregate determines whether it remains intact or sheds individual platelets or larger fragments (emboli). Our computational model tracks the formation and breaking of bonds between platelets and treats the thrombus as an evolving porous, viscoelastic material, which moves differently from the background fluid. This relative motion generates drag forces which the fluid and thrombus exert on one another. These forces are computed from a permeability-porosity relation parameterized from our groups experimental measurements. Basing this relation on measurements from occlusive thrombi formed in our flow chamber experiments, along with other physiological parameter values, the model produces stable dense thrombi on a similar timescale to the experiments.

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MS60

Towards a Mathematical Model of Platelet Aggregation and Fibrin Polymerization

The formation of a blood clot involves complex biophysical and biochemical processes that occur under flow. In the event of an injury, platelets become active and weakly aggregate to form a plug at the injury site. Activated platelets express binding sites for procoagulant species, and platelet surface-bound complexes convert zymogen prothrombin into enzyme thrombin; thrombin further activates platelets and converts soluble fibrinogen molecules in the blood plasma to fibrin monomers. These monomers then polymerize to form a gel that is a major structural component of a blood clot. Fibrin(ogen) interacts with activated platelets through surface integrins that allow platelets to adhere and cohere through bonds mediated by fibrin(ogen). Experimental evidence suggests platelet integrins interact differently with fibrinogen, fibrin, and fibrin oligomer. We propose a mean field mathematical model of fibrin branch formation which tracks fibrinogen, fibrin, and platelet species in either a bound or unbound state. Fibrin oligomers form in both the bulk and on the surface of platelets, and flow-mediated transport will affect fluid-phase species. A kinetic fibrin polymerization model is used to model fibrin gel formation; this model is studied up until gelation, which is defined as the emergence of an oligomer of infinite size. In this presentation, we show how the gel time depends on model parameters and how platelet-fibrin(ogen) interactions affect the gel structure.

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MS62

A Systems Pharmacology Model of Gene Therapy for Sickle Cell Disease

We developed a mathematical model for autologous stem cell gene therapies to cure sickle cell disease by transplanting stem cells containing a curative gene. Successful transplantation is expected to produce a lifelong supply of red blood cells (RBCs) containing an anti-sickling hemoglobin. There is limited patient data available from early clinical trials for this complex multi-step therapy. We set out to quantify the impact of key treatment parameters, such as initial stem cell dose, efficiency of lentiviral transduction, and degree of bone marrow preconditioning on engraftment efficiency, peripheral RBC numbers, and anti-sickling hemoglobin levels. Using ODEs we modeled erythropoiesis in the bone marrow, and hemoglobin assembly within RBC. Model simulations match observed RBC and hemoglobin levels in healthy and SCD phenotypes. Treatment simulations predict stem cell engraftment and RBC dynamics. Post-treatment dynamics show an early phase of reconstitution due to short lived stem cells, followed by a sustained RBC production from stable engraftment of long-term stem cells as previously reported. Using local sensitivity analysis, the initial dose of transduced stem cells and the intensity of bone marrow preconditioning are predicted to most positively impact long-term outcomes. The quantitative systems pharmacology approach used here demonstrates the value of model-assisted therapeutic design for gene therapies.

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MS62

Integration of a Machine Learning Method with a Hemoglobin (Hb) Solubility Model for Inferring Hb Polymer Mass and Fetal Hb Distribution in Sickle Red Blood Cells

Sickle cell disease (SCD) is an inherited hematologic disorder and is an important cause of childhood mortality in many countries, mainly in sub-Saharan Africa. SCD is caused by a single mutation from A to T in the β-globin gene of adult hemoglobin (HbA). This mutant hemoglobin (hemoglobin S [HbS]) polymerizes upon deoxygenation in the tissues and causes red blood cell (RBC) deformation. Increased levels of fetal hemoglobin (HbF) and or HbA can inhibit polymer formation in RBCs. Here, we assessed single-RBC images and their oxygen saturation using a previously reported microfluidic system (DOI:10.1073/pnas.1914056116). We developed a machine learning method that detects Hb polymer in single RBCs based on the cell morphology and the oxygen saturation measurements. This method uses the principle that Hb polymer decreases RBC oxygen saturation in proportion to polymer concentration. We estimated single-RBC Hb polymer mass by integrating single-RBC oxygen saturation measurements with a hemoglobin solubility model (DOI:10.1073/pnas.1922004117) that describes cooperative oxygen binding to Hb. Then we used the polymer mass estimates for different oxygen tensions to infer the distribution of HbF across RBCs for patients treated with hydroxyurea and patients who underwent a gene therapy that enhances HbF production (DOI:10.1056/NEJMoa2029392). We also estimated the distribution of HbA between RBCs for patients with sickle cell trait.

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MS62

Mathematical Model of Hemoglobin Oxygen Saturation to Determine Optimal Oxygenated Hemoglobin Stabilization to Minimize Sickling While Maintaining Adequate Oxygen Carrying Ca-

pacity

In sickle cell disease (SCD), red blood cell sickling is driven by concentration dependent polymerization of deoxygenated hemoglobin (deoxHb). Multiple drugs in development aim to reduce sickling by stabilizing oxygenated hemoglobin (HbO2), thereby decreasing the concentration of deoxHb to prevent polymerization. However, by stabilizing HbO2 these compounds also reduce the blood oxygen carrying capacity. A mathematical model accounting for the complex interrelated factors affecting hemoglobin oxygen saturation is required to determine the optimal level of HbO2 stabilization that minimizes RBC sickling while maintaining adequate oxygen carrying capacity. We revised and extended the model of Dash et al. 2016 so that the effect of 2,3-BPG on oxygen saturation is a function of the ratio of 2,3-BPG to available Hb and therefor reflective of the 2,3-BPG-Hb binding equilibrium. Additionally, we added equations to include expression of fetal hemoglobin (HbF). The extended model enables exploration of polymerization sensitivity to individual variability in total Hb expression, percent HbF expression, and 2,3-BPG levels in the presence or absence of HbO2 stabilizers. The model predicts oxygen carrying capacity becomes critically low when there is both low 2,3-BPG and high HbO2 stabilization. In the future, our model can be used to select responsive patient populations for new treatments and to explore additive and synergistic effects of combination therapies.

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MS62

Shedding Light to Sickle Cell Disease Using Quantitative Approaches

This talk will provide an introduction to the biology of sickle cell disease and its downstream sequelae. Sickle cell disease is a rare genetic disorder caused by mutations in the beta-globin chain which result in hemoglobin polymerization upon deoxygenation and subsequent red blood cell sickling. Sickling events trigger a cascade of downstream effects including hemolysis, inflammation, and obstructions of small blood vessels leading to ischemia, pain crisis, organ damage, and reduced life expectancy for sickle cell patients. In this minisymposium, we highlight a broad range of mathematical approaches that have been used to further understanding of different aspects of disease pathophysiology and to develop new treatment options for patients. Multi-scale models have been utilized to understand the regulation of red blood cell production, blood flow mechanics and rheology, and formation of vaso-occlusions. Statistical analysis and machine learning have also been employed to investigate frequency of pain-crises and mechanisms promoting disease progression in sickle cell patients.

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MS63

The Gibbs-Donnan Effect and Cell Volume Stabilization in Unexcitable Cells

The presence of impermeant molecules within a cell establishes a Donnan effect that, if left unchecked, will increase the cell volume due to the osmotic flux of water until it lyses. The Donnan effect can be counteracted by actively pumping Na+ out of the cell. This effectively stabilizes the cell by equalizing the osmolarity across the membrane but demands the continuous expenditure of energy to preserve this dynamic steady-state. In this talk, we introduce a system of five algebraic and differential equations, the so-called pump-leak model, that describes a cell's ion and water fluxes and membrane potential. First, we show that the model admits a stable steady state in the presence of a sodium pump, which constantly pumps Na+ out- and Cl- inside the cell. Then, using the model, we show that extracellular impermeant molecules can stabilize a cell in the absence of sodium pumps. We show how a cell may use both mechanisms to control its volume with less energy. Besides sodium pumps and extracellular impermeant molecules, we incorporate into our model a family of the Solute Carrier transporter superfamily called Cation-Coupled Cotransporters (CCCs), which transport Na+ and/or K+ and Cl across the cell membrane. We will show how CCCs can assist cells in regulating ion levels and cell volume. **This is joint work with Alan Kay from the Department of Biology at the University of Iowa. **

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MS63

Pattern Formation in a Synthetic Quorum-Sensing Toggle Switch

Differentiation within multicellular organisms is a complex process that helps to establish spatial patterning and tissue formation. Often, the differentiation of cells is governed by morphogens and intercellular signaling molecules that help to guide the fate of each cell. Here, we couple a synthetic co-repressive toggle switch to intercellular signaling pathways to create a quorum-sensing toggle. Our experimental results suggest that this circuit alters the emergent patterns of differentiation in colonies grown on agar containing an externally supplied morphogen. To understand the observed patterns, we developed a coupled 3D PDE-ODE system that takes into account colony expansion. Our bifurcation analysis and simulation results suggest that degradation, diffusion, and sequestration of the signaling molecules are critical to the observed patterns.

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MS63

Flow Sensing in Cancer from the Molecular to the Multicellular Scale

Cell sensing is fundamentally multi-scale, as information is propagated from molecules to cells to cell groups. I will describe a fascinating sensory mechanism in cancer metastasis where cells use self-guided chemotaxis to follow fluid flows in the body. We derive the limit that diffusive molecular noise places on the precision of this process. Comparing to experiments, we find that cells operate remarkably close to this limit. We then move up in scale to crowded cell populations. We predict a cell density at which this sensory mechanism fails, which agrees with that observed in experiments. Our work elucidates the fundamental limits of sensory biology from the nanometer to millimeter scale.

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MS63

Floral Patterns in Multi-Strain Bacterial Colonies

Diverse interactions among species within bacterial biofilms often lead to intricate spatiotemporal dynamics. The spatial structure of biofilms can determine the growth and survival of different species, but the mechanisms driving formation of these structures are not fully understood. Here, we describe the emergence of complex structures in a biofilm grown from a mixture of motile and non-motile strains of bacteria on a semi-solid agar surface. Time-lapse imaging shows that non-motile bacteria hitchhike with the motile bacteria as the latter grow and expand. The non-motile bacteria accumulate at the moving colony boundary and trigger a mechanical instability of the colony boundary that leaves behind striking flower-like patterns. The mechanism of the front instability governing this pattern formation can be elucidated by a mathematical model describing frictional interface motion with friction that depends on the local concentration of the non-motile strain at the interface. We also developed a detailed two-dimensional phase-field model that explicitly accounts for the cell growth and migration driven by self-generated mechanical stresses. Our findings highlight the importance of mechanical interactions in shaping the spatial structure of multi-strain biofilms.

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MS64

Rotor Localization and Phase Mapping of Cardiac Excitation Waves Using Deep Neural Networks

The analysis of electrical impulse phenomena in cardiac muscle tissue is important for the diagnosis of heart rhythm disorders and other cardiac pathophysiology. Cardiac mapping techniques acquire time-series and combine them to visualize the spread of nonlinear waves of electrical excitation in the heart. However, low spatial resolution, sparse measurement locations, noise, and other artifacts make it challenging to accurately visualize spatio-temporal activity. Here, we demonstrate that deep learning can be used to compute phase maps and detect phase singularities in optical mapping videos of ventricular fibrillation, as well as in very noisy, low-resolution, and extremely sparse simulated data of reentrant wave chaos mimicking catheter mapping data. Rather than encoding a phase signal from time-series data, a convolutional neural network (CNN) instead learns to directly associate phase maps and phase singularities with short spatio-temporal sequences of electrical data. Predictions can be performed across different data, with models being trained on one species and then successfully applied to another, or being trained on simulated data and then applied to experimental data. Neural networks are a promising alternative to conventional phase mapping and rotor core localization methods. Future uses may include the analysis of optical mapping studies in basic cardiovascular research, as well as the mapping of atrial fibrillation in the clinical setting.

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MS64

A Phase Defect Framework for the Analysis of Cardiac Arrhythmia Patterns

During heart rhythm disorders, complex spatiotemporal patterns of electrical excitation emerge in the heart muscle. Among these patterns are self-sustaining rotating waves called rotors, spiral waves or scroll waves. In the classical description, rotors are turning around a phase singularity point that extends into a filament curve in 3 spatial dimensions. Recent results defy this viewpoint and suggest that

rotor cores that form around a conduction block line are in fact extended phase discontinuities or phase defects, similar to a branch cut in complex analysis. Here we present a new topological framework in 2 and 3 spatial dimensions that unifies the concepts of conduction block, rotor cores, phase defects and filaments. We show how different building blocks of co-dimension 0, 1 and 2 are topologically related and shed new light on the processes of rotor creation and annihilation. Our framework is applied to analyse in silico and real-life experiments.

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MS64

Dynamics Study of Constant DI and Constant TR Control for Cardiac Alternans Based on a Two-Dimensional Cellular Automata Model

A computer model based on cellular automata principles has been developed to simulate 1-D and 2-D dynamics of cardiac electric waves. Local and global control strategies have been explored to suppress cardiac alternans in the model. Various stability and control issues are discussed.

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MS64

Novel Approaches and Similarity Score for the Identification of Active Sites during Patient-Specific Catheter Ablation of Atrial Fibrillation

Atrial fibrillation (AF) is the most common cardiac arrhythmia and precursor to cardiac diseases. Catheter ablation is associated with limited success rates in patients with persistent AF, and existing mapping systems fail to identify target sites for ablation. We evaluated the performance of multiscale frequency (MSF), kurtosis (Kt), and multiscale entropy (MSE) techniques to identify the AF drivers using unipolar and bipolar electrograms (EGMs) obtained from numerical simulations under different clinical scenarios: in the presence of noise, scar, and various catheters. We also developed a similarity score to identify the spatial location of active sites of arrhythmia in patients with AF. Our numerical simulation results demonstrate that MSF, MSE and Kt were able to accurately identify AF drivers from EGMs for the case of Multielectrode Multispline and Grid catheters. The presence of noise and scar tissue did not significantly affect the performance of the techniques. In patients, similarity score was proposed and validated to identify spatial active AF sites that were observed only in patients with unsuccessful AF termination, suggesting that these active sites were missed during the ablation procedure. In summary, AF drivers can be successfully identified in numerical simulations from EGMs under various clinical scenarios using MSF, MSE and Kt techniques, and in patients with unsuccessful AF termination after catheter ablation using similarity score.

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MS65

Chasing a Ghost: The Role of Ca2+ Mobilization on Burst Oscillation in Pyramidal Cells

Pyramidal cells (PCs) in the brain are known to encode incoming sensory information to give rise to perception and behavior. Understanding how this works is complicated by the fact that neural activities are governed by both the combined activities of interacting neuronal populations and by individual neurons that show different firing patterns (including tonic spiking and bursting) in response to incoming signals. We have recently expanded a previously developed HH model of PC neurons to include not only the intrinsic electrical properties of the cell, but also Ca2+ mobilization across the cell and ER membrane (i.e., the various calcium fluxes through channels and pumps), the small conductance calcium-activated potassium (SK) channels as well as the overall synaptic inputs (i.e., mean activity of EPSPs and IPSPs). Our goal was to explore how these four factors affect bursting in PCs. The model was parametrized using in vivo recordings of PCs in the ELL, including interspike interval distribution. Using bifurcation theory and slow-fast analysis, we explained how the firing activity of PCs switch between different states (including quiescence, bursting and tonic spiking) when modifying the calcium dynamics and what the underlying mechanism of burst oscillation is. Our results align with experimental findings that show neuromodulatory serotonergic input can strongly enhance burst firing by downregulating SK channels. In this talk, I will provide a summary of these findings.

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MS65

Classification of Bursting Patterns: A Tale of Two Ducks

In this talk, I will first briefly review existing classifications of bursting patterns. Then I will generalise a recent example that falls outside of these classification systems and present an extended classification, which requires the analysis of both fast and slow subsystems of an underlying slow-fast model and allows the dissection of a larger class of bursters. This new class of bursters with at least two slow variables will be denoted *folded-node bursters*, to convey the idea that the bursts are initiated or annihilated via a *folded-node singularity*. Key to this mechanism are so-called *canard* or *duck* orbits, organizing the underpinning excitability structure. I will describe the two main families of folded-node bursters, depending upon the phase (active/spiking or silent/non-spiking) of the bursting cycle during which folded-node dynamics occurs. I will classify both families and give examples of minimal systems displaying these novel bursting patterns. Finally, I will provide a biophysical example by reinterpreting a generic conductance-based episodic burster as a folded-node burster, showing that the associated framework can explain its subthreshold oscillations over a larger parameter region than the fast-subsystem approach.

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MS65

Understanding the Neuronal Response to Current Ramps Using Fast-Slow Analysis

The standard protocol for studying neuron spiking is to monitor voltage response to the application of current steps. However, a jump in applied current is artificial. A more physiological input is to ramp the applied current to reflect chemosensory input. Unsurprisingly, neurons can respond differently to the protocols since ion channel activation and inactivation are affected differently. The mathematical techniques necessary to analyze and understand the effects of current ramps are under-developed. We demonstrate how current ramps can be analyzed in single neuron models. The primary issue is the presence of gating variables that activate on slow time scales and are far from equilibrium throughout the ramp. The use of fast-slow analysis allows us to understand the neural response to ramps of different slopes. This study is motivated by data from olfactory bulb dopamine neurons, where both fast ramp (tens of milliseconds) and slow ramp (tens of seconds) protocols are used to understand the spiking profiles of the cells. The slow ramps generate experimental bifurcation diagrams with the applied current as a bifurcation parameter, thus establishing asymptotic spiking activity patterns. The faster ramps elicit transient behavior that is of relevance to most physiological inputs, which are short in duration. The two protocols together provide a broader understanding of the neurons spiking profile and the role that slowly activating ion channels can play.

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MS65

Multiple Time Scales in the Control of Progression Through the Eukaryotic Cell Cycle

The sequence of events by which a eukaryotic cell proceeds through repeated cycles of DNA replication and cell division is controlled by periodic activation and inactivation of a family of cyclin-dependent protein kinases (CDKs) and auxiliary proteins that regulate CDK activities. The molecular regulatory network is dauntingly complex, confounding efforts to understand its intricate behaviors by intuitive, biochemical reasoning alone. In principle, mathematical simulations of the biochemical reaction network could reliably predict its behavior, but only if we knew beforehand the values of the kinetic rate constants of the underlying reactionswhich, of course, we do not. To make sense of this confusion, we have studied the cell-cycle control system by traditional methods of dynamical systems theory, including time-scale separation, bifurcation theory and pseudo phase-plane analysis. JJT will show how these methods continue to deliver significant mechanistic insights on current problems of cell physiology.

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MS66

Impact of Within Host Heterogeneity on Malaria Transmission

Malaria is a disease endemic in areas encompassing over half the worlds population. It remains detrimental to the health and livelihood of millions of individuals causing over 200 million cases a year and nearly half a million deaths. *Plasmodium* parasites, the causative agents of malaria, have a complex life cycle requiring two hosts a vertebrate, such as a human, and the *Anopheles* mosquito. During the time in each of these hosts, the population dynamics of the parasite are quite variable in density and stage. In earlier work, we showed how density of parasite stages alters the timing and probability of disease spread at both interfaces of transmission: human to mosquito and mosquito to human. Here, we bridge previous stochastic

within-host modeling of parasite dynamics and diversity in the human and the mosquito to investigate consequences for transmission. We use a multi-scale model that tracks parasite dynamics and diversity, represented as genetically different variants, through the cycle of malaria infection. We track the density and persistence of these genetically diverse parasites. The extent of parasite diversity has important implications not only for disease severity but also for spread of the disease within the human and mosquito populations.

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MS66

Mathematics of Malariology: a Genetic-Epidemiology Framework

Malaria, a deadly disease caused by protozoan Plasmodium parasites, is spread between humans via the bite of infected adult female Anopheles mosquitoes. Over 2.5 billion people live in geographies whose local epidemiology permits transmission of P. falciparum, responsible for most of the life-threatening form of malaria. The widescale and heavy use of insecticide-based interventions, notably long-lasting insecticidal nets and indoor residual spraying), during the period 2000-2015, resulted in a dramatic reduction in malaria incidence and burden in endemic areas, prompting a renewed effort to eradicate the parasitic disease. Numerous factors, such as Anopheles resistance to all currently-available insecticides, potentially pose important challenges to the eradication efforts. In this talk, I will discuss a genetic-epidemiology framework for assessing the impact of insecticide resistance on malaria. Specifically, questions on whether eradication can be achieved using existing insecticide-based control resources will be addressed.

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MS66

A Mathematical Model for Onchocerciasis and Resistance in Treatment

Neglected tropical diseases are diseases that affect mainly developing countries and in turn are poorly funded and under researched. Onchocerciasis is a neglected tropical disease that exists primarily in Sub-Saharan Africa and South America. This is because the black flies that spread this disease are common to these regions and since these flies bite humans they can infect humans at a noticeable rate. When the black fly bites you it can pass a filarial nematode parasite, called Onchocerca volvulus, which is transmitted solely by black flies during blood feeding. Some people do not experience symptoms while infected with Onchocerciasis as the larvae can migrate through the human body without provoking a response from the immune system. But many people do have symptoms, which include itchy skin rashes, nodules under the skin, and vision changes Onchocerciasis is currently being treated with ivermectin through mass drug administration. The goal of this project is to find out the optimal way to distribute the treatment to eradicate the disease and to find if the current approach will eventually lead to drug resistance. Our focus was to model this situation and data fit our model to the country of Cameroon. Our research showed that the current treatment plan of Onchocerciasis may never completely eradicate the disease from the population due to resistance. We also found evidence that there may already be resistance in the population.

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MS66

TGF-Beta Inhibition Can Overcome Cancer Primary Resistance to PD-1 Blockade: a Mathematical Model

Immune checkpoint inhibitors have demonstrated, over the recent years, impressive clinical response in cancer patients, but some patients do not respond at all to checkpoint blockade, exhibiting primary resistance. Primary resistance to PD-1 blockade is reported to occur under conditions of immunosuppressive tumor environment, a condition caused by myeloid derived suppressor cells (MDSCs), and by T cells exclusion, due to increased level of T regulatory cells (Tregs). The present paper introduces two cancer-specific parameters and, correspondingly, develops a mathematical model which explains how primary resistance to PD-1 blockade occurs, in terms of the two cancer-specific parameters, and how, in combination with anti-TGF-β, anti-PD-1 provides significant benefits; these parameters may serve as predictive biomarkers. The model is represented by a system of partial differential equations and the simulations are in agreement with the recent mice experiments. The mathematical model also predicts that hyperprogression diseases may be reversed by combining anti-TGF-β to anti-PD-1. The model can be used to evaluate the efficacy of different protocols in combination therapy with PD-1 and TGF-β inhibitors. In particular, it is demonstrated that combined therapy may either decrease or increase tumor growth depending on the two cancer-specific parameters and the amount of, and the ratio between, the two drugs.

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MS67

Using Evolutionary Game Theory to Understand Multispecies Ecological Communities

Ecological communities are fundamentally governed by the interactions by individual organisms. These interactions are partially governed by the traits of the organisms, traits which are created and shaped by evolution. As such, integrating evolutionary processes such as natural selection with ecological processes may help us understand ecological communities. One useful framework that seamlessly integrates ecology and evolution is evolutionary game theory. In evolutionary game theory, individual organisms use their adaptations as strategies to achieve ecological ob-

jectives and receive a fitness payoff. Beyond interactions between individual organisms, evolutionary game theory can be used to model eco-evolutionary dynamics in and of multispecies ecological communities. In this presentation, I will demonstrate how using evolutionary game theory can help us to understand properties of multispecies communities. Using evolutionary game theory, we can generate in silico communities and compare their structure and properties to real ecological communities like niche packing, coexistence, nestedness, rank abundance, and average interaction strength. We can also explore how these measures change with shifting environmental conditions by analyzing the resulting evolutionary pressures. I present work that I have done and am currently doing on this topic and speculate on evolutionary game theorys utility in understanding ecological communities.

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MS67

Invasion of Cooperative Parasites in Moderately Structured Host Populations

Certain defense mechanisms of phages against the immune system of their bacterial host rely on cooperation of phages. Motivated by this example we analyse invasion probabilities of cooperative parasites in host populations that are moderately structured. More precisely we assume that hosts are arranged on the vertices of a configuration model and that offspring of parasites move to nearest neighbours sites to infect new hosts. We consider parasites that generate many offspring at reproduction, but do this (usually) only when infecting a host simultaneously. In this regime we identify and analyse the spatial scale of the population structure at which invasion of parasites turns from being an unlikely to an highly probable event.

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MS67

Fixation Probability in Network-Structured Metapopulations

The effect of population structure on evolutionary dynamics is a long-lasting research topic in evolutionary ecology and population genetics. Evolutionary graph theory is a popular approach to this problem, where individuals are located on the nodes of a network and can replace each other via links. We study the effect of complex network structure on the fixation probability, but instead of networks of individuals, we model a network of sub-populations with a probability of migration between them. We ask how the structure of such a meta-population and the rate of migration affect the fixation probability. Many of the known results for networks of individuals carry over to meta-populations, in particular for regular networks or low symmetric migration probabilities. However, when patch sizes differ we find interesting deviations between structured meta-populations and networks of individuals. For example, a two-patch structure with unequal population size suppresses selection for low migration probabilities.

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MS68

Life in a Tight Spot: How Bacteria Use Chemotaxis to Migrate Through Crowded Spaces

Bacterial motility and growth play central roles in agriculture, the environment, and medicine. While bacterial behavior is typically studied in bulk liquid or on flat surfaces, many bacterial habitats–e.g., soils, sediments, and biological gels/tissues–are complex and crowded spaces. In this talk, I will describe my group's work using tools from soft matter and applied mathematics to address this gap in knowledge. In particular, using studies of E. coli, we demonstrate how confinement in a crowded medium fundamentally alters bacterial behavior. In particular, we show how the paradigm of run-and-tumble motility is dramatically altered by pore-scale confinement, both for cells performing undirected motion and those performing chemotaxis, directed motion in response to a chemical stimulus. Furthermore, we show how spatial variations in the ability of cells to perform chemotaxis enable populations to autonomously stabilize large-scale perturbations in their overall morphology. Taken together, our work thus helps to reveal new principles to predict and control the organization of bacteria, and active matter in general, in complex and crowded environments.

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MS68

Long-Time Behavior of a Chemotaxis Model with Logarithmic Sensitivity and Logistic Growth

In this talk, we discuss the global existence and uniqueness and long-time behavior for solutions to a repulsive chemotaxis model with logarithmic sensitivity and logistic growth. In particular, we establish global existence and uniqueness of solutions to the corresponding initial value problem with Neumann boundary conditions, as well as demonstrate asymptotic convergence to constant states of the corresponding population and chemical concentration densities. Time permitting, we additionally discuss results concerning the vanishing chemical diffusivity limit.

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MS68

Understanding Collective Behavior of Bacterial Chemotaxis

Bacterial swimming mediated by flagellar rotation is one of the most ubiquitous forms of cellular locomotion, and it

plays a major role in many biological processes. A typical swimming path of flagellated bacteria looks like a random walk with no purpose, but the random movement becomes modified as environmental conditions change. Modified random movement is particularly characterized by their motility pattern or a combination of their swimming modes. Further, such individual swimming patterns characterize the collective behavior of a population of the bacteria. In this talk, we present several distinct motility patterns exhibited by bacterial species. We also discuss how to analyze the collective behavior of bacteria from the individual swimming pattern, particularly, by using an example of E. colis swimming behavior in response to chemical signals.

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MS68

A Brief Review of Density-Suppressed Motility Models

In this talk, I will discuss several mathematical models with density-suppressed motility describing different biological processes, like chemotaxis, bacterial pattern formation, predator-prey models, and introduce some theoretical and numerical results obtained for them.

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MS69

Multiscale Modeling of Microtubule Binding Domain to Microtubule

Multiscale modeling of microtubule binding domain to microtubule Emil Alexov Department of Physics, Clemson University, Clemson, SC 29634 Electrostatic interactions dominate other interactions in molecular biology because practically all atoms carry partial charge while being situated at Angstroms distances, thus resulting in large electrostatic force and energies. Furthermore, the electrostatic force is a long-range force and thus is very important not to be truncated since many biological phenomena involve binding of proteins to a large object. Because the electrostatic forces that guide binding act over large distances, one should consider the contribution of atoms situated at large distances. Here we report a multiscale approach that implements a computational focusing method that permits computation of large systems without truncating the electrostatic potential and achieves the high resolution required for modeling macromolecular interactions, all while keeping the computational time reasonable. We tested our approach on the motility of various kinesin motor domains. We found that electrostatics help guide kinesins as they walk: N-kinesins towards the plus-end, and C-kinesins towards the minus-end of microtubules. Our methodology enables computation in similar, large systems including protein binding to DNA, viruses, and membranes.

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MS69

Higher Order Implicit Boundary Integral Methods for Solving the Poisson-Boltzmann Equation

We present new higher-order quadratures for a family of boundary integral operators re-derived using the approach introduced in [Kublik, Tanushev, and Tsai. J. Comp. Phys. 247: 279-311, 2013]. In this formulation, a boundary integral over a smooth, closed hypersurface is transformed into an equivalent volume integral defined in a sufficiently thin tubular neighborhood of the surface. The volumetric formulation makes it possible to use the simple trapezoidal rule on uniform Cartesian grids and relieves the need to use parameterization for developing quadrature. Consequently, typical point singularities in a layer potential extend along the surfaces normal lines. We propose new higher-order corrections to the trapezoidal rule on the grid nodes around the singularities. This correction is based on local decompositions of the singularity and is dependent on the angle of approach to the singularity relative to the surfaces principal curvature directions. The proposed decomposition, combined with the volumetric formulation, leads to a special quadrature error cancellation.

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MS69

A New Diffuse-Interface Approach to Ensemble Average Solvation Energy

Variational implicit solvation models (VISM), because of their relatively low computational cost and satisfactory accuracy, are of paramount importance in the solvation analysis of biological and chemical systems at molecular level. Central in the construction of VSIM is an interface separating the solute and the solvent, which is obtained by optimizing a solvation energy functional. However, due to the random conformational changes of macromolecules, the disposition of a separating interface cannot be unique. Further, the idea of using the value of a solvation energy functional computed at a fixed interface to predict experimentally observed solvation energies is undermined by the fact that experimentally observable quantities are ensemble averaged. In this talk, we will introduce how to use a VISM with a "diffuse interface" to calculate ensemble average solvation energy. The new model is rigorously analyzed and new numerical methods are developed.

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MS69

A Regularization Approach for Solving the Super-Gaussian Poisson-Boltzmann Model with Heterogeneous Dielectric Functions

The recently developed Gaussian Poisson-Boltzmann (PB) models can not only provide a surface-free approach for electrostatics, but also capture the atomic details in the continuum modelling by using atom-specific heterogeneous dielectric values. In this talk, we will focus on singular point charges of the Gaussian PB model, which are Dirac delta functions. The usual trilinear interpolation of partial charges is known to introduce large numerical artifact or grid energy. To completely eliminate the grid energy, a novel regularization method is developed. In particular, a dual decomposition of potential and dielectric function is carried out, so that the charge singularities can be analytically captured by the Coulomb potential, while the reaction field potential satisfies a regularized PB equation with a new source term. Mathematical analysis has been conducted to show that a super-Gaussian density, instead of a Gaussian one, is required for the source term being well defined in the sense of distribution. Moreover, the well-posedness of the regularized formulation has been proved, and the regularity of the weak solution has been clarified. Numerical tests have been conducted to demonstrate the accuracy and robustness of the proposed regularization.

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MS70

An Immersed Boundary Model of Aortic Stenosis with Biochemical Interactions

Recent clinical studies have shown that subclinical leaflet thrombosis (SLT) is a common finding after a transcatheter aortic valve replacement, and if left untreated, SLT can lead to serious complications. Models are needed to determine the underlying cause of SLT and to predict which patients will develop SLT. To this end, we develop a model of aortic stenosis that combines fluid-structure interaction and a continuum thrombosis model that allows for deposition along the moving leaflets. The build-up of material on the leaflets in turn increase the stiffness of the leaflets. We quantify the model's ability to realize changes in stroke volume and pressures, and discuss improvements to model growth of a thrombus on a moving surface. These new approaches represent an important advancement in thrombosis modeling. Additionally, the techniques developed herein can be adapted to model deposition or absorption along other moving boundaries, such as drug absorption in the gut or particulate deposition in the lungs.

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MS70

Multiphysics and Multiscale Modeling of Microthrombosis in Covid-19

Emerging clinical evidence suggests that thrombosis in the microvasculature of patients with Coronavirus disease 2019 (COVID-19) plays an essential role in dictating the disease progression. Herein, we employ a novel multiscale and multiphysics computational framework to perform predictive modeling of the pathological thrombus formation in the microvasculature using data from patients with COVID-19. Our simulation results show that among the coagulation factors considered, antithrombin and factor V play more prominent roles in promoting thrombosis. Our simulations also suggest that recruitment of WBCs to the endothelial cells exacerbates thrombogenesis and contributes to the blockage of the blood flow. Additionally, we show that the recent identification of flowing blood cell clusters could be a result of detachment of WBCs from thrombogenic sites, which may serve as a nidus for new clot formation. These findings point to potential targets that should be further evaluated, and prioritized in the anti-thrombotic treatment of patients with COVID-19. Altogether, our computational framework provides a powerful tool for quantitative understanding of the mechanism of pathological thrombus formation and offers insights into new therapeutic approaches for treating COVID-19 associated thrombosis.

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MS70

Computational Modeling of Platelet Aggregation in An Extravascular Injury Geometry

Hemostasis is the process by which a blood clot forms to prevent bleeding at the site of an injury. The formation time, size, and structure of a blood clot depends on the local hemodynamics and the nature of the injury. We have previously developed computational models to study intravascular clotting, a process confined to the interior of a vessel. Modeling extravascular injuries, where blood leaks from a vessel into extravascular space, requires a set of new computational tools for the complex geometries that simulate the injury. Similar to our previous intravascular model, our new model of extravascular clotting uses a continuum approach to track the advection, diffusion, and aggregation of platelet densities in a dynamic fluid environment. The transport of platelet densities into any spatial location is limited by the platelet fraction that already resides within that location, i.e., the densities satisfy a maximum packing constraint using a hindered transport coefficient. We use a finite volume method on a nonuniform mesh in an H shaped geometry. Our computational model simulates platelet aggregation in an analogous in vitro microfluidic model. We use kinetic and occlusion time data from the microfluidic model to develop and validate our computational model. Results from the computations and experiments showed that the formation of a blood clot occludes the injury channel and stops flow from escaping while blood in the main vessel retains its fluidity.

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MS70

Mathematical Modelling of Platelet Signaling

The anuclear blood cells, platelets, form blood clots in human vessels. Dysfunction of platelets is observed in various hereditary and acquired diseases. Our team developed a system of experimental tests that allows us to characterize platelet functioning in healthy donors and patients. In parallel, a mechanistic computer model of intracellular signaling in platelets was developed, simulating the main functional responses of platelets to activation by thrombin, ADP, collagen and podoplanin. Platelet responses are known to have stochastic nature; therefore, we integrated the developed model by means of the tau-leap stochastic modeling approach and thus described platelet subpopulation formation. Further analysis of the model allowed us to determine the number of activated receptors as the origin of stochasticity in the platelet signaling network. To facilitate incorporation of the platelet signaling model in models of thrombus formation, we performed a reduction of the core system of ordinary differential equations using the Tikhonov's theorem. The constructed computational model allowed identification of mechanisms of platelet dysfunction in patients with immune thrombocytopenia and with Wiscott-Aldrich syndrome. Therefore, we utilized a set of experimental techniques to observe patient-specific features in platelet functioning and developed a pipeline for the construction of patient-specific platelet signaling model.

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MS71

Effects of Reward History on Decision-Making and Movement Vigor

During foraging, animals decide how long to stay and harvest reward, and then abandon that site and travel with a certain speed to the next reward opportunity. One aspect of this behavior involves decision-making, while the other involves motor-control. A recent theory posits that control of decision-making and movements may be linked via a desire to maximize a single normative utility: the sum of all rewards acquired, minus all efforts expended, divided by time. If this is the case, then the history of reward, and not just its immediate availability, should dictate how long one decides to stay and harvest reward, and how slowly one travels to the next opportunity. We tested this theory in a series of experiments in which humans used their hand to harvest tokens at a reward patch, and then used their arm to reach toward a subsequent opportunity. Following a history of poor rewards, people not only foraged for a longer period, but also moved slower to the next reward site. Thus, reward history had a consistent effect on both the decision-making process regarding when to abandon a reward site, and the motor control process regarding how fast to move to the next opportunity.

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MS71

Stochastic Dynamics of Foraging Behaviors

Foraging is a ubiquitous behavior performed by all animals as search for food is crucial for survival. When the animal is foraging throughout its environment searching for resources, it is employing a variety of cognitive computations from decision making to planning to learning in addition to adjusting its bodily dynamics. Foraging as a behavior allows studying cognitive dynamics in a natural context and opens up the opportunity for evolutionary comparison across species. In my presentation, I will provide a conceptual framework for an integrative understanding of patch foraging focusing on recently developed bayesian mechanis-

tic models, that delineate the potential decision strategies an animal might employ to decide when and how to leave a patch of food across environments with different statistics. I will discuss how these models can be extended to the social foraging realm. I will also contextualize the theoretical models in relation to field data from a variety of species and their potential to design large scale naturalistic experiments in traditional laboratory animal models.

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MS71

Effective Adaptation in Human-Agent Teaming

The ability to collaborate with different types of unseen human teammates is crucial for artificial agents to be effective in human-agent teams (HATs). On one hand, individual human difference and complicated team dynamics makes it difficult to develop a one-size-fits-all agent policy a priori. On the other hand, developing agent models in HATs that consider human individual variation is challenging and has not been well studied. This talk describes research into both human-human and human-agent teams in Coop Space Fortress, a dyadic cooperative task with an adversary and heterogeneous player roles. Results for human-human teams demonstrate that team performance is influenced by both players individual skill level, as well as their ability to collaborate with different team mates by adopting complementary policies. An agent team member was developed for the Coop Space Fortress scenario which employs a library of diverse agent policies developed using a mixture of learning approaches, and a novel similarity metric is used to select a complementary agent policy based on inference of human policy. The combination of the policy library and similarity metric allows the agent to adapt in real-time to new human team members. Experimental results demonstrate the contributions of adaptation in both human-human and human-agent team experiments.

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MS71

Correlation and Accuracy in Multi-Agent Two-Alternative Forced Choice Tasks

When making decisions, we often rely on a mix of information that we have acquired individually and information that is commonly available. Neglecting the effect of social information exchange, does the fact of information being individual or common affect the quality of the decisions we make? To answer this question we assume that multiple non-interacting agents make observations and decide between two options when they gathered sufficient information to reach one of two symmetric thresholds. Some observations are made in common by all agents and some privately by each agent. Common observations result in the first agents to reach threshold being less likely to make the correct choice compared to when all observations are private. We observe this phenomenon even when private and common observations are equally informative. Therefore, it is only the order of a decision that impacts its accuracy. Indeed, later deciders become progressively more accurate, and last deciders will be more accurate than those using only private information. We explain this counterintuitive observation, and conclude that access to common information increases accuracy for those with uninformative or contradictory early information and decreases accuracy for those whose early private information coincides with the common information.

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MS72

Understanding the Role of Autonomic Control in Sickle Cell Disease: Application of Computational Modeling and Signal Analysis

Painful vaso-occlusive crises (VOC) are a hallmark of sickle cell disease (SCD). The mechanism by which VOC is triggered remains elusive but we believe that the autonomic nervous system plays a role in the genesis of VOC. We hypothesized that abnormal autonomic control of peripheral vasoconstriction in SCD could lead to higher probability of rigid sickled cells getting lodged in the microcirculation. Collective microvascular obstruction could then lead to large scale VOC. To test this hypothesis, we employed a Laguerre-Volterra model to decompose the pain-induced vasoconstriction response. The most salient features of the identified dynamics were extracted to represent the biophysical markers of autonomic and vascular impairment in SCD and healthy controls. This approach allowed us to deduce which (functional) mechanisms contributed to the stronger pain-induced vasoconstriction response observed

in SCD compared to controls. Next, we sought to determine whether there is a causal link between naturally-occurring peripheral vasoconstriction during sleep and the incidence of VOC. We detected vasoconstriction events from fingertip photoplethysmograms acquired from SCD subjects in a prospective multi-center cohort sleep study. Using a statistical model, we found that a higher propensity to vasoconstrict, quantified by the median of overnight vasoconstriction magnitude, predicted more frequent VOC events.

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MS72

A Modeling Framework for Pediatric Sickle Cell Pain

Sickle cell pain presents in acute episodes in pediatric patients, as opposed to the chronic pain observed in adults. The episodic nature of pain events in pediatric patients necessitates a distinct approach from what has been used to mathematically model pain severity levels in adults. Statistical studies have examined interactions between sleep actigraphy measurements — like sleep quality and sleep efficiency — and pain levels in pediatric populations, and we propose a framework for modeling pediatric pain dynamics that incorporates the effects of sleep actigraphy and electronic survey data over varying time windows. We hypothesize that cumulative effects of these measurements will be more important than daily measurements in both replicating pain severity levels and determining markers of a pain episode. The ability to identify markers preceding the onset of a pain episode will be crucial in improving patient quality of life. We present work in progress towards developing this modeling framework.

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MS72

Quantitative Systems Pharmacology Model of Vaso-Occlusion Formation in Sickle Cell Disease

Sickle cell disease (SCD) is caused by a mutation in the beta-hemoglobin chain which results in hemoglobin polymerization. In turn, polymerization events lead to red blood cell (RBC) sickling and hemolysis triggering a cascade of inflammatory signals and endothelial cell activations (ECs). Neutrophil and RBC aggregation on ECs can lead to vaso-occlusions, obstructing blood flow within the micro-vasculatures. Vaso-occlusion is a major pathologic consequence of SCD as it can further lead to hypoxia, acute/long-term organ damages, and pain crisis. An important component of the development of vaso-occlusion is the role of fluid/blood flow and biophysical aspects of cell-cell interaction specifically through mediation by the selectin family of cell surface receptors. Our project focuses on developing a quantitative systems pharmacology model that computationally tracks the formation of vaso-occlusion in SCD. Our model consists of a system of partial differential equations that incorporates the effects of cell-cell interactions (neutrophils, RBCs, and ECs), blood flow, and biochemical reactions, on the formation of cellular aggregates in vaso-occlusion. The model will be used to investigate the vital roles of selectins as therapeutic targets for the treatment of SCD. We will quantitatively and mechanistically link the relationship between the circulating biomarkers and disease risk factors with an aim of aiding the design and development of future therapies for SCD.

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MS72

Classification of Patient Experiences with Pain in Sickle Cell Disease

Sickle cell disease is an inherited blood disorder which causes patients to experience both acute and chronic pain. Recent work has sought to use modern mobile or wearable technology to monitor and model patient pain and vital signs over time. Here, we develop and test various methods for partitioning irregularly and sparsely sampled histories of pain over time into distinct groups, seeking also to rigorously examine the consistency of the clustering methodology. In this work, we use self-reported pain data from

mobile apps and electronic hospital records to examine patient pain experiences. We use network-based unsupervised learning methods to identify underlying groups of pain trajectories (i.e., reported pain values over time). Our results indicate that patients' experiences fall generally into three classes—those with low pain, those with persistent high levels of chronic pain, and those who generally have moderate pain which varies greatly day to day. The results of this work have the potential to help both doctors and patients better categorize and manage pain levels over time. Further, the methods we develop and apply may be useful in any application where data is sparsely and irregularly sampled.

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MS73

A Closed-Loop Multi-Scale Model for Intrinsic Frequency-Dependent Regulation of Axonal Growth

Recent experimental studies indicated the existence of intrinsic control of axonal length by neurons. A possible underlying mechanism relies on mutual delayed feedback between two oscillatory signals, which are transport by molecular motors in an axon. However, many aspects of this mechanism remain unexplored. As a theoretical investigation, we propose a delayed feedback model built on existing theoretical studies and connect it to motor dynamics. Bifurcation analysis on the model indicates that the oscillation inhibits axonal growth and the inhibition becomes stronger as the oscillation period increases. We then provide a generic signaling pathway to illustrate how a neuron can decode the length information from the oscillatory signals and use it to control its axonal length. The pathway and the delayed feedback model form a closed loop system, which predicts step-like changes in axonal length that can be linked to the initiation/termination of the oscillation.

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MS73

Computational Models of Human Word Recognition

Despite (i) overlapping acoustic patterns of phonemes, (ii) boundaries that shift with speaking rate, talker characteristics, phonetic context, coarticulation, and novelty of message, and (iii) a many-to-many mapping between acoustics and precepts, listeners generally achieve phonetic constancy and understand speech. Relatively simple cognitive models have guided theories of the time course of human spoken word recognition (HSR) for decades, but generally have small vocabularies, do not use real speech as input, and set aside the problem of learning. Automatic speech recognition (ASR) systems provide robust, real-world computer speech recognition, but often contain many layers of richly connected neurons (making introspection difficult) and require carefully engineered training regimens and architectures that are not typically constrained by biological considerations. I will discuss efforts by myself and my collaborators to partially bridge this gap with the EARSHOT model: a shallow neural network model which can learn to map real speech from multiple talkers to semantic targets with high accuracy, with a human-like time course of lexical access and phonological competition. Analysis of the models internal representations and tests on secondary tasks suggest that the model develops a distributed phonological code despite no explicit training on phonetic or phonemic targets. The ability to work with real speech is a major advance for cognitive models of HSR.

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MS73

Spatial Dynamics of COVID-19: from PDEs to Metapopulation Models

We will present results on the spatial dynamics of COVID-19 in Andalusia, Spain using two distinct modeling approaches. First, we will report on a PDE-based model of the spread during the first wave of the pandemic (spring of 2020). Time-varying transmission and diffusion coefficients are incorporated to account for the mitigation measures imposed during the period we consider. Then, we will show results on a metapopulation model for the period before the second wave (summer and early fall of 2020). No mobility restrictions were in effect during this period, so we incorporate data-driven population flows among the eight provinces. These mobility flows are time-dependent due to weekend travel and for other reasons. One of our main findings is that the trends observed in the reported data cannot be reproduced by models without human mobility. We will conclude the talk with ideas for future directions and alternative ways to analyze the reported data.

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MS73

Spatially Inhomogeneous Stochastic Cyclic Competition Models: Stabilizing Vulnerable Ecologies Through Immigration Waves

We study the induction and stabilization of spiral structures for the cyclic three-species stochastic MayLeonard model with asymmetric predation rates on a spatially inhomogeneous two-dimensional toroidal lattice using Monte Carlo simulations. In an isolated setting, strongly asymmetric predation rates lead to rapid extinction from coexistence of all three species to a single surviving population. However, when the asymmetric competing system is coupled via diffusive proliferation to a fully symmetric MayLeonard patch, the stable spiral patterns from this region induce transient plane-wave fronts and ultimately quasi-stationary spiral patterns in the vulnerable asymmetric region. Thus, the endangered ecological subsystem may effectively become stabilized through immigration from a smaller stable region. To describe the stabilization of spiral population structures in the asymmetric region, we compare the increase in the robustness of these topological defects at extreme values of the asymmetric predation rates in the spatially coupled system with the corresponding asymmetric MayLeonard model in isolation. We delineate the quasi-stationary nature of coexistence induced in the asymmetric subsystem by its diffusive coupling to a symmetric MayLeonard patch, and propose a (semi-)quantitative criterion for the spiral oscillations to be sustained in the asymmetric region.

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MS74

Modeling Antiarrhythmic Drug Electrophysiology in iPSC-Derived Cardiomyocytes

Current drugs used to treat abnormalities in cardiac rhythm, or arrhythmia, often lack therapeutic efficacy and have significant side effects. Difficulty in connecting molecular drug interactions to patient phenotypes is due to nonlinear and stochastic behaviors that drive emergent cardiac phenomena. This challenge is further exacerbated by the limited experimental availability of healthy human cardiac cells and tissues, requiring suboptimal animal model surrogates. Amiodarone is an example of a widely prescribed but poorly understood therapy. Its mechanistic complexity, which includes time dependence and different modes of block, could be elucidated with detailed computational models. Human induced pluripotent stem cell-derived cardiomyocytes (hiPSC-CMs) treated with amiodarone were analyzed using automated planar patch clamp (single cells/currents) or optical fluorescence microscopy (confluent monolayers) to assess drug response. These data and literature parameters were integrated into a computational ventricular myocyte model to create drug models based on either hiPSC-CM or animal model amiodarone electrophysiology. Virtual cardiomyocyte cables treated with a therapeutic dose of hiPSC-CM- and animal-parameterized amiodarone exhibited differential impacts on action potential and calcium transient morphology. Our ability to identify these discrepancies may inform the translation of drug response in hiPSC-CMs and animal models to adult human multiscale electrophysiology.

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MS74

An in Silico-in Vitro Pipeline for Drug Cardiotoxicity Screening Identifies Ionic Proarrhythmia Mechanisms

Before advancing to clinical trials, new drugs are screened for their proarrhythmic potential using a method that is overly conservative and provides limited mechanistic insight. The shortcomings of this approach can lead to the misclassification of beneficial drugs as proarrhythmic. We developed an in silico-in vitro pipeline using mathematical models and human induced pluripotent stem cell-derived cardiomyocytes (iPSC-CMs) to circumvent this problem. A computational iPSC-CM model was used with a genetic algorithm to design experiments, specifically electrophysiological voltage-clamp (VC) protocols to identify which of several cardiac ion channels were blocked during in vitro drug studies. Such VC data, along with dynamically clamped action potentials (AP), were acquired from iPSC-CMs before and after treatment with a control solution or a low- (verapamil), intermediate- (cisapride), or high-risk (quinidine or quinine) drug. We identified significant AP prolongation (a marker of proarrhythmia) in response to both high-risk drugs and, from the VC data, determined ion channel targets that were likely responsible for these AP changes. In summary, we developed an in silico-in vitro pipeline that simultaneously identified proarrhythmia risk and underlying mechanism for cardiac ion channel-blocking drugs, illustrating the pipelines value in the preclinical drug screening phase.

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MS74

Cardiac Alternans: A Biomarker of Dynamic Elec-

trophysiological Changes in Diseased Substrates

Cardiac alternans has been associated with an increased propensity to malignant tachyarrhythmias such as ventricular tachycardia and fibrillation (VT/VF). Preclinical and clinical studies have demonstrated the utility of alternans in predicting the onset of VT/VF, with heightened levels of alternans reported to occur in conjunction with arrhythmic episodes. Sharp upsurges in alternans have been documented in patients with coronary artery disease, myocardial infarction, as well as acute heart failure. Moreover, increase in alternans has been shown to correlate with elevated sympathetic activity in humans, while the amplitude of alternans has been shown to diminish with -blockers. It has been proposed that prevention and control of alternans could inhibit the onset of impending lethal tachyarrhythmias. Here, in a series of preclinical and clinical studies, the utility of cardiac alternans as a biomarker of disease progression was investigated. Preclinical data investigating the potential of alternans in characterizing the electrophysiological substrates that predispose the heart to malignant arrhythmias, specifically during chronic myocardial infarction is presented. Furthermore, the use of alternans to serve as a marker for guiding anti-arrhythmic treatment in patients susceptible to tachyarrhythmias, both atrial and ventricular, by identifying dynamic changes in diseased substrates and quantifying the response to therapy, is evaluated.

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MS74

Modeling Neurophysiology and Cardiac Electrophysiology via Delay Differential Equations

Since the pioneering works of Hodgkin and Huxley (HH), cell electrophysiology has been modeled via ordinary differential equations. In this talk, we will show how the classic HH model can be replaced by a single delay differential equation (DDE). In addition, we present some benefits (e.g., for modeling Alternans) and challenges (e.g., new numerical methods) associated with the use of DDEs in cardiac modeling.

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MS75

Fast-Slow Analysis of a Stochastic Mechanism for Electrical Bursting

Electrical bursting oscillations in neurons and endocrine cells are activity patterns that facilitate the secretion of neurotransmitters and hormones, and have been the focus of study for several decades. Mathematical modeling has been an extremely useful tool in this effort, and the use of fast-slow analysis has made it possible to understand bursting from a dynamic perspective, and to make testable predictions about changes in system parameters or the cellular environment. It is typically the case that the electrical impulses that occur during the active phase of a burst are due to stable limit cycles in the fast subsystem of equations, or in the case of so-called "pseudo-plateau bursting', canards that are induced by a folded node singularity. In this paper, we show an entirely different mechanism for bursting that relies on stochastic opening and closing of a key ion channel. We demonstrate, using fast-slow analysis, how the short-lived stochastic channel openings can yield a much longer response in which single action potentials are converted into bursts of action potentials. Without this stochastic element, the system is incapable of bursting. This mechanism can describe stochastic bursting in pituitary corticotrophs, which are small cells that exhibit a great deal of noise, as well as other pituitary cells such as lactotrophs and somatotrophs that exhibit noisy bursts of electrical activity.

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MS75

A Simple Stochastic Model of Bleb-Driven Cell Migration

Blebs are pressure-driven protrusions that have been observed in cells undergoing apoptosis, cytokinesis, or migration, including tumor cells that use blebs to escape their organs of origin. Mathematical models have been previously developed to understand either bleb expansion (using fluid mechanics) or the bleb life cycle including both expansion and healing by cortex reformation (using an excitable dynamical system). Here, we introduce a simple stochastic pressure-driven cell migration model in 1D, which connects sub-cellular adhesion process and cell migration dynamics. We focus on how intrinsic noise from molecular interaction of cortex components can generate stochastic membrane-cortex separation, which allows cells to migrate by hydrostatic pressure. The incorporation of this stochastic initiation mechanism allows for the simulation of repeated blebbing events and thus continuous cell movement. We study the statistics of the blebbing events using a renewal process approximation and then derive a Langevin equation of cell migration by matching the asymptotic moments of the approximation process.

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MS75

The Role of Mixed Mode Oscillations in Defining Cellular Motility

Cellular motility is essential for many (patho)physiological processes, including immune responses, embryonic development and cancer metastasis. The two members of the Rho-family of GTPases, Rac1 and RhoA, have been implicated in defining the key signaling motif responsible for generating cellular polarity and directionality through their mutual inhibition. Their spatiotemporal dynamics are partially regulated by the phosphorylation of an adaptor protein called Paxillin. A 6D partial differential equation model describing the interactions of these proteins, along with other auxiliary proteins, was previously developed by our group to decipher their role in generating bistability between uninduced (active Rho) and induced (active Rac) states, as well as wave-pinning underlying cellular polarization. We have recently simplified this model into an excitable 3D model possessing three different time scales. The new model produced not only bistability and wave-pinning, but also relaxation oscillations (ROs) and mixed-mode oscillations (MMOs). Simulating the dynamics of this model using the cellular potts model produced outcomes in which protrusions in cell membrane changed localization, resulting in membrane oscillations and fast directionality variations similar to those seen in Chinese hamster ovary cells. Performing slow-fast analysis revealed that dynamic Hopf and canards are responsible for generating ROs and MMOs. In this talk, I will provide a summary of these findings.

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MS75

Complexity in Multi-Delay Physiological Feedback Systems

We investigate transitions to simple dynamics in first-order nonlinear differential equations with multiple delays. With a proper choice of parameters, a single delay can destabilize a fixed point, a common mechanism that leads to oscillatory and even chaotic behaviour in physiological systems. The distributed delay case corresponds to an infinite number of delays, and is known to typically yield solutions of relatively lesser complexity, all other parameters being equal. We focus on the intermediate regimes of multiple discrete delays, embodying many parallel feedback pathways. The dynamics are found to depend on the precise distribution of the delays in mixed feedback systems. A narrow spacing between delays induces chaotic behaviour, but a larger spacing (lower delay density) promotes a collapse in complexity towards stable periodic or fixed point behaviour. The behaviour of the unstable characteristic roots around the fixed point exhibits an astonishing parallel with that of the Lyapunov exponents and the Kolmogorov-Sinai entropy for these multi-delay systems, and thus serves as a proxy of solution complexity. Inverse period-doubling can also occur as the number of delays increases beyond a threshold that depends on the separation of time scales, namely between the mean delay and the intrinsic response time.

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MS76

Malaria Modeling and Incorporated Treatment Waiting Times with a General Integral Equation Model

Many epidemiological models assume an exponentially-distributed waiting time in each of the population classes in order to simplify the model formulation and its analysis. This may not always be the most accurate assumption depending on context, and some methods have been developed to account for the variability in class waiting times such as the linear chain trick. It is especially important to capture the correct waiting times in models dealing with pharmacological responses due to treatment in order to better understand the interaction between drug concentration and pathogen load within hosts. Capturing these interactions can help us model the within-human pharmacodynamics and pharmacokinetics which will then enable us to inform drug development and treatment in human populations. It will also help us reduce the spread of drug-resistant strains. We will present a two-strain SITR integral equation model for Malaria that incorporates general waiting time distributions and explore the treatment-related parameters and their relationship with population disease dynamics.

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MS76

Staged HIV Transmission and Treatment in a Dynamic Model with Long-Term Partnerships

The transmission dynamics of HIV are closely tied to the duration and overlap of sexual partnerships. There are many issues at play. A serodiscordant long-term partnership presents repeated exposures to the infected partner. If concurrency exists, an increase in partnership duration can increase infection rates. However, non-infected monogamous pairs are protected. We develop an autonomous population model that can account for the possibilities of an infection from either a casual sexual partner or a long-term partner who was either infected at the start of the partnership or was newly infected. The impacts of the long-term partnerships on the rate of infection are captured by calculating the expected values of the rate of infection from these extended contacts. The model has three stages of infectiousness: acute, chronic, and virally suppressed. We calculate HIV incidence and the fraction of new infections attributed to casual contacts and long-term partnerships allowing for variability in the condom usage, the effect of achieving and maintaining viral suppression, and early intervention by beginning HAART during the acute phase of infection. We present our results using data on MSM HIV transmission from the CDC in the U.S. While the acute stage is the most infectious, most of the new infections will be transmitted by long-term partners in the chronic stage

when condom use is infrequent.

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MS76

The Effects of PrEP on the Spread of HIV in the presence of Casual and Long-Term Partnerships

A classic approach for modeling the spread of the sexually transmitted diseases is to assume a zero inherent length infection contact. However, in the population with long-term partnerships, the infection status of the partners, the length of the partnership, and the exclusivity of the partnership, all affect the rate of infection. Additionally, the presence of the pre exposure prophylaxis (PrEP) also impacts the dynamics of the disease. Our goal is to develop a compartmental model that accounts for various partnership scenarios as well as the uptake and adherence to the PrEP treatment. Reproduction numbers are calculated and global stability of both disease-free and endemic equilibria will be shown with appropriate conditions. Sensitivity and PRCC analysis are performed on the key parameters to determine the degree to which each affects the disease transmission dynamics. The results suggest that increasing the adherence among the current PrEP users is a more effective (and likely more cost-efficient) strategy in the fight against the HIV epidemic than increased coverage with poor adherence. However, when both casual and long-term partnerships are accounted for in the population, even with the maximum level of compliance and full PrEP coverage, stopping the spread of HIV will require additional interventions.

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MS77

Cooperation, Partisanship, and Madisons Cure for Mischiefs of Faction

Political theorists have long argued that a pluralistic republic can combat the dangers of factions by enlarging the political sphere to include a greater diversity of interests. While the scope of politics has expanded over the past 75 years, polarization is markedly worse. Motivated by this paradox, we take a bottom-up approach to explore how partisan individual-level dynamics in a multidimensional issue space can shape collective-level factionalization. We extend a model of cultural evolution grounded in evolutionary game theory, in which partisanship determines the likelihood of cross-party learning and the interaction network changes endogenously according to individual interests. We find that while expanding interest diversity can indeed improve both individual and collective outcomes, increasingly high partisan bias promotes a reduction in issue dimensionality via party-based assortment, promoting polarization. Extreme partisan bias can boost interindividual cooperation, creating a tug-of-war between individual cooperation and societal cohesion. These dangers of extreme partisanship are highest when interests are heavily shaped by peer learning, with little independent exploration. Our results highlight the need to study polarization in a coupled, multilevel context.

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MS77

Environmental Feedbacks from the Warburg Effect in Pre-Metastatic Neoplasms

Cancer cells can forego using available oxygen in favor of less efficient glycolytic (GLY) metabolism. This is a hallmark of cancer known as the Warburg effect. As a by-product, this GLY pathway increases tumor acidity which can help the cancer cells out-compete healthy tissue and increase vasculature (angiogenesis). Prior work modeled acidity and vasculature as public or club goods, but did not explicitly track the acidity and amount of vasculature. Our evolutionary game theoretic model explicitly represents these environmental feedbacks as dynamic variables ($a(t)$ for acidity and $v(t)$ for vasculature) alongside the distribution of strategies ($x(t)$ for proportion of GLY cells). The relative fitness of the two strategies (oxidative phosphorylation vs GLY) is determined by competition at the level of metabolic rates and efficiencies due to the Michaelis-Menten kinetics of ATP production. This leads to non-linear fitness functions for the two strategies, allowing the system to have dynamic regimes with several interior fixed-points. We classify the number and stability of fixed-points based on the initial amount of vasculature and metabolic parameters. In particular, we note the importance of lower uptake rates of glucose in the GLY cells for maintaining a less dangerous non-glycolytic tumor. We hope that our model of in situ pre-metastatic neoplasms gives insights into early tumor progression and potential avenues for cancer treatment and prevention.

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MS77

Memetic Sin and Complex Contagion

Recently, information dynamics have taken center stage in our collective understandings of science, risk, and decision making. Surprisingly, while a great deal of studies have addressed information dynamics in human populations, the scope of mathematical theory on the topic is quite limited and often overly complex. Here, I'll present a simplified theoretical model that captures several well-known aspects of information dynamics within a single model and can be adapted to represent a wide set of phenomena and their resolutions.

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MS77

Evolutionary Dynamics of Cooperation Between Epithelial Cells

Cells can cooperate by producing diffusible growth factors that confer a fitness benefit on surrounding cells. For example, several mutations associated with malignancy rely on growth factor production. The evolution of cooperation has been extensively studied using game-theoretic models, and it is known that population structure and update dynamics play an important role in the resulting dynamics. Cell populations within the body are organised into tissues, such as epithelia, which form skin and the linings of our organs. These are dynamic structures, not easily represented by evolutionary graph theory models, which are traditionally used to incorporate population structure into evolutionary modelling. We thus use the Voronoi tessellation model to more realistically represent the population dynamics of an epithelium. Considering evolutionary games within this context, we are able to explore how the properties of an epithelium, in particular, the coupling of death and division, affect the evolutionary dynamics of cooperation.

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MS78

Chemotactic Navigation of Bacterial Swimmers with Multiple Run Modes

Bacterial chemotaxis – a fundamental example of directional navigation in the living world – is key to many biological processes, including the spreading of bacterial infections. Many bacterial species were recently reported to exhibit several distinct swimming modes – the flagella may, for example, push the cell body or wrap around it. How do the different run modes shape the chemotaxis strategy of a multimode swimmer? Here, we investigate chemotactic motion of the soil bacterium *Pseudomonas putida* as a model organism. By simultaneously tracking the position of the cell body and the configuration of its flagella, we demonstrate that individual run modes show different chemotactic responses in nutrition gradients and, thus, constitute distinct behavioral states. On the basis of an active particle model, we demonstrate that switching between multiple run states that differ in their speed and responsiveness provides the basis for robust and efficient chemotaxis in complex natural habitats, for details see Alirezaeizanjani et al. *Sci. Adv.* 2020; **6** : eaaz6153.

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MS78

Simulating Microbial Behaviors in Physically Relevant Environments

Simulating Microbial Behaviors in Physically Relevant Environments As biological machines, bacteria can exhibit a broad spectrum of processes ranging from petrochemical degradation to human health maladies which make them agents of interest across several bioengineering disciplines. While modern profiling tools have greatly advanced interrogations into how these processes emerge in bacteria, approaches to elicit specific responses from a bacteria population in situ remain difficult to achieve. The seminal work from Keller and Segel has demonstrated that a populations motility behaviors can be mathematically modelled and even predicted under certain stimuli. In this presentation, I will report the work accomplished by the Ford Group in applying similar models to predict microbial responses inside settings that mimic physical environments. First, I will illustrate how the Keller-Segel system can be expanded in order to interrogate bacteria motility behaviors in chemically heterogenous spaces. Second, I will discuss our investigations into how external porous media conditions influence a bacteriums navigational capabilities as well as how these factors translate back into the continuum perspective. Lastly, I will describe our extension of bacterial transport in porous media into the biomedical discipline in order to influence the progression of pathogenic infections.

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MS78

A Quantitative, Mechanistic Approach to Bacterial Infections: from Bacterial Exploration to Infection and Aggregation

Combining mathematical models and bacterial experiments, we have learned how pathogenic bacteria explore surfaces, infect cells, and form early aggregates. I will provide a brief summary of the obtained results and show that a mechanistic approach to bacterial infection is possible.

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MS79

Geometric Algebra Generation of Molecular Sur-

faces

Geometric algebra is a powerful framework that unifies mathematics and physics. Since its revival in the middle of the 1960s by David Hestenes, it attracts great attention and has been exploited in many fields such as physics, computer science, and engineering. This work introduces a geometric algebra method for the molecular surface generation that utilizes the Clifford-Fourier transform which is a generalization of the classical Fourier transform. Notably, the classical Fourier transform and Clifford-Fourier transform differ in the derivative property in $\mathbb{R}_k$ for k even. This distinction is due to the noncommutativity of geometric product of pseudoscalars with multivectors and has significant consequences in applications. We use the Clifford-Fourier transform in $\mathbb{R}_3$ to benefit from the derivative property in solving partial differential equations (PDEs). The Clifford-Fourier transform is used to solve the mode decomposition process in PDE transform. Two different initial cases are proposed to make the initial shapes used in the present method. The proposed method is applied first to small molecules and proteins. To validate the method, the molecular surfaces generated are compared to surfaces of other definitions. Applications are considered to protein electrostatic analysis. This work opens the door for further applications of geometric algebra and Clifford-Fourier transform in biological sciences.

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MS79

Machine Learning Analysis of Cocaine Addiction Informed by Dat, Sert, and Net-Based Interactome Networks

Cocaine addiction is a psychosocial disorder induced by the chronic use of cocaine and causes a large of number deaths around the world. Despite decades of effort, no drugs have been approved by the Food and Drug Administration (FDA) for the treatment of cocaine dependence. Cocaine dependence is neurological and involves many interacting proteins in the interactome. Among them, the dopamine (DAT), serotonin (SERT), and norepinephrine (NET) transporters are three major targets. Each of these targets has a large protein-protein interaction (PPI) network which must be considered in the anti-cocaine addiction drug discovery. Our work presents DAT, SERT, and NET interactome network-informed machine learning/deep learning (ML/DL) studies of cocaine addiction. We collected and analyzed 61 protein targets out of 460 proteins in the DAT, SERT, and NET PPI networks that have sufficiently large existing inhibitor datasets. Utilizing autoencoder (AE) and other ML/DL algorithms, we built predictive models for these targets to predict the potential of drug repurposing potentials and possible side effects. We further screened their absorption, distribution, metabolism, and excretion, and toxicity (ADMET) properties to search for leads having potential for developing treatments for cocaine addiction. Our approach offers a new systematic protocol for artificial intelligence (AI)-based anti-cocaine addiction lead discovery.

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MS79

The Role of Electrostatics in Machine Learning Assisted Structural Biology

Electrostatics plays a significant role in bimolecular structure, interaction, and dynamics. However, due to its long range and pairwise natures, consideration of electrostatics is often challenging in accuracy and computational cost. In this talk, we present a novel efficient and accurate approach to include electrostatics into the framework of topological network for predicting protein binding affinities. The simulation results demonstrate the significance of involving electrostatics.

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MS79

Persistent Sheaf Laplacians

The aim of this paper is to introduce persistent sheaf Laplacians (PSLs) as an extension of persistent Laplacian theory to cellular sheaves. This work is motivated by the need to elegantly fuse geometric and non-geometric information. The geometric shape can be successfully captured by persistent topology, while local non-geometric properties requires additional treatment. Cellular sheaves offer an ideal tool for this task. Recall that the theory of persistent Laplacian theory provides us a workflow to study a point cloud (1) generates a filtration of simplical complexes; (2) builds a persistence module of simplicial chain complexes; and (3) calculates persistent Laplacians and their spectra. We modify the second workflow and define the notion of PSLs for a persistent module of sheaf cochain complexes. Given a point cloud with nonzero real number associated to each point, we first generate a Rips complex or alpha complex filtration, and define a sheaf for each simplicial complex in the filtration. These sheaves will give rise to a persistent module of sheaf cochain complexes. Given a persistence module of sheaf cochain complexes, one can calculate PSLs, just as one can calculate persistent Laplacians for a persistent module of simplicial chain complexes. The spectra of PSLs can be used in the same way as persistent Laplacians.

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MS80

Combined Computational Modeling and Experimental Study of the Biomechanical Mechanisms of Platelet-Driven Contraction of Fibrin Clots

While blood clot formation has been relatively well studied, little is known about the mechanisms underlying the subsequent structural and mechanical clot remodeling called contraction or retraction. Impairment of the clot contraction process is associated with both life-threatening bleeding and thrombotic conditions, such as ischemic stroke, venous thromboembolism, and others. Recently, blood clot contraction was observed to be hindered in patients with COVID-19. A novel three-dimensional multiscale computational model is developed and used to quantify biomechanical mechanisms of the kinetics of clot contraction

driven by platelet-fibrin pulling interactions. These results provide novel biological insights since filopodia have been thought of previously as performing mostly a sensory function. The biomechanical mechanisms and modeling approach described can potentially apply to studying other blood clotting processes as well as to other systems in which cells are embedded in a filamentous network and exert forces on the extracellular matrix modulated by the substrate stiffness.

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MS80

Uncertainty Quantification of Biochemical Models for Coagulation

Mathematical models for coagulation consist in a set of ordinary differential equations whose parameters (reaction rates) and initial conditions (species concentrations) are uncertain due to physiological variability, limited knowledge of some mechanisms and measurements inaccuracy. Making the models useful in the current efforts towards a better understanding of coagulation requires knowing how thrombin production depends on these uncertain inputs. The Monte Carlo approach, where about $10^4 - 10^5$ simulations are performed with randomly selected input values, is generally used in the literature. This methodology is accurate but time consuming and hardly tractable for complex models (e.g. including spatial heterogeneities due to flow). A more efficient strategy is investigated in this study. Sensitivity coefficients are first assessed at low cost by solving a properly designed set of adjoint linear differential equations; the accuracy of the method is demonstrated from comparisons with derivatives assessed by finite differences. The dimension of the problem is then reduced to overcome the curse of dimensionality of uncertainty quantification analysis. In the case of a model of the extrinsic pathway with 79 input [Butenas et al., 2004], it is shown that one or two independent active variables are enough to represent the variability of thrombin production. A low order model based on these active variables can then be used to perform a Monte Carlo analysis at low cost.

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MS80

A Parallel Multiscale Model for Platelet Aggregation Under Flow

Modeling thrombus growth in pathological flows allows evaluation of risk under patient-specific pharmacological, hematological, and hemodynamical conditions. We have developed a 3D multiscale simulation framework for the prediction of thrombus growth under flow on a spatially resolved surface presenting collagen and tissue factor. The multiscale framework is composed of four coupled modules: a Neural Network (NN) that accounts for platelet signaling, a Lattice Kinetic Monte Carlo (LKMC) simulation for tracking platelet positions, a Finite Volume Method (FVM) simulator for solving equations describing agonist release and transport, and a Lattice Boltzmann (LB) flow solver for computing the blood flow field over the growing thrombus. Computationally efficient parallel simulations were achieved by using open-source software where applicable: Palabos (LB), OpenFOAM (FVM), and Multiscale Universal Interface for module-coupling. Parallel versions of LKMC and NN were achieved by employing a novel parallel platelet-decomposition approach. The model accurately captured the evolution of the growing thrombus observed in microfluidics experiments of whole blood perfusion with various antiplatelet agents. The generalizability of the 3D model enabled simulations of important clinical situations, such as cylindrical blood vessels and stenoses. Overall, the approach allows consideration of patient-specific platelet signaling and vascular geometry for the prediction of thrombotic episodes.

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MT1

Koopman Operator Methods for Analysis Design of Synthetic and Natural Gene Networks

See session abstract.

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MT2

Data-Driven Mathematical Modeling

See session abstract.

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See session abstract.

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Data-Driven Mathematical Modeling

See session abstract.

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PP1

A Computational Rule-Based Semi-Automatic Method For Creating Left Atrial Fiber Architec-

ture

With an aging population, atrial fibrillation (AF) affects 2.7 million to 6.7 million people in the United States [Du, X et al, J Am Coll Cardiol., 69(15):1968-1982, 2017]. Although the CHA_2DS_2VASC score is the most used risk-stratification scoring system to guide AF treatment, the measurement lacks personalization. To overcome this limitation, many researchers have started creating patient-specific computer simulations of AF. One of the challenges faced in creating such models is the complexity of the atrial muscle arrangement. This work proposes a semi-automated rule-based algorithm for left atrial (LA) myofiber construction. The transmural fibers produced by our algorithm generate similar electrical activation patterns compared to those generated using existing approaches that are more complex. Current approaches for defining the orientation of the atrial fiber bundles either require the definition of hundreds of landmarks or are overly simplistic. The notable advantage of our approach is the ability to capture the main LA fiber bundles while solving only seven harmonic fields, leading to a straightforward and reproducible approach. Finally, our method is easily extendable to non-trivial configurations of pulmonary veins that are common among AF patients.

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PP1

Simulation of Circulation Response to Accelerational Forces During Spaceflight

This project presents zero-dimensional computer models for blood flow in the context of spaceflight, focusing on launch and landing. In contrast to previous attempts at first-principle modeling of the cardiovascular systems behavior during spaceflight have emphasized the circulation in microgravity or post-spaceflight orthostasis. Our methodologies consist of a steady-state model that considers averaged values for physiological parameters and a multi-compartmental pulsatile blood flow model that is fully time-dependent. Systemic and pulmonary arteries and veins are modeled as compliance chambers, and the elements that connect these chambers operate as linear resistors, equipped with valves as needed. The systemic circulation is partitioned into upper and lower parts to allow for the effects of gravity and the acceleration forces of launch and landing. We consider the case of partial collapse of the systemic veins as they enter the thorax, allowing for changes in intrathoracic pressure from anti-G-straining maneuvers (AGSM). Both models include a feedback controller that monitors upper systemic arterial pressure as well as stroke volume and adjusts heart rate and systemic venous reserve volume to keep the monitored variables constant. The model was calibrated using biometric data from human centrifuge simulations of various spaceflight scenarios.

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PP1

Migratory Border Cell Cluster Adaptations to Chemical Gradients in Fruit Fly Egg Chamber

The migration of clustered border cells in recent experiments and modeling shows variable progression. Rotation, pausing, acceleration all are characteristics of wild-type migration. Genetic mutations can further alter any suggestion of a smooth uniform progression. We construct a minimal model for the transmembrane Receptor Tyrosine Kinases RTK as they respond to the chemicals secreted from the oocyte in a reduced geometrical setting to show how recycling of receptors can allow the cluster to adapt to chemical gradients that are sometimes dramatic.

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PP1

The Ecological Stoichiometry of Infection Dynamics in Primary Producers: Implications of a Nitrogen Dependent Host Growth and Immunity Tradeoff

Pathogens rely on their host for reproduction and changes in primary producer nutrition can thus alter their disease dynamics. Pathogens such as viruses, bacteria, and fungi, generally have higher nutritional demands and are stoichiometrically less flexible than primary producers. Increases in nutrient supply may thus more strongly enhance the performance of pathogens relative to their host. The conse-

quences of shifts in nutrient availability for disease dynamics also will depend on changes in host immunity. For example, a growth-defense trade-off may lead to reduced resistance when increased nutrient availability enhances host growth and thus further increases disease prevalence. In contrast, host immunity may also rely on nutrients directly, for example on nitrogen that is used to produce nitrogen-based compounds or build nitrogen-rich enzymatic machinery, which may lead to enhanced host resistance with increasing nitrogen availability. Here, we explored the role of nitrogen availability on infection dynamics of a primary producer host and its pathogen using a stoichiometric, disease model. Specifically, we tested how changes in nitrogen investments in host immune response will alter host biomass build-up and pathogen infection rates.

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PP1

How Excitation and Inhibition Shape Bump Wandering in Neural Fields

Localized regions of persistent cortical neural activity have been repeatedly validated as a neural substrate of parametric working memory. Anatomical evidence suggests these activity bumps can represent the continuous location of a cue location over several seconds. Continuous bump attractor models can represent such activity, linking neural dynamics to behavioral inaccuracies observed in memory recall. Both pyramidal (excitatory) and interneuronal (inhibitory) subpopulations exhibit tuned bumps of activity. However, many models collapse these into a single joint excitatory/inhibitory population, and do not consider the role of spatial cross-population noise. In our study, we separate excitatory/inhibitory neural populations and leverage asymptotic analysis to understand how network architecture and noise correlations shape stochastic bump movement. We observed that features of the inhibitory bump profile affect the stability and diffusion of the excitatory bump. Additionally, correlated noise across the two populations generally decreases diffusion of the bumps. A separate inhibitory population and noise correlations can greatly influence memory of initial conditions in the excitatory subpopulation. Finally, the nonmonotonic trends observed in our results indicate that memory diffusion may be further minimized by tuning parameters of neural architecture or considering a more detailed account of excitatory/inhibitory interactions.

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PP1

A Model for Bleb Expansion Using the Level Set Method

There are two main structures which cells use to migrate, blebs and F-actin driven pseudopods. Blebs are spherical protrusions of the cell memberane driven in-part by intracellular fluid pressure while pseudopods use rapid polymerization of actin to move the membrane forward. Depending on their environment, cells are able to switch between movement with F-actin and blebs . While F-actin driven pseudopods have been well characterized, there are still a lot of open questions about the physical and chemical mechanisms that regulate bleb-driven motility. Of particular interest is the translation of mechanochemical cues into coordinated movement. The focus of our research is to use mathematical modeling and computer simulation to clarify the underlying mechanisms that drive blebbing. In this work, we present preliminary efforts to model the expansion of blebs in confined *Distyostelium discoideum* cells using the level set framework to guide shape changes.

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PP1

Mathematical Model of Cell Migration Through Complex Boundaries and Force Balances

Cell migration is the movement of cells responding to chemical gradients acting as signals. It is integral to daily functions like development and healing; also, progress in studies can lead to findings in cancer metastasis. This research centers on movement of a cluster of migratory cells among nurse cells toward the oocyte in the egg chamber of Drosophila melanogaster. This organism has a well-studied history and many human homologs in genetics. We ask: How to model cell migration through force balances, and what changes to parameters, equations, and geometry are needed? To answer this, we capture heterogeneous cells of the egg chamber: including nurse, epithelial, and migratory border cells using interactions between cell membranes and arising via forces, including adhesive, repulsive, and spring forces. We use a volume force to include heterogeneously sized cells and realistic sizing. When cells fill the chamber, we enact the migratory force, which stems from a chemical gradient signaling, allowing border cells to climb through nurse cells. We solve the force balance equation with a Eulers step to capture progression in time. In MATLAB, we code cell boundaries around cell centers to represent membranes while adapting parameters, equations, and coefficients in order to realistically simulate cell migration. Acknowledgements to NSF-NIGMS (#1953423) for their grant and funding, Dr. Starz-Gaiano, and Simon Ishanathan Guteng Jr for help in initial stages.

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PP1

Assessing the Role of Model Choice in Parameter Identifiability of Cancer Treatment Efficacy

There are currently seven commonly used mathematical models that describe how cancer replicates. Comparison of these model predictions to experimental data has so far failed to determine which model is the most accurate, although it is well-known that the different models can result in vastly different predictions of how the cancer grows. There is growing interest in using mathematical models to help predict the efficacy of chemotherapy, so it is crucial that we understand how the underlying choice of cancer growth model affects estimates of treatment effectiveness. In this study, we generate synthetic treatment data using each of the growth models and fit the data sets using the other growth models to determine the robustness of efficacy parameter estimates. We find that chemotherapy efficacy parameters are fairly insensitive to the choice of cancer growth model, offering hope that mathematical models can be used to help predict chemotherapy outcomes.

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PP1

Variation of Best Fit Distributions in Single Cell Virus Dynamics Models

Mathematical modeling of viral kinetics can be used to gain further insight into the viral replication cycle and virus-host interactions. However, many of the virus dynamics models do not incorporate the cell-to-cell heterogeneity of virus yield or the time-dependent factor of virus replication. A recent study of vesicular stomatitis virus (VSV) kinetics in single BHK cells determined that both virus production rate and yield of virus particles varies widely between individual cells of the same cell population. Here we use the results of the previously mentioned study to determine the distribution that best describes the time course of viral production within the single cells. We determined a list of eight potential distributions that are commonly used in viral kinetics models to fit to each data set by minimizing the sum of squared residuals. The model of best fit for each individual cell was determined using Akaikes Information Criterion (AICC). Results of this study show that the distribution that best describes viral production varies from cell to cell. This finding could have further reaching implications for incorporating time-dependent viral production into a standard model of virus kinetics in order to better reproduce the diversity of viral replication that occurs over time within a population of cells.

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Insulin Action Models Applied to Glycerol and Glucose Yield Different Dynamics in Adolescent Girls with Obesity

In response to a glucose challenge, the pancreas releases insulin which, under healthy conditions, 1) suppresses lipolysis in adipose tissue to decrease glycerol concentration, and 2) regulates glucose concentration through action in muscle and liver. Insulin resistance (IR) occurs when more insulin is required to achieve the same control, and IR may be tissue-specific. Adipose, liver, and muscle tissue exhibit distinct dose-dependent responses to insulin in multiphase hyperinsulinemic-euglycemic (HE) clamps, but the HE clamp protocol does not address potential differences in the dynamics of tissue-specific insulin responses. To investigate metabolic dynamics in adipose tissue, we developed a differential-equations based model that describes the coupled dynamics of glycerol and insulin action during an oral glucose tolerance test in female adolescents with obesity and IR. To quantify the metabolic dynamics in muscle and liver, the oral minimal model was applied to applied to glucose and insulin data collected under the same protocol. We found that the action of insulin on glycerol peaks earlier and more closely resembles the dynamics of plasma insulin compared to insulin action on glucose. These findings suggest that the dynamics of insulin action show tissue-specific differences in our IR population. Improved understanding of the tissue-specific dynamics of insulin action may provide novel insights into the progression of metabolic disease.

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PP1

Speciation and Evolution in MacArthur Type Population Models

In classic MacArthur models, the number of consumers and resources is fixed from the onset. However, nature itself is never this static, and in real-life experiments, consumers (e.g. bacteria) can quickly acquire adaptations to increase their consumption. In this project, we set certain parameters of the model free by adding new species that are a

small perturbation of their ancestors, mimicking evolution. In such an approach, individual species become less interesting and we need to study the long time average dynamics to understand how the modelled ecosystem behaves. The goal is to find interesting, or the 'right', measures to quantify the average dynamics, allowing us to draw conclusions on the structure of the ecosystem and make comparisons with experiments possible.

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PP1

Infrared Detection of Cancer Mirna

The occurrence and mortality of cancer around the world is growing and will continue to grow. Most common cancer treatment approaches include surgery, radiation, and chemotherapy, all of which work best when the cancer is detected early. Developing systems of early detection of cancer will help to mitigate the negative aspects of cancer treatment since cancer found at an early stage, when it is small and before it has spread to other parts of the body. Cancer cells are known to release little pieces of RNA, known as miRNA, that circulate throughout the body, particularly in the bloodstream. Nanoparticles can be designed to bind to select miRNA. Upon binding, the emission spectrum of the nanoparticle shifts, particularly in the infrared. Infrared light passes quite easily through many tissues, so this system could allow for non-invasive detection of circulating cancer miRNA and potentially improve early diagnosis potential for cancer. The purpose of this research is to use mathematical analysis and computer simulation of mathematical models to study the efficacy of this type of detection system and what parameters make it viable for cancer detection.

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PP1

Discovering the Inherent Dynamics of Biological Systems via an Artificial Neural Network

Once we design a mathematical system that could explain our biological phenomena, it still requires additional work such as determining system parameters or nonhomogeneous terms, called system variables. This study provides a method for estimating system variables using deep neural networks equipped with mathematical theories. We also present our results using simulation and experimental data.

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PP1

A Mathematical Model of the Transient Receptor Potential Ion Channel in Urinary Bladder Smooth Muscle

Enhanced spontaneous contraction of the urinary bladder smooth muscle (UBSM) is associated with overactive bladder (OAB), a pathophysiological syndrome that affects millions of individuals. The anticholinergic drug "Oxybutynin", used for OAB, causes several side effects such as dry mouth, complications in visual functions and constipation. Therefore, the current research is focused to identify alternative pathways with the potential to reduce DSM contractility for the treatment of OAB. Recently, transient receptor potential melastatin-4 (TRPM4) channels have been identified in regulating DSM cell excitability which is the aim of this study. We have used a mathematical model to describe the AP to help us understand the role of ion channels. In this model, the TRPM4 channel current (Itrp) is computed upon the steady-state values of the activation and inactivation parameters. All ionic conductance were tuned to set the resting membrane potential (RMP) at - 50 mV and maximum conductance was set to 0.00001 mho/cm2. As the value of maximum conductance is increased, the DSM cell model generates AP with the higher RMP value. After increasing the maximum conductance to 0.0001 mho/cm2, the simulated AP showed a more depolarized RMP value. This simulation showed that the activation of more TRPM channels will cause OAB by increasing the excitability of DSM cells. Hence, TRPM4 channel blocker 9-phenanthrol may play a novel approach for the treatment of bladder overactivity.

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PP1

A Mathematical Model for Skeletal Muscle Using MRI Data

Skeletal muscle is a complex and heterogeneous biological material that is important for both movement and structure. A unique aspect of muscle is its ability to activate and produce force. Many properties of muscle can influence the amount of force produced during activation, including muscle composition and volume. Muscle consists of muscle fibers embedded in a matrix of collagen fibers, and this structure can be substantially influenced by muscular diseases. For instance, cerebral palsy (CP) is a disorder resulting from an upper motor neuron lesion in the brain and can affect muscle in several ways, such as altering the microstructural properties, increasing fat infiltration, and changing the whole muscle architecture. In this work, we develop a mathematical model for skeletal muscle that can capture the influence of CP on the mechanics of skeletal muscle. We capture the muscle mechanics using a finite-strain nonlinearly elastic continuum model of a fiber reinforced composite with the activation in the along-fiber direction. To include the effects of CP into the model, we utilize experimental data obtained with MRI. The experimental data gives realistic muscle geometries to understand the effects of CP on the muscle architecture, as well as information about the material composition including the volume fraction of fat. This study combines mathematical, clinical, and experimental work to produce a comprehensive model to better understand how CP influences muscle

mechanics.

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PP1

Odor-Evoked Increases in Olfactory Bulb Mitral Cell Spiking Variability

At the onset of sensory stimulation, the variability and co-variability of spiking activity is widely reported to decrease, especially in cortex. Considering the potential benefits of such decreased variability for coding, it has been suggested that this could be a general principle governing all sensory systems. Here we show that this is not so. We recorded mitral cells in olfactory bulb (OB) of rats and found increased variability and co-variability of spiking at the onset of olfactory stimulation. Using models and analysis, we predicted that these increases arise due to network interactions within OB, without increasing variability of input from the nose. We tested and confirmed this prediction in awake animals with direct optogenetic stimulation of OB to circumvent the pathway through the nose. Our results establish increases in spiking variability at stimulus onset as a viable alternative coding strategy to the more commonly observed decreases in variability in many cortical systems.

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PP1

Modeling Enzyme Kinetics in the Presence of Lipid

Blood coagulation is a network of biochemical reactions whereby dozens of proteins act collectively to initiate a rapid clotting response. Coagulation reactions are lipid-surface dependent, and this dependence is thought to help localize coagulation to the site of injury and enhance the association between reactants. Current models of coagulation fail to agree with laboratory studies under variations in lipid concentrations. Models overestimate conversion efficiencies of critical coagulation proteins and fail to capture spatial limitations of lipid surfaces. We developed a mathematical model of lipid-mediated enzyme reactions where the association rate between lipid-bound reactants is modified by an interaction probability (IP). The IP is derived by considering the fraction of the lipid surface that is occupied by any lipid-bound species, and accounts for surface crowding. We performed constrained optimization to estimate a set of intrinsic rates for the enzyme-substrate pair. Preliminary results agree with experiments and reveal a critical lipid concentration where the conversion rate of the coagulation protein is maximized, inferring that the model can describe the dilution effect where, as lipid is increased, proteins are physically separated, and reaction rates decrease. Further refinements of the model, including product inhibition due to experimental design, are also incorporated to better understand the impacts of the dilution effect in more complex reaction networks.

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PP1

The Nature of Correlated Variability in Segregated Cortical Excitatory Subnetworks

Understanding the basis of shared, across trial fluctuations in neural activity in mammalian cortex is critical to uncovering the nature of information processing in the brain. This correlated variability has often been related to the structure of cortical connectivity since variability not accounted for by signal changes likely arises from local circuit inputs. Recordings from segregated networks of (excitatory) pyramidal neurons in mouse primary visual cortex reveal that across-network noise correlations are larger than predicted given the weak cross-network connection probability. We aim to uncover the circuit mechanisms responsible for these enhanced correlations through biologically-motivated cortical network models. In particular, we use a Wilson-Cowan-type firing rate model with weakly connected subpopulations to study the impact of cross-population connection strength on cross-population interactions. Preliminary findings suggest that scaling excitatory connections scales correlations proportionally, but that inhibition may play a key role in shaping the enhanced correlations observed in the absence of strong excitatory-excitatory subnetwork connectivity. We are working to extend this rate-based approach to a more realistic spiking neuronal network with clustered excitatory subpopulations with weak cross-cluster connection probability.

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PP1

Activity Patterns of a Two-Timescale Neuronal Ring Model with Voltage-Dependent, Piecewise Smooth Inhibitory Coupling

We present an analysis of activity patterns in a neuronal network that consists of three mutually inhibitory neurons with voltage-sensitive piecewise smooth coupling. One of the observed propagating solutions appears to be contrary to the network architecture and is characterized by a sudden turn-around of trajectories during fast transitions between quasi-stable states. Standard fast-slow analysis fails to describe the mechanism underlying this activity pattern due to the voltage-sensitive nature of the coupling. We exploit the piecewise smooth nature of the coupling and consider a sequence of fast subsystems defined in a piecewise way. Our analysis shows that there are three possible scenarios during fast jumps, which may depend on both the fast dynamics and the slow dynamics. First, the fast dynamics may succeed to equilibrate at (or near) a critical manifold, after which the slow dynamics relaxes to its own fixed point. Second, while the fast dynamics tries to equilibrate to a critical manifold, the slow dynamics may push the fast system through a bifurcation, which forces a second fast jump to a new critical manifold. Third, the presumed critical manifold may be lost prior to fast subsystem equilibration, through effects that may relate to either the slow dynamics or the fast dynamics, in which case the fast dynamics is forced to approach a new critical manifold directly. In the second and third cases, we observe the sudden turn-around during fast jumps.

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PP1

Mixed Mode Oscillations in a Three-Timescale Coupled Morris-Lecar System

Mixed mode oscillations (MMOs) are complex oscillatory behaviors of multiple-timescale dynamical systems in which there is an alternation of large-amplitude and small-amplitude oscillations. It is well known that MMOs in two-timescale systems arise either from a canard mechanism associated with a folded node singularity or a delayed Andronov-Hopf bifurcation (DHB) of the fast subsystem. While MMOs in two-timescale systems have been extensively studied, less is known regarding MMOs emerging in three-timescale systems. In this work, we examine the mechanisms of MMOs in a coupled Morris-Lecar model neurons with three timescales. Define the critical manifold M_s as the set of equilibria of the fast subsystem consisting of equations for fast variables. The reduced problem on M_s is itself a slow-superslow system exhibiting its own critical manifold M_{ss}. We show that when the upper fold surface L_s of M_s intersects M_{ss}, the canard and DHB mechanisms can coexist and interact to produce a type of MMOs that exhibits properties of both mechanisms and is robust to changes of parameters that control timescales. Decreasing the strength of the coupling from one neuron to another neuron can shift the upper L_s and M_{ss} so they no longer intersect. As a result, there is only one mechanism contributing to MMOs and the resulting MMOs appear to be less robust than MMOs arising in the first scenario.

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PP1

Fine Temporal Patterning of Gamma Oscillations Synchronization

Synchronization of neural activity in the gamma frequency band is associated with various cognitive phenomena. Abnormalities of gamma synchronization may underlie symptoms of several disorders. Properties of oscillations are known to depend on the synaptic properties of circuits expressing this activity. This study explores how synaptic properties affect the fine temporal patterning of neural synchrony. If two signals show only moderate synchrony strength, it may be possible to consider these dynamics as moving in between synchronized and desynchronized states. We use connected networks expressing pyramidal-interneuronal gamma (PING) to explore the temporal patterning of synchronized and desynchronized intervals. Synaptic strength changes may alter the temporal patterning of synchronized dynamics even if the average synchrony strength is not changed. Larger values of both excitatory and inhibitory synapses between excitatory and inhibitory neurons tend to promote short desynchronizations; stronger synapses between inhibitory interneurons tend to promote longer desynchronizations. Furthermore, circuits with different patterning of synchronization in time may have different sensitivity to synaptic input. Thus, the alterations of synaptic strength may mediate physiological properties of neural circuits not only via change in the average synchrony level of gamma oscillations, but also via change in how synchrony is patterned in time over very short time scales.

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PP1

Modelling the Steady Flow-Wave Transition in Contractile Actomyosin Networks

Cytoskeletal contraction is central for cell motility, divi-

sion, and intracellular transport. This contraction is generated by myosin in dynamically cross-linked viscoelastic actin networks. Experiments of our collaborators show that cell extracts encapsulated in water-in-oil droplets self-organize to form actomyosin networks that contract and flow for hours. In small droplets, these systems exhibit a dynamic steady-state characterized by radially symmetric inward flow. As the droplet size increases, the networks transition to a state of contractile waves or spirals. Motivated by these experiments, we developed a model of the actomyosin network as a compressible, viscous fluid governed by reaction-transport and force balance equations; the latter is nontrivial as this is an active fluid with density-dependent stresses. Analysis and numerical simulation demonstrate that our model successfully reproduces key experimental results. We capture the size-dependent transition from continuous contraction to waves and how this transition depends on contraction rate. Our model also predicts waves with periods which are roughly size-independent. These results shed light on the mechanics of cell waves and contractions.

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PP1

Epidemic Conditions with Temporary Link Deactivation on a Network SIR Disease Model

The spread of an infectious disease depends on intrinsic properties of the disease as well as the connectivity and actions of the population. This study investigates the dynamics of an SIR type model which accounts for human tendency to avoid infection while also maintaining preexisting, interpersonal relationships. Specifically, we use a network model in which individuals probabilistically deactivate connections to infected individuals and later reconnect to the same individuals upon recovery. To analyze this network model, a mean field approximation consisting of a system of fourteen ordinary differential equations for the number of nodes and edges is developed. This system of equations is closed using a moment closure approximation for the number of triple links. By analyzing the differential equations, it is shown that, in addition to force of infection and recovery rate, the probability of deactivating edges and the average node degree of the underlying network determine if an epidemic occurs.

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PP1

Mathematical Optimization in Bioimpedance Spectroscopy

Bioimpedance spectroscopy uses the frequency-dependent resistance presented by a biological system to an induced sinusoidal current. Its applications include the analysis of electrochemical biosensors and physiological variables of plants (many of which are relevant to agriculture) and animals (e.g. biomedical). Equivalent circuit models (ECM) are a long-standing standard tool in bioimpedance spectroscopy. They are effective in modern large-scale or small-scale (in-field or point-of-care) settings where computational resources are limited. ECMs are also efficient feature extractors for regression models. This presentation concerns two optimization problems relating to ECM: i) Fitting the circuit parameters to a system's impedance spectrum. The choice of the cost function is important here, as disregarding frequency information by simply using the mean squared error causes the introduction of undesired implicit weighing effects. As for the optimization algorithm itself, we present alternatives to the slow and initial-value-dependent complex non-linear least squares. ii) Identifying an appropriate equivalent electrical circuit topology for a given electrochemical system using state-of-the-art evolutionary algorithms, in addition to the incorporation of domain knowledge to ensure adequate interpretability. We take several precautions (specific to bioimpedance spectroscopy) to provide the least complex circuit model capable of generating a given measurement data set.

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PP1

Multicellular Modeling of mRNA Vaccine-Loaded Lipid Nanoparticles for Cancer Immunotherapy

The interactions between biological systems and engineered nanomaterials has become an important area of study due to recent applications of nanomaterials in medical applications. Mathematical modeling of nanoparticles (NPs) for cancer treatment can be used to explore NP, cell, tissue, and anti-cancer agent response parameters for a growing tumor, allowing for designers to see the impact of their design choices. In this work, we propose an agent-based model (with *PhysiCell*. Ghaffarizadeh et al. (2018). DOI: 10.1371/journal.pcbi.1005991) of mRNA vaccine-loaded lipid nanoparticles (LNPs) for cancer immunotherapy. The model is extended by a cancer nanotherapy model (https://nanohub.org/resources/pc4nanobio) and multiscale model of SARS-CoV-2 (https://doi.org/10.1101/2020.04.02.019075). The nano-immunotherapy model is used to perform explorations of activation and immune response through exploring tumor cell growth, LNP-dendritic cell interactions (LNP bind-

ing dynamics, intracellular mRNA message translation dynamics), activation of immune systems (recruitment of CD8+, CD4+ T cells and antibody), and interactions between CD8+ T cells, antibody, and tumor cells. The model of this work can be run on a cloud-hosted platform at: https://nanohub.org/resources/mrnatumor.

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PP1

Optimization of Dosing Strategy to Induce Anovulation

Despite the many benefits of hormonal contraceptives composed of exogenous estrogen and/or progesterone, some go beyond contraception, adverse side effects with high doses such as thrombosis and myocardial infarction, cause hesitation to usage. This work considers a menstrual cycle model that can predict the mean daily levels of pituitary and ovarian hormones throughout a normal menstrual cycle. Our modeling framework utilizes optimal control theory to determine minimum total exogenous hormone dose, and timing of administration that lead to contraception. Simulation results show a reduction in dosage of about 92% in estrogen monotherapy and 43% in progesterone monotherapy. In addition, combination therapy significantly lower doses further. These results may give clinicians insights into optimal dosing scheme for contraception.

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IP1

Opening Remarks and Presentation: A Surrogate-based Strategy for Analyzing Post-fire Debris Flow Hazards

Wildfire is a catalyst for landcover change that can substantially increase the potential for devastating and destructive debris flow hazards. Debris flows, or fast-moving landslides that consist of a mixture of water, mud, and rock, initiate after fires when surface water runoff rapidly erodes sediment on steep slopes. Numerical models of post-fire debris flow bulking and runout are computationally intensive. These models depend on poorly constrained and difficult to measure parameters related to fire-altered soil and vegetation, some of which change in time. Further, the development of debris flows (as opposed to clear flows) also depends on the rainfall intensity of potential storms. To date, modeling-based hazard analysis has focused on if" a debris flow might be triggered on a given fire scared hillside, and not on the extent or footprint of potential debris flow runouts. We employ Gaussian process emulators to high-dimensional debris flow model output to quantify uncertainties and aid in model-based hazard assessments of post-fire debris flow inundation.

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IP2

Climate Modeling in the Age of Machine Learning

Climate simulations remain our best tools to understand and predict global and regional climate change. Climate projection uncertainty stem, in part, from the poor or lacking representation of processes, such as ocean turbulence and mixing which impact the uptake and transport of heat and carbon. The representation of these unresolved processes has been one of the bottlenecks in improving climate projections. The explosion of climate data and the power of machine learning algorithms are suddenly offering new opportunities. Can data-driven machine learning methods help us deepen our understanding of these unresolved processes and simultaneously improve their representation in climate models to reduce climate projections uncertainty? In this talk, I will present some of our recent work in which we leverage tools from machine learning to learn representations (or closures) of unresolved ocean processes, and subsequently implement these closures into ocean models. I will contrast equation-discovery and convolutional neural network approaches and discuss advantages and pitfalls of both. Our work suggests that machine learning could open the door to discovering new physics from data and enhance climate predictions. Yet, many questions remain unanswered, making the next decade exciting and challenging for hybrid climate modeling.

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IP3

Viability Theory for Computing Tradeoffs in Sustainability Issues

From the conceptualization of sustainable development, many quantitative methods, metrics, and criteria have been proposed and discussed to operationalize sustainability. For example, the discounted utility approach is criticized because this criterion neglects long-run utility, entailing unsustainable trajectories. In that regard, the account for biological, ecological, or social constraints to fulfill throughout time emerges as a crucial issue. Nevertheless, multiple constraints may be incompatible, so tradeoffs in what constitutes sustainability must be made. Accounting for the tradeoffs between multiple objectives or constraints is also relevant in epidemics control, where epidemiological and budgetary constraints must be compatibilized. From an intergenerational equity perspective, if the constraints induced by reference points, thresholds, or tipping points must be satisfied over time, such problems related to sustainability can be formulated into the mathematical framework of viability theory. In this talk, I will present a general framework for introducing how the viability theory can study this kind of problem. In particular, I will introduce the set of sustainable thresholds, a concept created to visualize tradeoffs between constraints in a given system. Along with showing the latest results associated with this concept, I will present some examples of applications related to fishery management and epidemics control.

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IP4

Data Driven Stochastic Models of Geophysical Flows

In this seminar, we will describe the application of a range of data driven approaches to modelling geophysical flows. Starting with the multivariate stochastic models first developed by Hasselmann, then moving beyond assumptions of statistical stationarity to develop more general regularised approaches incorporating optimization and numerical methods from applied mathematics. These new methods have been developed to generate data driven stochastic models whose parameters are time dependent, thereby allowing for the identification of evolving metastable states in nonstationary flows and the exogenous drivers of these coherent states and their underlying dynamics. Applying concepts from dynamical systems, such as hyperbolicity and local attractor dimension, these reduced order stochastic models are shown to provide a theoretical basis for the specification of forecast covariances and selection of initial forecast perturbations in operational weather prediction. Lastly, we consider machine learning classification problems in the small data regime i.e., when the size of the data statistic is relatively small with respect to the feature space dimension. Where standard methods tend to show a lack of robustness such that the overfitting bound is rapidly reached and predictions are poor with respect to validation data, we describe recent work to overcome these limitations in application to climate prediction.

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SP1

Closing Remarks and SIAM Activity Group on Mathematics of Planet Earth Prize Lecture: Mathematics for the Climate Crisis

Modern ideas coming from dynamical systems theory and statistical mechanics allow for a much-improved under-

standing of the relationship between climate variability and climate response to to forcings. This is also leading to the possibility of finding a synthesis between Hasselmann and Lorenzs visions of climate, the first based on stochasticity, the latter rooted in deterministic chaos. I will describe how the Ruelle response theory can be used to perform climate projections on a hierarchy of models, ranging from low dimensional to state-of-the-art Earth system models. I will then associate the divergence of the response operators with the proximity to tipping points. Finally, I will discuss the global stability properties of the climate, focusing on the dichotomy between the co-existing warm and snowball states, which has had a key importance for the development of life. When stochastic forcing is included, one observes transitions between the competing basins of attraction. For weak Gaussian noise laws, large deviation laws define the invariant measure, the statistics of escape times, and typical escape paths called instantons. The Melancholia state, the chaotic saddle embedded in the boundary between the basins of attraction, is the gateway for noise-induced transitions. The metastability can be understood in terms of an energy-like landscape with valleys and mountain ridges defined by the Graham's quasipotential.

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JP1

Joint Plenary Speaker with the 2022 SIAM Annual Meeting (AN22): How Machine Learning can Improve Projections of Future Climate

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CP1

Multirate Partitioned Runge-Kutta Methods for Coupled Compressible Navier-Stokes Equations

The Earth system model is a complex integrated model of atmosphere, ocean, sea-ice, and land surface. Coupling the components can be a significant challenge due to the difference in physics, temporal and spatial scales. This study concerns new coupling strategies for the fluid-fluid interaction problem based on multirate partitioned Runge-Kutta methods. We consider a coupled compressible NavierStokes equations with gravity. We assume that the interface is rigid-lid, where no mass flux is allowed, but horizontal momentum and heat flux are exchanged. We numerically observe that multirate partitioned Runge-Kutta coupling schemes 1) conserve total mass; 2) have the second-order accuracy in time; and 3) provide favorable strong and weak scaling behaviors in modern computing architectures. We also show the speedup factors of multirate partitioned Runge-Kutta methods over their base (single rate) method.

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CP1

A Minimal SDE Model of D-O Events with Multiplicative Noise

The abrupt transitions in the last glacial period between cold stadial and warmer interstadial climate states found in Greenlandic ice-core records, known as Dansgaard-Oeschger (D-O) events, are a rich topic of study not only due to their potential similarities in time scales to present and near-future climate transitions but also since their underlying physical mechanisms are not fully understood. The dynamics of the climate can be described by a Langevin equation $dx = -\frac{\partial U}{\partial x}dt + \eta(t)$ where the potential $U(x)$ has a bimodal distribution to represent the stable stadial and interstadial states and the stochastic process $\eta(t)$ is usually realized as a Gaussian white noise process that causes jumps between these two states. From the steady-state of the Fokker-Planck equation associated with this Langevin equation, the potential $U(x)$ can be determined from the probability distribution of the ice-core record time series. Thus this minimal model simulates time series with statistics similar to those of the original ice-core record. Novel to this study, we introduce a multiplicative noise term $\eta(t, x)$ to represent the different statistical properties of the noise in the stadial and interstadial periods. The discrepancy between the Itô and the Stratonovich integration of the Langevin equation results in differences in the attribution of the drift and diffusion terms for a transformed variable. This is illustrated by performing both.

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CP1

Using Bayesian Methods for Parameter Estimation and Uncertainty Quantification of Cloud Microphysics Schemes

The Bayesian Observationally Constrained Statistical-Physical Scheme (BOSS) project uses Bayesian inference to tune parameterizations of cloud microphysical processes using simple functional forms, and to quantify the uncertainty in the resulting parameter values. This application has a number of features that make the use of Bayesian methods challenging: (1) Most microphysical process rates are not directly observable, so microphysics parameterizations can only be constrained by either incorporating them into a time-evolving "host" model to translate process rates into observable effects, or by comparing their rates to those of a reference model acting as a proxy for real-world observations. (2) We do not know the true (or even "true-ish") functional form for most process rates, so no single tuning will be optimal or near-optimal in all regimes. (3) Different reference microphysical models strongly disagree

in most cloud regimes. (4) Even when comparing to the same reference model, the optimal set of parameters may be very different depending on whether scheme tuning is performed based on instantaneous process rates or time-evolving model outputs. We present the methodologies used to navigate these challenges involving imperfect models and incomplete data in the BOSS project. We summarize how our evaluation of BOSS schemes can inform future parameterization development in weather and climate models, for microphysics as well as other model physics parameterizations.

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CP1

Reducing Co_2 Emissions for Aircraft Flights Through Complex Wind Fields Using Dynamic Programming

During last years UN Climate Change Conference the international aviation community agreed to advance actions to reduce CO_2 emissions. Adopting more fuel efficient routes will achieve this quickly and economically, with the largest reductions possible on long haul flights. In this talk, dynamic programming is used to find time and fuel-optimal routes across the North Atlantic. The method relies on solving an associated HamiltonJacobiBellman equation providing optimal feedback controls for the route planning problem, from whence globally optimal trajectories are retrieved. For this, a time-optimal control formulation penalizing fuel burn subject to arrival constraints is developed. This formulation includes an aerodynamic fuel-burn model and a data-driven background wind field. The control variables are expressed as a set of position-dependent aircraft headings, true airspeeds and pitch angles. Fuel consumption is modelled with a new physics-driven fuel burn function, which is aircraft model specific. The performance index is based on both fuel use and flight time. Cruise phase flights between London Heathrow Airport and JFK Airport in New York are simulated across wind fields taken from re-analysis data from 1st December, 2019 to 29th February, 2020. The fuel use from these is compared to actual data recorded by flights on these days and reduction in fuel and thus CO_2 is calculated.

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CP2

Earthquake Forecasting from the Elementary Catastrophes Theory

Based on some ideas developed by the authors in recent years, a new method for earthquake forecasting is envisioned. The foremost role in the proposed methodology is played by the Elementary Catastrophes Theory applied to a relevant seismograms analysis. A series of fold catastrophes are traced using the tangents slopes to the null points of the seismograms and analyzed its increments inside appropriate sectors of the p waves reconstructed by the three signals of a standardly oriented seismograph. The data acquisition and processing period are assumed to include a time-lapse starting several hours (even days) before the main earthquake until the appearance of its first peak. Since the earthquakes are (quasi) periodic phenomena it is expected, immediately before their main peaks, that there will be detection of certain regularities in the behavior of the afore mentioned slopes, which are exactly the "fold" catastrophe's critical values. Application of heuristics programming is considered in order to search for said regularities. There is a real possibility of relating this type of attempt to the efforts carried out by the Earthquakes Early Warning Systems researching groups because the use of the Elementary Catastrophe Theory will provide essentially complementary information, not taken into account until now.

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CP2

Long-Range Dependence in Low-Frequency Earthquake Catalogs

Low-frequency earthquakes (LFEs) are small magnitude (less than 2) earthquakes, with reduced amplitudes at frequencies greater than 10 Hz relative to ordinary small earthquakes. They are usually grouped into families of events, with all the earthquakes of a given family originating from the same spot at a few dozens km depth. They tend to occur in bursts, that is dozens of earthquakes are detected within a few hours or days, followed by weeks or months of quiet, with just a few earthquakes occurring. Long-range dependence is a phenomenon that may arise in the statistical analysis of time series data. It relates to the slow rate of decay of the statistical dependence between two points with increasing time interval between the points. In this study, I look for evidence of long-range dependence in low-frequency earthquake catalogs. For each family of events, the dataset contains the timing of each earthquake associated with this family. I thus translate the list of earthquake occurrence times into a discrete time series defined by the number of earthquakes per unit of time. I then use graphical methods to compute either the Hurst parameter H or the fractional differencing parameter d associated with each time series. For most families of the catalogs studied, I find that 0 ¡ d ¡ 0.5, which is characteristic of long-range dependence in the time series. The statistical characterization of LFE occurrence could provide important constraints on future mechanical models of

LFEs.

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CP2

Direct Seismic Inversion of Das and Geophone Data Using Energy Fluxes, Virial Theorem and Deep Learning

Spacing between conventionally placed geophones does not allow to fully sample the seismic wavefield and exploit all its features for high-resolution analysis of elastic subsurface properties. Fiber optic distributed acoustic sensing (DAS) technologies have progressed rapidly and emerged in vertical seismic profiling (VSP). DAS channels represent densely sampled linear sensors recording average strain induced upon the fiber cable by the seismic wavefield. High density of DAS channels allows for a new method of inversion directly at the location of the sensors. Elastic subsurface parameters can then be reconstructed and monitored at much higher resolution than in conventional VSP. We discuss key steps of the new method below. New energy-driven DAS inversion method links geophone measurements are to potential and kinetic energy, respectively. Classic virial theorem applied in the context of continuous elastic media links these energies averaged over time leading to a new method for P-wave velocity estimation. Then using energy balancing along the well we invert density and velocity simultaneously. The energy-driven inversion of DAS data in a blind synthetic test and a field VSP example. Finally, velocity and density estimates are enhanced using a probabilistic deep learning framework. The new methodology delivers much higher resolution and accuracy than conventional zero-offset VSP processing workflow.

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CP3

Predicting Ensemble Simulations of Geophysical Models Using Reservoir Computing

In this talk, we analyze the performance of reservoir computing in predicting trajectories of chaotic prototype systems mimicking the long-term climate simulations. In particular, we analyze how including memory and/or removing the seasonal fluctuations affect the performance of the predictions. We illustrate the performance of reservoir computing with respect to ensemble simulations as well.

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CP3

A Multi-Model Ensemble Kalman Filter for Data Assimilation and Forecasting

Data assimilation (DA) aims to optimally combine model forecasts and noisy observations. Multi-model DA generalizes the variational or Bayesian formulation of the Kalman filter, and we prove here that it is also the minimum variance linear unbiased estimator. However, previous implementations of this approach have not estimated the model error, and have therewith not been able to correctly weight the separate models and the observations. Here, we show how multiple models can be combined for both forecasting and DA by using an ensemble Kalman filter with adaptive model error estimation. This methodology is applied to the Lorenz96 model, and it results in significant error reductions compared to the best model and to an unweighted multi-model ensemble. We discuss applications to hybrid prediction using dynamical and machine learning forecasts.

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CP3

Evaluating Simulated Vegetation Status of Earth System Models Using Satellite Climate Data Records

The change of the Earth system is assessed with a suite of models developed by international agencies to understand climate trends and plan for mitigation actions. There is a need to assess the quality of vegetation status simulated by these Earth system models to ensure global carbon flux is accurately estimated. Leaf Area Index (LAI), the one-sided green leaf area per unit ground surface area, is a key variable characterizing vegetation status and has strong impacts on multiscale biogeochemical and biogeophysical interactions. Comparisons of the simulated historical LAI provided by the latest Coupled Model Intercomparison Project (CMIP6) to satellite-based observations were made with monthly data for the period 1981-2014 at three spatial resolutions: 1, 2.5, and 5 degree. A total of 49 CMIP6 models were evaluated individually and as ensembles when multiple realizations were available. Two long-term global satellite time series, NOAAs LAI Climate Data Record and Global Inventory Modeling and Mapping Studies (GIMMS) LAI3g, were used for benchmarking model accuracy. Basic comparison metrics of root mean squared error (RMSE), mean bias error (MBE), and R-squared were evaluated in addition to careful examinations of density distributions, seasonal patterns, and geospatial patterns of differences. This comprehensive analysis serves the larger Earth system modeling community by identifying where improvements to the simulations of terrestrial

components are needed.

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CP4

Green Security Games for Natural Reserves in Ecuador

Recently computer scientists have made important contributions assisting wildlife conservation. A key example is the design of patrolling agendas in protected areas aimed to maximize the frequency with which rangers thwart environmental crimes. The vast majority of these Green Security Games has focused on the open spaces of the African Savanna and it is not readily adapted to the reality of South American parks where, due to the density of vegetation and the ruggedness of the terrain, traveling (by both rangers and poachers) is done only over the collection of available trails (a graph). In this talk we will present the early results of our project, aiming to develop a theory of green security games on graphs. The games we consider take place in the trail map of the reserve and the objective of the ranger is to choose the most convenient circuit-like path starting and ending at the unique point on the map at which she resides. In the talk we will present two results: (1) We prove that the construction of Stackelberg equilibria (optimal strategies for the ranger, taking into account the informational advantage of poachers) can be formulated as a mixed integer quadratic problem on the circuit polytope of the graph of trails and (2) We provide Computational demonstrations showing that this approach can be scaled so as to be of practical interest, allowing us to construct optimal patrolling agendas for the Jamacoaque reserve in Ecuador, using real poaching data.

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CP4

A New Framework for Harnessing Reactivity

As a system that supports life, it is important that our planet and its subsystems maintain healthy regimes not just at dynamic attractors but also during transient excursions. In particular, even the existence of a global asymptotic attractor within a desirable regime does not ensure the transient health of the system; disturbances to the system may be amplified to an unhealthy state before returning to the attractor. This is not due only to nonlinearities. We can study amplification in the linearization through the lens of reactivity: the maximum instantaneous rate of radial amplification. In this talk, we present a new framework for analyzing the radial and tangential dynamics of two-dimensional linear systems that uncovers a dual relationship between reactivity and eigenvectors. This leads to easily-calculated conjugate matrices that - unlike the diagonalization - make the reactivity explicit. We illustrate how these results provide insights into how reactivity in the linearization can accumulate to magnify disturbances and contribute to excursions from an attractor.

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CP4

Preferred Timescales for Phase Tipping in Predator-Prey Systems

Cyclic predator-prey dynamics can react sensitively to changing environmental conditions, even collapsing to extinction given a well-timed perturbation—a phenomenon known as phase tipping. In phase-tipping, a transition from a limit cycle to a stably coexisting steady state happens without any bifurcations associated with the parameter jumps modeling environmental change. We probe how timescales of the problem impact the frequency of the rare extinction events, and identify certain timescale separations required for phase tipping. For instantaneous environmental changes, with timing drawn from an exponential distribution, we find that phase tipping occurs most readily when the frequency of changes is on an intermediate timescale compared to inherent system timescales. When environmental changes are not instantaneous, but instead take place over some interval of time, we find that the dangerous phases for tipping events may shift and that there is a well-defined cut-off for how slow the environment may change and still be at risk for phase-tipping. Our work highlights the important role of timescales for environmental shifts in determining whether there are risk-of-extinction phases in the oscillatory population dynamics. We also introduce an example of phase tipping in a fishery model, where harvesting events take the place of environmental shifts.

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CP4

Understanding Mass Extinction Events: Can Mathematics Help?

Climate change may have an adverse impact on the biosphere resulting in species mass extinction and considerable biodiversity loss worldwide. Species are going extinct all the time at a certain baseline rate, but there have been several events in the past when the extinction rates increased by more than two orders of magnitude. Mathematical models may provide tools to connect ecosystem-scale processes to global-scale processes. However, due to the complexity of the processes, we need to make a difficult choice of what methods of mathematical modeling will be suitable to crack a problem. In this talk, we would like to discuss the advantage of integrating mathematical models with standard geological, geochemical, and ecological methods towards better utilization of these methods in mass extinction studies.

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CP5

Ecological Dynamics on Large Metapopulation Graphs

In this presentation, we discuss reaction-diffusion models for predator-prey dynamics in patch-structured populations with between-patch dispersal on large graphs. We aim to unify two classical approaches for studying spatial dynamics in ecological systems: spatially-continuous models where dispersal typically follows a local diffusion operator and spatially-discrete patch models with more general network connectivity between the patches. Making use of the recently-developed formalism of graph limits, or graphons, we derive a continuum analogue of patch reaction-diffusion models which can describe the role of dispersal in the presence of non-local connectivity schemes like small-world or power law networks. A useful feature of these continuum limits is that one can find threshold quantities for the onset of pattern formation in predator-prey models and for persistence of a disease outbreak in terms of the non-local dispersal kernel, and therefore the qualitative behavior of these metapopulation dynamics is intricately linked to the topology of the dispersal network. We will place particular emphasis on the nonlinear stability of patterned states and regimes in which patterned steady states can coexist bistably with spatially uniform states.

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CP5

Mathematical Modeling and Analysis of Wind Turbine Dynamics and Control: Recent Results

Mathematical modeling and analysis of how wind turbines work in terms of dynamics and control, among many renewable energies, have given interesting new insights and information that should help developing the efficient implementation and utilization of wind energy. We present a state of the art mathematical model that has been cited in the news recently and verified vs. real measured data. We also provide some important information this modeling work is providing in terms of possible solution-solving to existing challenges facing stable, efficient and better-managed connection between the wind farms and the power grid.

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CP5

Criteria to Assess Reliability of Divergence Estimates from Drifter Triplets

Measuring velocity gradients of a flow field is challenging. In the ocean, such measurements are generally either subject to stationarity assumptions or restricted to small areas where moored instruments can be maintained. Dense drifter deployments offer another option. E.g., the change in the area defined by the convex hull of a triplet of drifters provides an estimate of the divergence averaged over that area and the elapsed time. Unfortunately, this computation can be subject to large errors, especially when the triangle shape is far from equilateral. Here we explore what characteristics of the triangle shape can be used to remove estimates that are likely to be erroneous while retaining good estimates as much as possible. The primary tool is a very-high-resolution regional ocean model simulation, where it is possible to compute a baseline divergence field and therefore actual errors. We also discuss the impact of removing estimates from the sample on the distribution of divergence estimates.

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CP5

Stochastic Models of Infectious Diseases in a Periodic Environment with Application to Cholera Epidemics

Seasonal variation affects the dynamics of many infectious diseases including influenza, cholera and malaria. The time when infectious individuals are first introduced into a population is crucial in predicting whether a major disease outbreak occurs. In this investigation, we apply a time-nonhomogeneous stochastic process for a cholera epidemic with seasonal periodicity and a multitype branching process approximation to obtain an analytical estimate for the probability of an outbreak. In particular, an analytic estimate of the probability of disease extinction is shown to satisfy a system of ordinary differential equations which follows from the backward Kolmogorov differential equation.

An explicit expression for the mean (resp. variance) of the first extinction time given an extinction occurs is derived based on the analytic estimate for the extinction probability. Our results indicate that the probability of a disease outbreak, and mean and standard derivation of the first time to disease extinction are periodic in time and depend on the time when the infectious individuals or free-living pathogens are introduced. Numerical simulations are then carried out to validate the analytical predictions using two examples of the general cholera model. At the end, the developed theoretical results are extended to more general models of infectious diseases. This is joint work with Linda JS Allen.

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CP5

Bifurcations in a Schwarzschild Equation Model of the Arctic Atmosphere

We present a column model of the Arctic atmosphere that incorporates radiation flux governed by the two-stream Schwarzschild equations, water vapor concentrations governed by the Clausius-Clapeyron equation and nonlinear surface albedo response to temperature. Representative carbon pathways (RCPs) are used to model carbon dioxide concentrations into the future. The resulting nine-dimensional two-point boundary value problem is solved and various RCPs are applied to the solutions. The model predicts that under the highest carbon pathway, the Arctic climate will undergo an irreversible bifurcation to a warm steady state, which would correspond to an annually ice-free situation. Under the lowest carbon pathway, corresponding to very aggressive carbon emission reductions, the model exhibits only a mild increase in Arctic temperatures. Under the two moderate carbon pathways, temperatures increase more substantially, and the system enters a region of bistability where external perturbations could possibly cause an irreversible switch to a warm, ice-free state.

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CP6

Modeling the Spatial Aggregation of Adélie Penguins

Determining the drivers of abundance trends in populations is key to effectively implementing environmental policy and conservation. Much of the data necessary to understand these relationships are at fine spatial scales, and to accurately gauge trends it is imperative to include historical time series information. Antarctic seabirds are important indicators of climate change, but the costly resources required to travel to and gather data in Antarctica underline the need for heightened reliance on remote surveillance methods such as satellite imagery. Unfortunately, large proportions of long-term available imagery are of poor quality. We present methods to super-resolve information from low resolution satellite imagery to uncover the spatial dynamics of Adlie penguin colonies. Additionally, we use shape modeling to tie abundance trends to the spatial complexities of colonies in order to showcase the relationship between habitat suitability and topographic complexity. In this project, we aim to better equip scientists with tools to study population dynamics with data captured from satellite imagery when high-resolution images are limited or unavailable; furthermore, we seek to test the hypothesis that the destinies of Adlie penguin colonies are driven by their habitat topographies.

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CP6

Estimating Characteristics of Giant Kelp Gametophyte Populations Using Deep Leaning

Seaweed has served as food in a variety of cultures for a long time and marine algae may be cultivated on a larger scale as a source for food, feed or bio-fuel. For efficient operations domestication of appropriate species of algae is needed, that includes identifying species varieties with genotypes and phenotypes best suited for given environmental conditions. In this talk we report on an effort of developing imaging and computational tools to automate parts of this highly labor-intensive process. We focus on the problem of determining properties of giant kelp (Macrocystis pyrifera) gametophyte populations, that includes size distributions and sex and dead cell ratio, using data collected from imaging in a flowthrough system. We developed an image processing pipeline for labeling image data and to amass large enough datasets to train deep leaning models to be used as efficient, accurate and robust estimators of the required populations characteristics.

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CP6

Weakly Supervised Faster-RCNN+FPN to Classifysmall Animals in Camera Trap Images

Camera traps have revolutionized animal research of many species that were previously nearly impossible to observe due to their habitat or behavior. Deep learning has the potential to overcome the workload to the class automatically those images according to taxon or empty images. However, a standard deep neural network classifier fails

because animals often represent a small portion of the high-definition images. Therefore, we propose a workflow named Weakly Object Detection Faster-RCNN+FPN which suits this challenge. The model is weakly supervised because it requires only the animal taxon label per image but doesn't require any manual bounding box annotations and low accuracy drops by less than 5% compared to the supervised version. First, it automatically performs the weakly supervised bounding box annotation using the motion from multiple frames. Then, it trains a Faster-RCNN+FPN model using this weak supervision. Experimental results have been obtained on two datasets and an easily reproducible testbed. This method could boost camera traps adoption by tackling the inherent challenges. Additionally, we also hope it will shed light on the benefits of weakly supervised deep learning methods for all disciplinary communities.

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MS1

Nitrogen, Litter, and Biodiversity Loss in North American Grasslands

The global rise in anthropogenic reactive nitrogen (N) and the negative impacts of N deposition on terrestrial plant diversity are well-documented. Whether or not this biodiversity is reversible, however, remains unclear. Hypothesized mechanisms preventing recovery of biodiversity include nutrient recycling, seed limitation, and litter inhibition of plant growth. In this talk, we will present an ODE model that unifies these mechanisms, produces bistability at intermediate N inputs, and qualitatively matches data collected from a long-term N-enrichment experiment in Minnesota.

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MS1

Overview of Management Questions and Models for Grasslands and Savannas

In this talk, I will give an overview of issues facing management of grasslands and savannas including species coexistence, rainfall, nutrient deposition, and fires, and how these issues are encoded and addressed in models. The models discussed include spatial and biomass models with continuous and discrete disturbances. Alternative attractors and transient behavior play an important role in many of these models. I will also discuss an example of how to analyze the resilience of a savannas grazing potential to discrete fire disturbances.

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MS1

The Effect of Habitat Fragmentation on Plant Communities in a Spatially Implicit Grassland Model

The spatially implicit Tilman-Levins ODE model helps to explain why so many plant species can coexist in grassland communities. This now-classic modeling framework highlights the importance of tradeoffs between colonization and competition traits and also predicts that "extinction debts"—long transient declines—may occur following habitat destruction. Despite its strengths, the Tilman-Levins model does not explicitly account for landscape scale or the spatial configuration of viable habitat, two factors that may be decisive for population viability. We propose modifications to the model that explicitly capture habitat geometry and the spatial pattern of seed dispersal for individual species. The modified model retains implicit space and is in fact mathematically equivalent to the Tilman-Levins model in the single species case. But its novel interpretation of a habitat destruction parameter better quantifies seed loss due to edge effects in fragmented habitats. We explore the implications of these modifications the context of Midwestern grasslands.

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MS1

The Role of Fire in Shaping the Dynamics of Veg-

etation Mosaics in Fire-Prone Savannas

The savanna biome encompasses variations of vegetation physiognomies that traduce complex dynamical responses of plants to the rainfall gradients leading from tropical forests to hot deserts. Such responses are shaped by interactions between woody and grassy plants that can be either direct, disturbance-mediated (e.g. fire) or both. There has been increasing evidence that several (highly contrasted) vegetation physiognomies may durably coexist in humid savannas, which are fire-prone, suggesting multistability (i.e. mosaic of vegetation). Therefore, a major question consists of understanding/characterizing how fires may impact vegetation mosaic dynamics. This question has triggered several modeling efforts relying either on space-implicit or on space-explicit mathematical models. In this talk, I will present some recent space-explicit models designed to study the impact of fire on the long-term dynamics of a forest-grassland vegetation mosaic in humid savannas by the means of a bistable traveling wave. Notably, I show that depending on fire-return time as well as difference in diffusion potential of woody and herbaceous vegetation, fires are able to greatly slow down or even reverse the progression of forest in humid regions.

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MS2

A Look to the Role of Vegetation in Tipping Climate States: Simplified Modelling and Land Use in the Amazon

Soil moisture, terrestrial vegetation, and atmospheric flows are parts of a complex interacting system. Desertification and deforestation can generate a reduction in precipitation in many regions of the world, especially the tropics. Rainfall decrease might lead to vegetation dieback which can in turn lead to further rainfall reduction. In the first part of this talk, I show how such feedback can lead to the existence of multiple equilibria in the atmosphere-vegetation system, by mean of simplified, physically based models representing the planetary boundary layer, soil water and plant with ordinary differential equations. In the second part of this talk, I show how part of this feedback loop can be quantified for the Amazon basin. Land-use changes in the Amazon affect rainfall patterns, but to what extent remains unclear. Generally, it is assumed that rainfall decreases proportionally to the transpired portion of atmospheric moisture. Instead, the observed moisture in the atmosphere shows a steep increase in rainfall at large atmospheric moisture. Given this non-linear relationship, a complete deforestation of the Amazon could result in a 55%70% decrease in rainfall annually, despite contributing only 13% of the atmospheric moisture in the area. Consequences of this nonlinearity might be twofold: although the effects of deforestation may be underestimated, it also implies that forest restoration may be more effective for precipitation enhancement than previously assumed.

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MS2

A Quasipotential Approach to Tipping Cascades

We consider a general model of a bi-stable tipping element where each node has two stable states separated by an unstable gating state, transitions (tipping) between states are driven by white noise. Coupled together tipping at one node can influence other nodes to tip causing a cascade. The timing and order of these tipping cascades are emergent properties of the network. Analysis of the transient dynamics responsible for these cascades is crucial to understand their behavior and identify early warning indicators. Our previous work has shown how symmetrically coupled elements can be thought of as a gradient or potential system. We have classified the timing and order of tipping cascades in this case using geometric analysis via the computation of their potential landscape. For non-symmetrically coupled, i.e. more realistic coupling structures, the coupled elements do not form a potential system and there is no closed-form for the potential landscape. In these cases, an approximation of the potential called the *quasipotential* (QP) can be computed. Theoretically introduced by Friedlin and Wentzel in the 80s the QP has remained elusive as it is hard to compute. The recent development of a range of numerical algorithms has facilitated the computation of the QP in low-dimensional systems. Here we use the QP to explore the behavior of a chain of coupled tipping elements. We identify a range of behaviors that are not present in the symmetric/potential case.

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MS2

Green Sahara Tipping Points in an Ensemble of Transient Holocene Climate Model Simulations

The 'Greening' of the Sahara during the Holocene is a particularly dramatic natural environmental change. Although it is well understood that slow variations in Earth's orbit caused this transition, climate models have largely failed to convincingly reproduce it. Having conditioned one climate model with the climatic state in North Africa for the mid-Holocene at 6000 years ago, we performed a series of transient simulations covering the last 10,000 years. The results show abrupt changes that replicate features seen in long paleoclimate records. We will discuss how this approach differs from other paleoclimate modelling studies, how the results are sensitive to a range of climatic forcings operating during this time, and what it tells us about reproducing abrupt climate changes in models of the climate system.

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MS2

Dynamical Systems Approaches to Climate Response and Climate Tipping

The currently ongoing climate change and the debate about possible measures to be taken to limit the consequences of climate change, requires to know and understand the future response of the climate system to greenhouse gas emissions. Classical measures of climate change such as the Equilibrium Climate Sensitivity (ECS) are inherently linear and unable to account for abrupt transitions due to (interacting) tipping elements. In this presentation I will discuss more general notions of climate sensitivity defined on a *climate attractor* that can be useful in understanding the response of a climate state to changes in radiative forcing. For example, a climate state close to a tipping point will have a degenerate linear response to perturbations, which can be associated with extreme values of the ECS. While many identified tipping elements in the climate system are regional and may have no direct impact on the global mean temperature, cascades of tipping elements can potentially have an impact, initiated by the threshold of the leading tipping element in a cascade.

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MS3

Responsible Research and Ethical Professional Choices in Applied Mathematics I

The conversations around 'ethics in mathematics' are simultaneously divisive and fundamentally necessary for the field. More important is connecting the theory and practice - the conversations with action. During the ongoing climate crisis, this challenge becomes ever more urgent. Mathematics practitioners need ethical guidelines that are accessible, authentic, and usable, and which reflect the communitys sense of professional identity, culture of practice, and obligations to peers and the public. Many mathematics professional societies have ethics codes, but they are often incomplete and only address a narrow range of mathematical practices. The speakers will describe results of a recent survey of mathematical practitioners regarding the applicability of ethical provisions from various mathematics-adjacent professions to mathematics, highlighting those items which displayed the broadest agreement, and disagreement, as touchstones for further discussion. Additionally, they will look at current trends in ethical discussions from major societies and international communities, especially with respect to the climate crisis.

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MS3

Towards Professional Responsibility in Teaching Applied Mathematics II

The presenters will briefly summarize the main points of part I of this talk. They will then invite the audience to participate in the discussion and share their own experiences. Remote audience members will be able to do this using anonymous polling tools.

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MS3

Responsible Research and Professional Choices in Applied Mathematics II

The presenters will briefly summarize the main points of part I of this talk. They will then invite the audience to participate in the discussion and share their own experiences. Remote audience members will be able to do this using anonymous polling tools.

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MS3

Towards Professional Responsibility in Teaching Applied Mathematics I

The climate crisis and environmental challenges are increasingly of concern to many of our students. How does our knowledge of climate change and its urgency impact how we teach and train students? How should it have an impact? The speakers will discuss this important topic and identify areas of action and obligation. They will also identify potential changes that instructors can make, as well as ways to lower barriers to making changes in our professional practice.

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MS4

Stochastic Parametrization of Subgrid Fluxes in the Shallow Water Equations Using Generative Adversarial Networks (GAN)

Stochastic subgrid-scale parametrizations account for the bulk effects of unresolved processes in a reduced model by sampling from a distribution typically described in terms of

resolved modes. In this work, we evaluate the performance of conditional generative adversarial network (GAN) in parametrizing subgrid-scale effects in a finite-volume flux discretization of the Shallow water equations. The resolved modes are defined as local spatial averages while the unresolved variables are the fluctuations. We train a Wasserstain GAN to generate subgrid fluxes in the equation for the resolved modes. The optimized GAN generator is then used to perform numerical simulations of the effective model and reproduce statistical features of the local averages. In addition, we also demonstrate that once trained the neural network can be used in to perform simulations of effective equations in new regimes with increased forcing.

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MS4

A Data-Driven Approach to Climate Variability and Predictability

Reduced-order dynamical models play a central role in developing our understanding of predictability of climate. In this context, the Linear Inverse Modeling (LIM) approach (closely related to Dynamic Mode Decomposition DMD), by helping capture a few essential interactions between dynamical components of the full system, has proven valuable in being able to give insights into the dynamical behavior of the full system. While nonlinear extensions of the LIM approach have been attempted none have gained widespread acceptance. We demonstrate that Reservoir Computing (RC), a form of machine learning suited for learning in the context of chaotic dynamics, by exploiting the phenomenon of generalized synchronization, provides an alternative nonlinear approach that comprehensively outperforms the LIM approach. Additionally, the potential of the RC approach to capture the structure of the climatological attractor and to continue the evolution of the system on the attractor in a realistic fashion long after the ensemble average has stopped tracking the reference trajectory is highlighted. Finally, other dynamical systems based methods and probabilistic deep learning methods are considered and a broader perspective on the use of data-driven methods in understanding climate predictability is offered.

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MS4

Statistical Reduced-Order Models and Closure Strategies for Turbulent Geophysical Flows

The capability of using imperfect statistical reduced-order models to capture crucial statistics in turbulent geophysical systems is investigated. Much simpler and more tractable block-diagonal models are proposed to approximate the complex and high-dimensional turbulent dynamical equations using both parameterization and machine learning strategies. 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. In addition, new machine learning strategies are proposed to learn the expensive unresolved processes directly from data.

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MS4

Predicting Shallow Water Dynamics Using Echo-State Networks with Transfer Learning

We present how Echo-State Networks (ESN) can be used to predict the dynamics of the Shallow-Water Equations. Such ESN models represent a computationally efficient method as an initial-value solver. Therefore, they can be used for performing ensemble simulations and predicting evolution of averaged quantities or accessing uncertainty. Our approach also can be interpreted as equation learning where the same neural network is capable of reproducing dynamics of the initial-value problem for a large set of initial conditions. We also demonstrate that large-scale quantities such as momentum and averaged water height play an important role in predicting the dynamics. We introduce a transfer learning approach to quickly re-train the neural network and take such large-scale quantities into account.

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MS5

Interactions Between Host Traits and Temperature Drive Shifts in the Thermal Characteristics of Mosquito-Borne Pathogen Transmission

Recently, the role of temperature in mosquito-borne parasite (MBP) transmission has become a major area of focus as researchers work to assess how climate change may shift global patterns of mosquito-borne disease risk. Such research has focused almost entirely on mosquitoes and their parasites while mostly neglecting the role of the vertebrate host in the transmission system. In this talk, we explore

the connections between vertebrate host traits and MBP transmission dynamics, especially as these connections relate to temperature. We find that the population density of vertebrate hosts is a key factor determining the persistence of MBP populations at any temperature. Furthermore, vertebrate host population density can shift the thermal optimum for transmission in some systems. These results emphasize the importance of accounting for the full ecology of MBP transmission when deriving estimates of mosquito-borne disease risk in a changing climate.

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MS5

Temperature Fluctuations Impact Zika Dynamics

A dynamic temperature-dependent model for Zika virus (ZIKV) is developed and parametrized using experimental data. The model is used to assess the impact of temperature fluctuations and some parameters through which control measures can be implemented on disease burden quantified in terms of the basic reproduction number (R0) and the total infectious human population. It is shown that R0 is maximized at a single temperature, while the total infectious human population is maximized across a wider temperature range. Additionally, it is shown that seasonal temperature fluctuations impact ZIKV significantly and that the geographical range of ZIKV is wider than that predicted by previous R0 Models. Hence, the study highlights the critical role of climatic dynamics and variation on emerging vector-borne diseases.

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MS5

Changing Temperatures and the Risk of Dengue Outbreaks

With changing temperatures, we expect geographic distributions and competencies of infectious disease vectors to change. Dengue is a mosquito-borne virus that has historically been tropical, and has recently been expanding its range. To evaluate dengue outbreak risk in areas where its primary vector, Aedes aegypti, has been observed, we developed an SEIR-type model, simulated epidemics, and carried out sensitivity analyses. Our model focused on two key temperature-dependent parameters: mosquito extrinsic incubation period and mosquito lifespan. We found that changing temperatures significantly impact dengue risk. Our numerical simulations suggested that under scenarios with a 3 C air temperature increase, risk of summer outbreaks could double in Los Angeles and Houston, although risk could evaporate in Phoenix because of intense heat. This research was supported by an appointment to the Intelligence Community Postdoctoral Research Fellowship Program at Los Alamos National Laboratory, administered by Oak Ridge Institute for Science and Education through an interagency agreement between the U.S. Department of Energy and the Office of the Director of National Intelligence.

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MS5

Mosquito, Parasite, Malaria: Connecting Regional Temperatures to Mosquito and Parasite Developmental Traits in a Mathematical Model for Malaria

Shifting climatic patterns have been reported to have an effect on the abundance and redistribution of vectors that transmit vector-borne disease. With temperature a well-known factor affecting mosquito population dynamics and the rate of development of the malaria parasite forms within a mosquito, the consequences of increasing temperatures and such shifting climatic patterns may have serious consequences for malaria disease transmission in different regions. While a sinusoidal wave form is a common methodology used to embed temperature effects into malaria, and in general, disease models, it misses the within and between seasonal monthly and yearly variations in the disease-related parameter traits and temperature profiles. We address this in our seasonal malaria framework by proposing a different methodology which maps data on temperature-dependent mosquito traits and temperature-dependent parasite demographic traits to regional temperature data, using the info to create seasonal profiles unique to a given locality and based on regional recorded temperature data for that locality. This is done without forcing a sinusoidal fit to the data. I will discuss our methodology and illustrate its use in studying the impact of seasonality on malaria transmission dynamics and burden in two malaria regions in Malawi - one a high transmission region and the other a low transmission region.

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MS6

Rate and Noise-Induced Tipping in Tropical Cyclones

In dynamical systems, a tipping event is loosely defined as occurring when a sudden or small change to a variable or parameter induces a large change to the state of the system. Such events are often classified according to whether the underlying mathematical mechanism involves, predominantly, a bifurcation (B-tipping), noise induced transitions (N-tipping), or fast changes in parameters (R-tipping), i.e. rate induced tipping. However, in many climate applications the dynamical system is necessarily stochastic and non-autonomous and thus mechanisms which drive tipping must be a combination of these effects. In this talk, we present a study of tipping events in a low dimensional model of tropical cyclone formation that are induced by fast varying and stochastic parameters. The primary mathematical tool we use is the Freidlin-Wentzell (FW) theory of large deviations applied to a compactified system in which phase space is augmented so that asymptotic end states of the non-autonomous systems now correspond to fixed points of an autonomous system. The use of the FW theory allows us to extract scaling laws for the expected time of tipping that depends on noise strength as well as the time scale on which the time varying parameters change.

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MS6

Noise-Induced Tipping in Stochastic Piecewise-Smooth Systems

We develop a path integral framework for determining most probable paths in a class of systems of stochastic differential equations with piecewise-smooth drift and additive noise. This approach extends the Freidlin-Wentzell theory of large deviations to cases where the system is piecewise-smooth and may be non-autonomous. In particular, we consider an $n-$dimensional system with a switching manifold in the drift that forms an $(n-1)-$dimensional hyperplane and investigate noise-induced transitions between metastable states on either side of the switching manifold. We explore implications of our results through two case studies, which exhibit notable phenomena such as non-unique most probable paths and noise-induced sliding in a crossing region.

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MS6

Abundant Multistability and Intermediate Tipping Points in a Global Ocean Model

Tipping points (TPs) are thought to arise by the destabilizing effect of a single dominant positive feedback on a climate sub-system at a well-defined threshold of a forcing parameter. However, the large number of spatio-temporal scales in the climate, and associated second-order feedbacks, could lead to a variety of more subtle, but discontinuous reorganizations of the spatial climate pattern before an eventual catastrophic tipping. Such intermediate TPs could hinder predictability and mask generic early-warning signals (EWS). Here we consider a TP of the Atlantic meridional overturning circulation (AMOC) as a result of increased glacial melt. Using an ensemble of equilibrium simulations in a global ocean model, we map out the stability landscape of the circulation in high detail. While in a typical hysteresis experiment only one regime of bistability is found, subtle changes in forcing reveal an abundance of discontinuous, qualitative changes in the AMOC variability. These are used to initialize small-scale hysteresis experiments that yield a variety of multistable regimes with at least 4 coexisting alternative attractors. We argue that due to chaotic dynamics, non-autonomous instabilities, and complex geometries of the basins of attraction, the realized path to tipping can be sensitive to initial con-

ditions and the forcing trajectory. Further, we discuss to which degree the equilibrium dynamics are reflected in the transient dynamics for different rates of forcing.

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MS6

Permafrost via Budyko's Model

Climate change affects permafrost thaw depth and the extent of permafrost. As permafrost degrades, stored soil organic carbon gets released into the atmosphere as carbon dioxide and methane. This feedback cycle increases climate change. We will approximate carbon emissions from permafrost using a simple planetary energy balance model coupled with a heat equation. Under certain boundary conditions and parameters, we describe the degradation process.

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MS7

How Close and How Much? Linking Health Outcomes to Spatial Distributions of Built Environment Features

Built environment features (BEFs) refer to aspects of the human constructed environment, which may in turn support or restrict health related behaviors and thus impact health. In this talk we are interested in understanding whether the spatial distribution and quantity of fast food restaurants (FFRs) influence the risk of obesity in schoolchildren. To achieve this goal, we propose a two-stage Bayesian hierarchical modeling framework. In the first stage, examining the position of FFRs relative to that of some reference locations - in our case, schools - we model the distances of FFRs from these reference locations as realizations of Inhomogenous Poisson processes (IPP). With the goal of identifying representative spatial patterns of exposure to FFRs, we model the intensity functions of the IPPs using a Bayesian non-parametric view and specifying a Nested Dirichlet Process prior. The second stage model relates exposure patterns to obesity, offering two different approaches to accommodate uncertainty in the exposure patterns estimated in the first stage. Our analysis on the influence of patterns of FFR occurrence on obesity among Californian schoolchildren has indicated that, in 2010, among schools that are consistently assigned to a cluster, there is a lower odds of obesity amongst 9th graders who attend schools with most distant FFR occurrences in a 1-mile radius as compared to others.

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MS8

Closed-Form Discovery of Structural Model Errors by Integrating Bayesian Sparse Regression and Data Assimilation

Models used for many key processes of the climate system are imperfect. The discrepancy between the mathematical representations of a true physical system and its imperfect model is called the model error. These model errors can lead to substantial differences between the numerical solutions of the model and the observations of the system, particularly for nonlinear, multi-scale phenomena. Thus, there is substantial interest in reducing model errors, particularly through understanding their physics and sources and leveraging the rapid growth of observational data. Here we introduce a framework named MEDIDA: Model Error Discovery with Interpretability and Data Assimilation. MEDIDA only requires a working numerical solver of the model and a small number of noise-free or noisy sporadic observations of the system. In MEDIDA, first, the model error is estimated from differences between the observed states and model-predicted states. If observations are noisy, a data assimilation (DA) is used to provide an analysis state of the system, which is then used in estimating the model error. Finally, an equation-discovery technique, such as RVM (a sparsity-promoting Bayesian method), is used to identify an interpretable closed-form of the model error. Using the chaotic Kuramoto-Sivashinsky (KS) system as the test case, we demonstrate the excellent performance of MEDIDA in discovering different types of structural/parametric model errors, using noise-free and noisy observations.

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MS8

Prior Error Covariances in An Ensemble Kalman Filter Framework in Numerical Weather Prediction

We will discuss the sample error covariances used in ensemble Kalman filtering (EnKF) applications in numerical weather prediction (NWP). For these applications an ensemble may contain $O(10^2)$ members to represent a $O(10^7)$ domain. In this regime, it has been demonstrated that EnKFs are unable to represent non-Gaussian error statistics (Miyoshi et al 2016). Additionally the resolutions used in operational data assimilation are often coarser than the forecast model making the data assimilation less nonlinear. We will present an alternative covariance formulation, based on quadrature filtering, optimal for the case where the fourth order derivatives of the nonlinear model are small and the prior error is well approximated by Gaussian distributions. We will discuss and demonstrate the improved performance of this method for 1D 2D shallow water models with known error characteristics. Additionally we will discuss the rank issues inherent in NWP EnFK applications.

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MS8

Training Physics-Based Machine-Learning Param-

eterizations with Ensemble Kalman Methods

Most machine learning applications in Earth system modeling currently rely on gradient-based supervised learning. This imposes stringent constraints on the nature of the data used for training, and it complicates learning about the interactions between machine-learned parameterizations and other components of an Earth system model. Approaching learning as an inverse problem resolves many of these issues, since it allows parameterizations to be trained with partial observations or statistics that directly relate to quantities of interest in long-term climate projections. Here we demonstrate the effectiveness of ensemble Kalman methods in treating learning about parameterizations as an inverse problem. We consider two different algorithms: unscented and ensemble Kalman inversion. Both methods involve highly parallelizable forward model evaluations, converge exponentially fast, and do not require gradient computations. In addition, unscented Kalman inversion provides a measure of parameter uncertainty. We demonstrate this learning approach through the calibration of an eddy-diffusivity mass-flux scheme for subgrid-scale turbulence and convection, using data generated by large-eddy simulations. We find the algorithms amenable to batching strategies, robust to noise and model failures, and efficient in the calibration of hybrid parameterizations that can include empirical closures and neural networks.

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MS9

Remarks on the Hibler Model for Sea-Ice Dynamics

Sea ice dynamics remains one of the most uncertain factors in earth system models' ability to address the climate change problem. Hilbers model, which is based on a viscoplastic rheology, is widely accepted in the climate modeling community as representative of the large scale sea-ice dynamics and it is extensively used in earth system models, despite some major deficiencies in accurately representing fine features associated with leads and ridges and in the formation of melt ponds, to name a few. However, due the inherent nonlinearities the model is notoriously difficult to solve numerically and its behaviour as an initial value problem is poorly understood. In this talk I will discuss a few analytical issues related to the well posedness of this model as a system of nonlinear PDEs and present a family of numerical schemes for the goal of solving this highly challenging nonlinear problem in the most accurate and most efficient manner.

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MS9

Numerical Methods on Solving Sea Ice Dynamics Model Based on a Viscous-Plastic Formulation

Accurate modeling of sea ice dynamics is critical for predicting environmental variables, which in turn is important in applications such as navigating ice breaker ships, and has led to extensive research in both modeling and simulating sea ice dynamics. The most widely accepted viscous-plastic formulation introduced by Hibler is intrinsically difficult to solve numerically due to highly nonlinear features. In particular, sea ice simulations often significantly differ from satellite observations. To improve the numerical accuracy of the viscous-plastic sea ice model, I propose a potential function method, utilizing the idea of phase field method, which naturally incorporates the physical restrictions of ice thickness and ice concentration in transport equations. I also examine the poor convergence seen in existing numerical methods and demonstrate that using higher order methods for solving conservation laws, such as the weighted essentially non-oscillatory (WENO) schemes, is critical for yielding higher order convergence on smooth solutions as well as resolving the discontinuities in the sharp features of sea ice covers.

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MS9

An Introduction to Models and Observations of Sea Ice Dynamics

Sea ice is a defining feature of the Arctic and has broad impacts in fields ranging from maritime navigation and the global climate system. This talk will provide a brief introduction to models of sea ice dynamics, observational data that can help constrain model behavior, and the challenges of performing data assimilation in this setting. Our goal is to provide an approachable introduction that lays the foundation for the remaining research talks in this session.

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MS9

Fast and Robust Newton Solvers for Viscous-Plastic Sea-Ice Models

We present a novel Newton-Krylov solver for the viscous-plastic sea-ice model, which is commonly used in climate models to describe the large-scale motion of sea-ice. Due to the strong nonlinearity of the momentum equation, the development of fast, robust and scalable solvers is still a substantial challenge. We propose a novel Newton linearization for the momentum equation, which converges fast and robustly with respect to mesh refinement, and thus allows fully resolved sea-ice simulations. Combined with an algebraic multigrid-based preconditioned Krylov method for the linearized systems, the resulting solver scales well and can be used in parallel. We present highly resolved benchmark solutions and solve problems with up to 8.4 million

spatial unknowns.

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MS10

Stochastic Wind Modelling for Bushfire Simulation

The prediction of the rate of wildfire spread is vital for fire agencies to protect communities from possible damages. One environmental factor that is of great significance to understanding and predicting the fire behaviour is wind velocity. The intrinsic uncertainty associated with wind vectors can cause errors in the prediction of fire propagation across a landscape. By capturing the uncertainty using probabilistic approaches, more accurate and informative wildfire simulations can be produced. In this study, two stochastic processes: the Wiener process and the First-Order-Gauss-Markov (FOGM) process, are implemented to capture the natural stochasticity in the horizontal components of wind velocity. Each process is then calibrated using wind observation related to a specific spatial location recorded by 11 different weather stations in close proximity. These stochastic wind models are then implemented in a fire spread simulator called Spark. In comparison to an ensemble of deterministic simulations, the fire spread predicted by stochastically modelled wind is more limited in both direction and speed.

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MS10

Probabilistic Machine Learning, Bayesian Inference, and Remote Sensing for Environmental Data

There is a rapid increase in the availability of remote sensing data and other measurements that can be harnessed by machine learning (ML) techniques for real-time analysis or spatio-temporal forecasting of natural hazards, such as wildfires. This could, for example, consist of detecting the edges/contours of encroaching fire lines from aerial imagery, segmenting individual fallen trees in a forest using satellite imagery, or predicting future atmospheric pollutant concentrations at a fine scale. Given the important implications of such tasks, a crucial aspect of both analysis and forecasting is uncertainty quantification (UQ). Probabilistic ML, especially Bayesian methods, provide a flexible and natural framework that includes UQ to address these tasks. In this talk, I will discuss some of these ML methods in the context of environmental data and remote sensing, and the potential applications to/for fire science.

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MS10

Deep Learning Applied to A Coupled Fire-Atmosphere Spread Model

In this talk, we first introduce a physics-based computational model for wildland fire which includes fireinduced sinks and vorticities. Next, these fireatmosphere interactions are investigated using deep convolutional neural networks (CNNs). The training, validation, and test data sets are generated using the simplified computational model. The predictions are made to determine burning maps (first arrival time) in time increments after ignition. In addition, we use statistical methods and metrics to compare the performance of CNNs and the simplified model. Last, we will apply the learned model to real data by selecting proper models and training datasets.

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MS10

Hierarchical Level Set Dynamics for Inferring Wildland Fire Front Propagation

Level set dynamics have proven to be an effective and flexible technique for tracking the spread of wildland fire fronts. With a specified function that gives the rate of advance of a fire front, the method can produce realistic topological spread of the fire (e.g., merging fronts, absorbing "islands"). The limiting component of level-set dynamics is the specification of this spread function (velocity). Here, we investigate a Bayesian implementation specified in terms of signed-distance functions and advective dynamics that learns the spread function given spatial, temporal, and/or spatio-temporal covariates and random effects. There are several numerical challenges to this implementation. The approach is demonstrated on simulated data and observations of large wildland fires in the Western US.

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MS11

Investigating the 'Hothouse Narrative' with Dynamical Systems

The 'hothouse narrative' states that tipping cascades could lead humanity to a binary choice between a 'governed Earth' and a 'hothouse' with no midway alternative. To investigate this scenario, we construct a toy model of interacting tipping elements and ask the following questions: Given a continuous family of emission scenarios, are there discontinuities in the family of responses, as suggested by the 'hothouse narrative'? How realistic is this given knowledge provided by climate simulations and paleo-climate evidence? The relatively low complexity of our model allows us to easily run it for several thousand years and a large range of emissions scenarios, helping us highlight the fundamental role of the differenttime scales involved in answering our questions. On the one hand, we find that the near-linear relationship predicted by GCMs between global temperature and GHG emissions for the next century can break up at millennial time scales due to cascades involving slower tipping elements such as the ice sheets. This translates as a discontinuity in the family of responses of our model. On the other hand, we find that different emissions scenarios respecting the same carbon budget could potentially lead to different tipping cascades and thus qualitatively different outcomes.

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MS11

Critical Slowing Down in Coupled Stochastic Dynamical Systems

There has recently been rising interest in interdependent critical transitions in coupled nonlinear random dynamical systems. In the special case of a top-down hierarchy of systems, a causal chain of transitions, commonly called *tipping cascade, might be triggered. The classical statiscal indicators of critical slowing down in the observable of each system will still provide information about the advent of a bifurcation in that system, but will in general also be influenced by a change in the system driving it. We give an overview of simple modelling approaches and develop some first analytical formulas for anticipating critical transitions in these models. We also outline possible estimation methods based on these formulas.*

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MS11

Cascading Tipping in a Coupled Cryosphere-Ocean Model

In the climate system, many different large-scale components have been identified as tipping elements, i.e., components that may pass a tipping point, with a substantial and definitive impact on earth and societies. These climate components do not stand on their own, but are dynamically coupled, which leads to the issue of cascading tipping. One important example of cascading involves the Greenland Ice Sheet (GIS), the West Antarctica Ice Sheet (WAIS) and the Atlantic Meridional Overturning Circulation (AMOC). While the destabilizing effect of a GIS decline on the AMOC is well established, the consequences of adding a tipping WAIS is still unclear. In this project, we aim at getting a better understanding of the global behaviour of this connected system. Accounting for the different nature of both ice sheets, we use two models including their most important feedbacks, namely, the marine ice sheet instability for the WAIS and the height-accumulation feedback for the GIS. The AMOC is coupled to both ice sheets through meltwater fluxes. Finally, we consider the Southern Ocean temperature as the main driver of the marine ice sheet instability. With this conceptual interhemispheric model, we study the role of the AMOC as mediator of this potential cascading, as well as the involved time scales. As a new result we find that, in this model, the stability of the AMOC depends on the ratio between the GIS and WAIS tipping rates, as well as their delay in time.

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MS11

Relaxation Oscillations and Noise Induced Transitions in Ice Age Climate

The Atlantic Meridional Overturning Circulation (AMOC) has been implicated as a major tipping element in climates of the past and therefore is of great interest for understanding abrupt changes that may occur under future warming. Complex coupled climate models that simulate ice age climate are able to show millennial time-scale Dansgaard-Oeschger (D-O) oscillations that agree well with the observed climate record. These oscillations contain highly non-linear abrupt transitions between cold and warm states in the Northern Hemisphere driven by abrupt AMOC variations. These transitions can be modulated under changes in internal and external forcing such as atmospheric carbon dioxide concentration and the Earths orbitally controlled insolation. Using a physically based simple dynamical systems model that mimics the complex model behaviour, it can be shown that the D-O cycle is an internal stochastic climate oscillator that is controlled by atmospheric carbon dioxide level through the glacial. The D-O oscillation can exhibit regular cyclicity when the control parameter passes through a Hopf bifurcation into an unstable oscillatory state (at levels of intermediate atmospheric carbon dioxide concentration). The system can also exhibit infrequent noise-induced transitions when the system is stable at low and high carbon dioxide level. The modern AMOC therefore could possibly have a similarly high sensitivity to future anthropogenic global warming.

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MS12

Equitable Ridepooling Using Autonomous Electric Vehicle Fleets with Community-Driven Stops

We formulate and address a multi-agent control problem where a fleet of autonomous, multi-passenger electric vehicles (e.g. buses or shuttles) are coordinated by a cen-

tral transit agency to best serve a community of riders who choose routes based on a predetermined set of station stops. This novel autonomous ridepooling framework lays between existing public transit services with fixed station stops and routes and pure mobility-on-demand services (e.g. Uber) with dynamic and adaptive stops and routes. The transit agency is expected to act in the best interest of society, managing the autonomous electric fleet to maximize social good by satisfying as many passenger requests as possible. We develop a Multi-Agent Reinforcement Learning (MARL) simulation environment and test various heuristic and RL trained policies that can control a fleet of autonomous electric vehicles for ridepooling with stochastic requests from a community. Using domains with different graph sizes (i.e. number of stop locations) and request distributions, we observe that RL methods can outperform benchmark heuristics on larger, heterogeneous the domains. Pre-training RL policies with imitation learning based on the best heuristic method is explored to improve convergence times and learning stability. Our results indicate that no single RL method or heuristic method consistently outperforms all others across all domains, meaning selecting the best method for learning agent policies is domain-specific.

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MS12

Localized Urban Pollution Patterns and Environmental Justice Concerns: Lessons from a Long-Term Mobile Monitoring Campaign

Urban air pollution exhibits significant variation on the scale of city blocks (¡100 m). This hyperlocal variation is difficult to represent with statistical or mechanistic modeling, so the influence of hyperlocal variability on population exposure and racial/ethnic exposure disparity has been difficult to characterize. This presentation describes a set of uniquely extensive and high-resolution observations made in four counties of the San Francisco Bay Area using Google Street View cars equipped with the Aclima mobile platform. These data show that even for pollutants with steep localized gradients, differences in average outdoor concentrations among racial/ethnic groups are driven by regional variability. However, localized peaks contribute to disparity in extremes among groups.

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MS12

Statistical Inference of Travelers' Route Choice Preferences with System Level Data

Traditional network models encapsulate travel behavior among all origin-destination pairs based on a simplified and generic travelers' utility function. This study extends classical bilevel formulations to estimate travelers utility functions with multiple attributes using system-level data. We formulated a methodology grounded on nonlinear least squares to statistically infer travelers' utility function in the network context using traffic counts, traffic speeds, the number of traffic incidents and sociodemographic information obtained from the US Census. The analysis of the mathematical properties of the optimization problem and of its pseudo-convexity motivated the use of normalized gradient descent. More importantly, we developed a hypothesis test framework to examine statistical properties of coefficients attached to utility terms and to perform feature selection. Experiments on synthetic data showed that the coefficients of the travelers utility function can be consistently recovered and that hypothesis tests are a reliable statistic to identify which attributes are determinants of travelers route choices. Besides, a series of Monte-Carlo experiments showed that statistical inference is robust to noise in the Origin-Destination matrix or in the traffic count measurements. The methodology was also deployed at a large scale using real-world multi-source data in Fresno, CA collected before and during the COVID-19 outbreak.

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MS12

Design of An Improved Computational Model for Prediction of Traffic Flow

Transport emissions are a major contributor to the rise in air pollution today. Models that effectively predict congestion on critical traffic corridors provide crucial tools for advancing and evaluating mitigation strategies for the environmental and health consequences of traffic. We build on the traditional Lighthill-Whitham-Richards model for unidirectional traffic on a single road given by a partial differential equation (PDE). We derive desirable mathematical conditions for velocity functions to ensure L^1 contractivity for the PDE. Properly capturing driver behavior with a velocity function requires both modeling driver decisions and robust uncertainty quantification as a function of traffic densities. A particle-based traffic model is then crucial to obtain the desired velocity profile. Combining these models provides a general class of velocity functions that satisfy the desirable conditions for the stability of the PDE and fits the velocity profile obtained using the particle model. Finally, we compare the PDE and particle models ability to capture the observed traffic effects of real-world driving behaviors.

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MS12

Sources of Inequity in Exposure to Fine Particulate Air Pollution

Racial-ethnic minorities in the United States are exposed to disproportionately high levels of ambient fine particulate air pollution (PM2.5), the largest environmental cause of human mortality. This presentation will cover some of the mechanisms that underlie this disparity, including the spatial scales across which disparities are relevant, where disparities occur and which types of emissions sources contribute to them, and how disparities in exposure to air pollution are related to disparities in economic consumption activities. Although there are no easy solutions to this problem, we will also discuss considerations that could lead

to better outcomes in the future.

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MS13

Extended Theories of Geometric Thermal Shallow-Water Dynamics

Driven by growing momentum in two-dimensional geophysical flow modeling, a general family of "thermal' rotating shallow-water models is introduced. The models are capable of accommodating thermodynamic processes, such as those acting in the ocean mixed layer, by allowing buoyancy to vary in horizontal position and time as well as with depth, in a polynomial fashion up to an arbitrary degree. Moreover, the models admit Euler-Poincare variational formulation and possess Lie-Poisson Hamiltonian structure. Such a geometric property provides solid fundamental support to the theories described with consequences for numerical implementation and the construction of unresolved motion parametrizations. In particular, it is found that stratification halts the development of small-scale filament rollups recently observed in a popular model, which, having vertically homogeneous density, represents a special case of the models presented here. In this talk, I will describe the new model family after a brief recount of the history of thermal shallow-water modeling in the ocean, and Earth and planetary atmospheres.

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MS13

Theoretical and Computational Analysis of the Thermal Quasi-Geostrophic Model

I will present several theoretical results for the thermal quasi-qeostrophic (TQG) model of submesoscale geophysical fluid dynamics (GFD). Physically, the TQG model involves thermal geostrophic balance, in which the Rossby number, the Froude number and the stratification parameter are all of the same asymptotic order. The TQG model is shown to be well posed locally in time. Also solutions of its regularized α-TQG version converge to solutions of TQG as its smoothing parameter $\alpha \to 0$. I will also introduce the rate of convergence of α-TQG solutions to TQG solutions as $\alpha \to 0$ and present some simulations in appropriate GFD regimes. If time permits I will also introduce a stochastic variant of the TQG model. This is joint work with Darryl D. Holm, Erwin Luesink, Prince Romeo Mensah and Wei Pan and is part of the STUOD project (https://www.imperial.ac.uk/ocean-dynamics-synergy/).

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MS13

Structure-Preserving Discretization of the Thermal Shallow Water Equations with Boundaries

TRiSK-type discretizations, which are based on discrete exterior calculus (DEC), are widely used in both atmosphere and ocean models (such as Dynamico, MPAS-O, MPAS-A, ICON-IAP). This is principally for their desirable mimetic properties, which give useful features such as energy conservation, steady geostrophic modes, and an absence of spurious linear modes. However, in the case of domains with boundaries a suboptimal treatment is often used, losing mimetic properties and restricted to the case of no-flux or no-slip boundary conditions. In this talk, I will present a consistent extension of DEC to domains with boundaries and arbitrary boundary conditions, including inflow/outflow conditions, for the general case of unstructured grids. This extension preserves the desirable mimetic properties of DEC without boundaries, such as discrete integration by parts and product rules. The revised DEC is then used to develop a version of TRiSK for the thermal shallow water equations with boundaries that has the same properties as the case without boundaries, including energy conservation up to boundary fluxes, steady geostrophic modes and an absence of spurious linear modes.

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MS13

Well-Balanced Central-Upwind Schemes for the Thermal Rotating Shallow Water Equations

We introduce well-balanced central-upwind schemes for the thermal rotating shallow water model (TRSW) both on one- and two-dimensional cases. The scheme is designed using the flux globalization approach: first, the source terms are incorporated into the fluxes, which results in a hyperbolic system with global fluxes; second, we apply the Riemann-problem-solver-free central-upwind scheme to the rewritten system. We ensure that the resulting method is well-balanced by switching off the numerical diffusion when the computed solution is near (at) thermogeostrophic equilibrium. We verify the proposed schemes in some challenging one-dimensional examples and then use this novel method to investigate the similarities and differences in the predictions of the thermal and isothermal shallow water models for the fundamental dynamical processes: evolution of isolated vortices in the midlatitude β-plane in the presence of topography and relaxation of localized pressure and temperature perturbations in the equatorial β-plane.

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MS14

Detecting Physical Pathways with Software Profiling

Pathways, causal networks of physical processes, and their evolution are important for attributing climate affects to their sources. Modeling pathways in earth system models typically involves complex software projects that make use of large computers to approximate the state of the earth system and the changes it undergoes. Intuitively, the source code of an accurate climate model should encapsulate important physical pathways and there is a simulacrum of each model pathway and its evolution in the software code and infrastructure. In this talk we discuss using code profiling, employing statistics determined from software infrastructure, to trace a pathway and its evolution through the course of a simulation. We demonstrate the related numerical methods we develop on the quintessential example

of the 1991 Mt Pinatubo eruption.

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MS14

The Impact of Numerical Schemes on the Atmospheric Circulation in Weather and Climate Models

Atmospheric General Circulation Models (GCMs) consist of a fluid dynamics component, the so-called dynamical core, and a subgrid-scale physical parameterization package. The latter approximates the effects of unresolved motions on the resolved fluid flow. Both components contribute to the uncertainty of weather and climate simulations, but in fundamentally different ways. The paper sheds light on the impact of the dynamical cores and their numerical schemes on atmospheric motions. In particular, it is demonstrated how the computational grid, the characteristics of the numerical technique, and the dissipation mechanisms interact with a variety of physical flow phenomena. Examples from state-of-the-art weather and climate models are provided, such as the dynamical cores in the Department of Energys 'Energy Exascale Earth System Model' (E3SM), the Community Earth System Model (CESM) from the National Center for Atmospheric Research (NCAR), and NOAAs Unified Forecast System (UFS).

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MS14

Global Sensitivity Analysis Using the Ultra-Low Resolution Energy Exascale Earth System Model

For decades, the Arctic has been warming at least twice as fast as the rest of the globe. As a first step towards quantifying parametric uncertainty in Arctic feedbacks, we perform a variance-based global sensitivity analysis (GSA) using a fully-coupled, ultra-low resolution (ULR) configuration of version 1 of the Department of Energys Energy Exascale Earth System Model (E3SMv1). The study randomly draws 139 realizations of ten model parameters spanning three E3SMv1 components, which are used to generate 75-year long projections of future climate using a fixed pre-industrial forcing. We quantify the sensitivity of six Arctic-focused quantities of interest (QOIs) to these parameters using main effect, total effect and Sobol sensitivity indices computed with a Gaussian process (GP) emulator. A sensitivity index-based ranking of model parameters shows that the atmospheric parameters in the CLUBB (Cloud Layers Unified by Binormals) scheme have significant impact on sea ice status and the larger Arctic climate. We also use our GP emulator to predict the response of varying each variable when the impact of other parameters are averaged out. These results allow one to assess the non-linearity of a parameters impact on a QOI and investigate the presence of local minima encountered during the spin-up tuning process. Our study confirms the necessity of performing global analyses involving fully-coupled climate models, and motivates follow-on investigations involving the ULR model.

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MS14

Evaluation of Numerical Process Coupling Approaches in Global Atmosphere Simulation

The E3SM atmosphere model (EAM) consists of modular components that are each responsible for a different subset of processes: horizontal flow, cloud formation, etc. Primarily, the system state is advanced in time by sequential splitting: each component updates the state and passes it to the next component in the sequence. The associated splitting error of this approach depends heavily on the ordering of the sequence. One alternative is parallel splitting, where all components operate in parallel on the same state and then combine the results into a single updated state. Similarly, various approaches are applied for advancing components with differing time scales, including dribbling and multirate time integration methods. This work introduces an error analysis framework for identifying the coupling method splitting error independent of the other temporal discretization errors. The underlying semi-discrete approach, which assumes component integrations are done exactly, can help identify when better performance might be expected from one coupling approach over another. As a demonstration, the framework is used to evaluate sequential splitting, parallel splitting, dribbling, and multirate infinitesimal step integration methods applied to various components of EAM. The costs and benefits of the various methods are compared against the current sequential splitting approach. Prepared by LLNL under Contract DE-AC52-07NA27344.

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MS15

Structure-Preserving Finite Element Methods for

Fluids with Variable Density

This talk will discuss some recent work (joint with Francois Gay-Balmaz) on structure-preserving finite element methods for the incompressible Euler equations with variable density, as well as extensions to other systems like inhomogeneous, incompressible magnetohydrodynamics. Our numerical methods make use of the variational formulation of fluid dynamics on diffeomorphism groups. In this formulation, the fluid motion is regarded as a diffeomorphism of the fluid domain that extremizes an action functional: the time-integral of the fluid's kinetic energy minus its potential energy. It turns out that one can discretize this variational principle to construct finite element methods for fluid flow with several structure-preserving properties. In the case of magnetohydrodynamics, for example, our techniques lead to a method that exactly preserves energy, cross-helicity, magnetic helicity, incompressibility, and the divergence-free constraint on the magnetic field.

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MS15

Compatible Finite Element Spaces for Terrain Following Meshes

In this talk, we are presenting a new approach for compatible finite element discretizations for atmospheric flows on a terrain following mesh. In classical compatible finite element discretizations, the H(div)-velocity space involves the application of Piola transforms when mapping from a reference element to the physical element in order to guarantee normal continuity. In the case of a terrain following mesh, this causes an undesired coupling of the horizontal and vertical velocity components. We propose a new finite element space, that drops the Piola transform and introduce a hybridisable formulation with trace variables that are supported on horizontal cell faces in order to enforce the normal continuity of the velocity. Alongside the discrete formulation for various fluid equations, we discuss solver approaches that are compatible with them and present our latest numerical results.

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MS15

Conservative, High Order Reference Element Upwinding for Compatible Finite Element Methods in Geophysics

High frequency oscillations may be suppressed in Hamiltonian fluid systems without breaking energy conservation via the damping of additional invariants (eg: potential enstrophy, entropy). This may be achieved via the consistent upwinding of quantities that appear within the skew-symmetric operator of the Hamiltonian system. Such approaches include the well known anticipated potential vorticity method (APVM) and streamwise upwind Petrov Galerkin (SUPG) method. In this talk these methods will be compared to a new approach by which the basis functions are themselves upwinded within the reference element. This approach may be interpreted either as the Lagrangian advection of the basis functions themselves, or as a Taylor series correction that for higher order elements that includes both dissipative and backscatter terms. In the context of strong form differential operators, this new approach results in a consistent, conservative method, similar to SUPG (and unlike APVM, which is not consistent). When used in conjunction with weak form differentiation, the downwinded trial functions result in a method that is adjoint consistent. Comparisons against APVM and SUPG show that the results of the upwinded trial functions are almost indistinguishable from those for the SUPG method, in terms of both the kinetic energy spectra and potential enstrophy conservation, while both methods are clearly superior to APVM.

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MS15

Structure Preserving Transport Stabilized Finite Element Methods for Magnetohydrodynamics

The ideal magnetohydrodynamic equations, which can be used to study e.g. space weather, contain an underlying structure that leads to the conservation of quantities such as energy, cross-helicity, and magnetic helicity. Recently, there has been an effort to maintain these quantities after discretization in order to ensure more accurate long-term simulations. One way to achieve this is by means of mimetic methods, in which vector calculus identities hold discretely. In this talk, we consider the compatible finite element method, and review an existing discretization that conserves the aforementioned quantities, and further preserves the magnetic field's zero divergence property. We then discuss a shortcoming, given by a lack of transport stabilization, and consider possible paths of including the latter for the magnetic and velocity fields in the context of div- and curl-conforming finite element spaces. This is done while aiming not to compromise on the discrete structure preserving properties as much as possible. Finally, we present preliminary numerical results in terms of stabilization and structure preservation.

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MS16

Tipping in Spatially Extended Systems

In the current Anthropocene, there is a need to better understand the catastrophic effects that climate and land-use change may have on ecosystems, earth system components and the whole Earth system. The concept of tipping points and critical transitions contributes to this understanding. Tipping occurs in a system when it is forced outside the basin of attraction of the original equilibrium, resulting in a critical transition to an alternative, often less-desirable, stable state. The general belief and intuition, based on simple conceptual models of tipping elements (i.e. ordinary differential equations), is that tipping leads to reorganization of the full (sub)system. In this talk, I will review and explore tipping in conceptual, but spatially extended, and potentially spatially heterogeneous, models (i.e. partial differential equations). In these spatially explicit models, additional stable states can emerge that are not uniform in space, such as Turing patterns and coexistence states (part of the domain in one state, the rest in another state with a spatial interface or front between these regions), which can lead to a different tipping behaviour. In particular, in

these systems a tipping point might lead only to a slight restructuring of the system or to a tipping event in which only part of the spatial domain undergoes reorganization, limiting the impact of these events on the systems functioning.

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MS16

Rate-Induced Tipping of the Compost Bomb: Sizzling Summers, Heteroclinic Canards and Metastable Zombie Fires

The Arctic is the fastest warming region on Earth. Understanding how a rapidly changing climate change impacts Arctic systems is therefore an important challenge. This is the basis of the 'Compost-Bomb' instability, a theorized runaway heating of northern latitude peat soils when atmospheric temperature rises faster than some critical rate, first proposed in [Luke Cox, European Journal of Soil Science (2011), 62.1] and analysed in [Wieczorek et al, Proceedings of the Royal Society A (2011), 467.2129]. The Compost Bomb instability was one of the first examples of what is known as Rate-induced tipping or R-tipping. The key trigger for the compost bomb instability is heat produced by microbial respiration. Here, the original soil carbon and temperature model of Luke Cox is augmented with a non-monotone microbial respiration function, for a more realistic representation of the process. This gives rise to a meta-stable state, reproducing the results of [Khvorostyanov et al, Tellus (2008), 60B] where a complex PDE model is used. Two non-autonomous climate forcings are examined: (i) a rise in mean air temperature over decades (ii) a short-lived extreme weather event, with the rate-induced compost bomb observed in each. Using techniques of compactification, singular perturbation theory and desingularisation, we reduce the R-tipping problem to one of heteroclinic orbits, uncovering the tipping mechanism for each climate change scenario.

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MS16

Ice Ages as Tipping with Irregular Forcing

The Mid-Pleistocene Transition (MPT) is a shift from 41,000-year to about 100,000-year ice age cycles that occured roughly 1,000,000 years ago, as shown in proxy records. It is often considered as a change in internal climate dynamics and studied using simple conceptual models such as the one proposed by Saltzman and Maasch (1988). We show for such a simple model that the astronomical forcing (changes in effective solar radiation incoming to the Earth) and internal bistability can lead to a form of tipping that replicates features of the MPT in the records. The tipping observed in the model is connected to the theory of quasiperiodically forced dynamical systems and strange non-chaotic attractors. A key technique we use in our analysis is the computation of a non-autonomous saddle trajectory (a complement to a local pullback attractor and generalization to local pullback repeller). While for the model we use the technique relies on boundary-value solvers for delay-differential equations, it can be extended to more simulations of more complex systems.

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MS16

Extracting Tipping Criteria from Stochastic and Spatially Heterogeneous Ecosystem Simulations

Identification and classification of tipping points is based on the analysis of governing equations. Yet, one can only obtain these equations by taking a so-called mean-field approximation of the considered spatio-temporal stochastic process. This works when the number of system units is large, the environmental conditions are approximately spatially homogeneous, and random influences average out. In ecosystems such as tropical forests these assumptions are often violated: their size is finite, spreading processes such as plant dispersal or fire can generate large correlations and fluctuations, and environmental conditions are highly heterogeneous. For such cases, one could choose to work only with simulations of the spatio-temporal process in consideration, but due to the instability and intermittency near tipping points, this choice would turn out too computationally expensive. Hence, an approach is required that makes states that are rarely visited in conventional simulations accessible without relying on mean-field assumptions. We will show how feedback control applied to stochastic ecosystem simulations can be used to extract tipping criteria, even in more realistic heterogeneous settings, avoiding the mean-field altogether. We use as example a probabilistic cellular automaton of forest dynamics in the Amazon basin that includes fire percolation and rainfall feedback, and finally show which conservation scenarios can prevent collapse of the forest.

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MS17

Amplification of Flows and Waves under Simple Backscatter Closure

Motivated by numerical schemes for large scale geophysical flow, we consider the rotating shallow water and Boussinesq equations on the whole space with idealized horizontal kinetic energy backscatter source terms built from negative viscosity and stabilising hyperviscosity with constant parameters. We study the impact of this energy input through various explicit flows, including barotropic, parallel and Kolmogorov flows as well as monochromatic inertia gravity waves. With focus on stable stratification we find that the backscatter generates numerous solutions of this type that grow exponentially and unboundedly, which signifies the possibility of undesired energy concentration into

specific modes due to the backscatter.

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MS17

Data-Driven Modeling of Non-Local Mixing Phenomena in Geophysical Flows

Geophysical flows often feature mixing phenomena with a wide range of eddy sizes due to the effects of forcing and dissipation on large scales. In addition, many of them tend to exhibit mixing and no-mixing regions in statistically steady states, with eddies propagating finite distances between them. Therefore, a local closure model is sometimes not enough to accurately describe the mixing phenomena in geophysical flows, motivating us to explore non-local models that better account for mixing in geophysical flows. In this work, we propose an approach to construct neural-network-based model of non-local mixing that builds upon data-driven kernels. We test this approach by studying a barotropic flow driven by linear relaxation toward an unstable zonal jet. The results show that our approach achieves better extrapolation capability when training and testing on flows with different relaxation time and the reference unstable zonal jet. The approach also demonstrates the potential of constructing data-driven models of non-local mixing phenomena that can be generalized to different types of geophysical flows.

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MS18

The Theory, Science and Art of Data Assimilation for Earth System Prediction

Data assimilation is a powerful technique widely used for Earth system applications (atmosphere, ocean, sea ice, land, waves) to combine observations with a numerical model to produce forecasts that are better than observations or model alone. It is a multi-disciplinary science, combining elements of earth system science, remote sensing, instrumentation, applied mathematics, computer science, and electrical engineering. Data assimilation (DA) is a sequential process that mathematically combines observations with a model forecast (background) and their respective error estimates to obtain the best estimate of the current model state. These analyses have many applications, but are most often used to initialize the NWP model forecasts. Much of the art of DA involves estimating the observation and background error covariances, selecting a good mix of observations, and balancing system complexity against computational timing constraints. Over the past two decades, much of the increased weather forecast skill has been attributed to improvements in DA techniques and the effective assimilation satellite observations. Challenges for the next decade include DA for high resolution, coupled global earth system models. This will require development of computationally efficient methods to include non-Gaussian error distributions, allow for more nonlinearity and include additional probabilistic information from ensembles.

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MS18

Bridging Gaps in the Climate Observation Network: A Physics-based Nonlinear Dynamical Interpolation of Lagrangian Ice Floe Measurements via Data-Driven Stochastic Models

Modeling and understanding sea ice dynamics in marginal ice zones relies on acquiring Lagrangian ice floe measurements. However, optical satellite images are susceptible to atmospheric noise, leading to gaps in the retrieved time series of floe positions. This paper presents an efficient and statistically accurate nonlinear dynamical interpolation framework for recovering missing floe observations. It exploits a balanced physics-based and data-driven construction to address the challenges posed by the high-dimensional and nonlinear nature of the coupled atmosphere-ice-ocean system, where effective reduced-order stochastic models, nonlinear data assimilation, and simultaneous parameter estimation are systematically integrated. The new method succeeds in recovering the locations, curvatures, angular displacements, and the associated strong non-Gaussian distributions of the missing floes in the Beaufort Sea. It also accurately estimates floe thickness and recovers the unobserved underlying ocean field with an appropriate uncertainty quantification, advancing our understanding of Arctic climate.

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MS18

A Peridynamic Model of Sea Ice Dynamics

The Arctic has undergone significant changes in recent decades due to climate change, with substantial reductions in sea ice extent and multiyear ice, leading to thinner ice that is susceptible to breakup. This so called "New Arctic" presents many challenges including, but not limited to, accurately modeling sea ice dynamics, lead (crack) development, and ridge formation (sea ice floe collision). Particle methods, such as the discrete element method (DEM), can provide detailed descriptions of sea ice dynamics that explicitly model fracture and ridging, which can be challenging with typical continuum sea ice modeling approaches. However, large sea ice floes or consolidated pack ice can deform and break up under external forcing, which presents additional difficulties for a DEM to simulate these impor-

tant dynamics accurately. In this talk, we present our current efforts in extending sea ice DEM formulations to model sea ice mechanics with a novel peridynamic-DEM hybrid model. We will present results on idealized sea ice tests that examine the ability of the model to predict effective sea ice properties including effective stress, strength, and lead intersection angles. Lastly, we will present results from simulations of sea ice dynamics and lead formation in the Beaufort Sea and compare our results to optical satellite imagery to assess predictive capabilities.

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MS19

Modeling, Data Assimilation, and Forecasting of Fuel Moisture in Wildland Fires: From Kalman Filter to Deep Learning

The WRF-SFIRE modeling system couples a high-resolution multi-scale atmospheric model with a fire spread fire model by the level set method and a fuel moisture model. Modeling the evolution of fuel moisture is essential for the diurnal variability of wildfires over multiple days. The current fuel moisture code uses atmospheric variables (temperature, relative humidity, rain) to estimate the equilibrium fuel moisture contents, and then runs time-lag differential equation model of the time evolution of the moisture content, which is used in the computation of the fire progression. A version of the fuel moisture subsystem is first run for a spin-up period to estimate the state and the parameters at every grid node from weather data products and fuel moisture sensors on Remote Atmospheric Weather Stations (RAWS), using a combination of a spatial regression and an augmented extended Kalman filter. In the forecast mode, the differential equation model takes weather inputs from WRF. This talk is concerned with improvements of this fuel moisture model. A more sophisticated differential equation model can increase the accuracy. To increase the accuracy further, we replace the differential equation and the Kalman filter by a neural network to build a time-dependent model on a location from data. Satellite observations can be used to enhance the accuracy spatially.

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MS19

Valuating Fire Suppression Risk Data with a System of ODEs

Efficient and effective wildland fire response requires interregional coordination of suppression resources. We developed a mathematical model to examine how scarce resources are shared. Best-fit models describe regional resource allocation according to driving risk factors. By regressing a linear system of ordinary differential equations with GIS-data for demand predictors like suppression resource use, ongoing fire activity, fire weather metrics, accessibility, and population density onto pre-smoothed Resource Ordering Status System (ROSS) wildfire personnel and equipment requests, we fit a national scale model. We report statistical properties of the best-fit parameters and indicate how these findings might be interpreted for personnel and equipment sharing by examining test cases for national, central/southern Rockies, and California interregional sharing. Abrupt switching behavior across medium and high alert levels was found in test cases for national, central/southern Rockies, and California interregional sharing.

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MS19

A New Way to Look at Fire: Using AI to Describe Fire and Plume Behavior

When fire propagates through a fuel bed, there are a variety of structures and behaviors we wish to better understand. I will demonstrate how fire and plume behavior can be predicted by applying computer vision principles and adapted graph theory techniques to infrared and visual videos. The spatial and temporal scales resolved by this methodology are limited only by the cameras features. Data that quantifies the transport of heat and fire spread, turbulent statistical information, and near-field plume structure can be obtained from these videos and contribute to our understanding of fire and plume behavior. A statistical approach is used to analyze the data, and results indicate there are new ways of using statistical models to better describe the system dynamics. I will showcase analysis of sub-centimeter

scale results from an infrared video of fire spread. Current and future work that considers the fire-atmosphere coupling and heat transport will also be discussed.

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MS19

Bayesian Modelling of Wildfire Rate of Spread

Operational bushfire rate of spread models (ROS) are valuable assets in a fire behaviour analysts toolkit. Models are usually deterministic, meaning that a single predicted rate of spread value is produced for a given set of inputs (wind speed, temperature etc.). However, a great deal of uncertainty should be expected when predicting ROS, given the complex and chaotic nature of bushfires. A second issue is that historically, there has been a lack of bushfire observations available for model development, due to the difficulty involved in monitoring actual bushfires. In our work, we present an approach that can address these issues by: 1) using a Bayesian statistical approach that better accounts for ROS modelling uncertainty, 2) using ROS data acquired via aerial line scans over actual bushfires. Line scanning methods have been refined by fire agencies and aviation companies, and currently provide the most accurate way to measure ROS. We used fire agency (RFS and DELWP) line scans collected between 2002 and 2018 to create 223 ROS observations.

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MS20

Delayed Loss of Stability in Models for Glacial Cycles

In a series of papers in the 1990s, K. Maasch and B. Saltzman proposed a mechanism for the mid-Pleistocene transition based on a system of ordinary differential equations and on the combined effects of slow changes over time of some physical parameters, for example due to plate tectonics, and of orbital forcing. Maasch and Saltzman showed that the proposed mechanism leads to time series that share a number of central qualitative characteristics with the observed data from ice core samples over the entire Pleistocene Epoch. This talk will show that their model actually permits several different mechanisms for such a transition and will then focus on the most interesting one, namely delayed loss of stability in a dynamic Hopf bifurcation in the presence of periodic or quasiperiodic forcing. Evidence will be presented that nonlinear coupling can cause resonances in the case of multifrequency forcing which will then result in a shorter delay than in the case of single frequency forcing. The mathematical challenges for characterizing such scenarios rigorously will be outlined.

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MS20

Overshoots and Rate-Induced Tipping in Conceptual Climate Models

Previous studies report low global warming thresholds above pre-industrial conditions for key tipping elements such as ice-sheet melt. If so, high contemporary rates of warming imply that exceeding these thresholds is almost inevitable, which is widely assumed to mean that we are now committed to suffering these so called bifurcation-induced tipping events. Here we show that this assumption may be flawed, especially for slow-onset tipping elements (such as the collapse of the Atlantic Meridional Overturning Circulation (AMOC)) in our rapidly changing climate. We demonstrate, using conceptual climate models, that a threshold may be temporarily exceeded without prompting a change of system state, if the overshoot time is short compared to the effective timescale of the tipping element. On the other hand, systems may exhibit rate-induced tipping points instead of (or as well as) bifurcation-induced tipping, where a system fails to adapt to rapidly changing external forcing. Such tipping points are much less widely known, and yet are arguably even more relevant to contemporary issues such as climate change. We illustrate this phenomenon using a model for the AMOC and the possibility of avoiding tipping by reversing the forcing. This has the potential to lead to multiple critical rates for the same maximal change as the low rates required to avoid rate-induced tipping compete against the fast rates required for safe overshoots.

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MS21

Data-Driven Dynamics of Phytoplankton Blooms in a Reaction-Diffusion NPZ Model

Phytoplankton are the base of the marine food web. They

are also responsible for much of the oxygen we breathe, and they remove carbon dioxide from the atmosphere. The mechanisms that govern the timing of seasonal phytoplankton blooms is one of the most debated topics in oceanography. Here, we present a macroscale plankton ecology model consisting of coupled, nonlinear reaction-diffusion equations with spatially and temporally changing coefficients to offer insight into the causes of phytoplankton blooms. This model simulates biological interactions between nutrients, phytoplankton and zooplankton. It also incorporates seasonally varying solar radiation, diffusion and depth of the oceans upper mixed layer because of their impact on phytoplankton growth. The models predictions are dependent on the dynamical behavior of the model. The model is analyzed using seasonal oceanic data with the goals of understanding the models dependence on its parameters and of understanding seasonal changes in plankton biomass. A study of varying parameter values and the resulting effects on the solutions, the stability of the steady-states, and the timing of phytoplankton blooms is carried out. The models simulated blooms result from a temporary attraction to one of the models steady-states.

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MS21

Machine Learning Methods for Advancing Biogeochemical Modeling and Carbon Cycle Understanding

Machine learning (ML) methods are powerful in extracting patterns, discovering new knowledge from multi-scale, multi-types of data, and identifying underlying cause-effect relationships for predictive understanding. In this presentation, I will talk about how to leverage ML to advance biogeochemical modeling and carbon cycle understanding. First, I will discuss different ML-based surrogate modeling techniques for building fast-to-evaluate emulators of the simulation models and thus accelerating model calibration. These techniques include dimension reduction, neural networks learning and Bayesian optimization. Additionally, I will introduce an invertible neural network method that can solve model calibration problems directly and computationally efficiently. Lastly, I will describe an interpretable ML method for dynamical system learning from time series observations. I will demonstrate these methods using terrestrial ecosystem biogeochemical models for improving carbon flux prediction and carbon cycle understanding.

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MS21

A Network Theory Perspective on Ocean Dynamics and its Application to Marine Ecology and Climate

I will introduce a network framework developed for the characterization of fluid transport dynamics in the ocean. The discretisation of the sea surface in equal-sized cells brings to the construction of a new kind of networks, called Lagrangian Flow Networks, describing water exchanges between different regions of the seascape. Using Network Theory concepts tools we can study dispersion and mixing at both local and global scales evidencing relationships between network measures and dynamical properties of the flow. Among possible applications, I will show how such a framework could provide insights on marine metapopulation ecology and climate science.

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MS21

Mathematical and Computational Perspectives in Marine Biogeochemistry and the Oceans Carbon Cycle: an Overview

Over the past 40 years, our knowledge in marine biogeochemical cycles and processes (such as the biological carbon pump, hereafter BCP) has grown tremendously, particularly thanks to the fruitful combination of many dedicated expeditions that have been carried since the 1980s, and to the advent of marine biogeochemical models in the late 1980s and 1990s which are now integral part of the most advanced CMIP-like Earth System models used for climate modelling. Despite that, we are relatively far from understanding and quantifying important biogeochemical processes such as the BCP: for instance, the carbon fluxes from the ocean surface to deep ocean are only poorly quantified, and we also lack a consensual understanding of what processes might influence these fluxes particularly in the mesopelagic ocean. In this talk I will review these topics and will conclude by discussing some of the difficulties I have found in advancing in this area, as well as some ideas on how to overcome these difficulties - particularly with the aid of mathematical sciences. I aim to tailor this talk to a non-expert audience so that it should be accessible to anyone with a scientific background no previous knowledge of marine biogeochemistry should be required.

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MS22

Thermal Instability of Surface-Intensified Eddies as Precursor of Sargassum Inundation in the Caribbean Sea

Geometric fluid *mechanics* casts new light on the problem of *Sargassum* inundation in the Caribbean Sea. On one hand, recent nonlinear dynamical systems results pertaining to the fluid *kinematics* identify the carriers of *Sargassum* with coherent Lagrangian vortices whose (flow-invariant) boundaries defy stretching. These vortices possess finite-time attractors for the cargo, viz., *Sargassum* rafts modeled as elastic networks of inertial particles, which makes transportation by ocean currents and winds effective. On the other hand, a two-dimensional model of baroclinic Caribbean Sea eddy *dynamics* with buoyancy inhomogeneity and Lie-Poisson Hamiltonian structure identifies thermal instability mediated by bottom topography as a mechanism for filamentation and ensuing coastal inundation. The results are consequential for the prediction of *Sargassum* arrival, and thus for response and planning. This is joint work with F.J. Beron-Vera, G.J. Goni, D.

Karrasch, M.J. Olascoaga and J. Trinanes.

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MS22

Coherent Dipoles in a Mixed Layer with Variable Buoyancy: Theory Compared to Observations

Motivated by recent observations of long-living dipolar cycloneanticyclone structures in the ocean and their signature in the surface temperature field, we report the existence of an exact dipolar solution (modon) in the one-layer thermal quasi-geostrophic equation, which is an generalization of the standard quasi-geostrophic equations to include buoyancy or temperature as an active tracer. The properties of such "thermal modons, and especially their ability to carry heat anomaly over long distances, depend on the relative sign of the associated vorticity and buoyancy anomalies. We show using numerical simulations with the thermal shallow water equations, and their quasi-geostrophic version, that the evolution of the modons is consistent with the observations. The existence of a small scale instability that can lead to a complete destruction of the dipole and mixing of the associated buoyancy field is further discussed, supported by dedicated numerical experiments.

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MS22

Stochastic Modelling of Thermal Ocean Dynamics

Introducing stochasticity into models for thermal ocean dynamics is becoming a popular approach to help quantify uncertainty. This also comes with an important challenge. Many models of thermal ocean dynamics are derived from the Euler equations for a three dimensional ideal fluid under the influence of rotation and buoyancy stratification. Are such derivations consistent with the introduction of stochasticity? What would be a criterion for an admissible thermal ocean model with noise? The field of geometric mechanics helps to answer such questions and can give a road map overview of stochastic thermal ocean dynamics.

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MS23

Persistent Atmospheric Extreme Events from a Large Deviation Perspective: Typical Structures and Probability Estimates

Persistent atmospheric extreme events, like heatwaves, cold spells, rainfall events of several days, have a huge impact since they exert a long-lasting anomalous stress on human health, infrastructure and natural ecosystems. I will present in this talk a method to analyse persistent extreme events based on large deviation theory, discussing two applications: an analysis of heatwaves and cold spells as temporal averages of surface air temperature and a study of rare and persistent configurations of the North Atlantic jet stream based on temporal averages of jet indices. In both cases, the probability of persistent events can be obtained based on a large deviation principle for averaging block lengths larger or equal than 1-2 months. Furthermore, based on their spatial structure, we find that these events are very similar to each other, corresponding to the large deviation concept of typical unlikely events. Additionally, we assess the change in probability of heatwaves due to global warming, and the effect of persistent jet anomalies on the frequency of temperature and precipitation extremes over Europe.

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MS23

Facilitating Atmospheric Source Inversion via Operator Regression

Climate effects are caused by a combination of confounding sources which interact with the climate system through various feedbacks. The interaction of these sources makes it very challenging to attribute how much a given source contributed to the observed climate effect. A big picture goal to enable climate attribution is to characterize uncertainties and dependences in and between sources to understand their interaction. This may be posed as a Bayesian inverse problem constrained by a climate model. However, the computational cost of climate simulators mandate surrogate models to enable the many query algorithms required for exploration of the inverse problem. Traditional approaches construct surrogate models for quantities of interest known to be important in the climate system. Such approaches are insufficient for the source inversion problems of interest as they fail to capture the feedback mechanisms which are crucial for informing the inverse problem. We present work developing neural network based operator surrogates for flow maps which are used to trace pathways through the climate system and thus facilitate atmospheric source inversion. We consider a prototypical test problem inverting for SO2 emissions from volcanic eruptions. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525. SAND2022-0896 A.

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MS23

Eddy Saturation in a Reduced Two-Level Model of the Atmosphere

Eddy saturation describes the nonlinear mechanism in geophysical flows whereby, when average conditions are considered, direct forcing of the zonal flow increases the eddy kinetic energy, while the energy associated with the zonal flow does not increase. We present a minimal baroclinic model that exhibits complete eddy saturation. Starting from Phillips classical quasi-geostrophic two-level model on the beta channel of the mid-latitudes, we derive a reduced order model comprising of six ordinary differential equations including parameterised eddies. This model features two physically realisable steady state solutions, one a

purely zonal flow and one where, additionally, finite eddy motions are present. As the baroclinic forcing in the form of diabatic heating is increased, the zonal solution loses stability and the eddy solution becomes attracting. After this bifurcation, the zonal components of the solution are independent of the baroclinic forcing, and the excess of heat in the low latitudes is efficiently transported northwards by finite eddies, in the spirit of baroclinic adjustment.

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MS23

Monotone Remapping Schemes on Arbitrary Grids

Coupled climate models with multiple components, such as atmosphere and ocean models, involve remapping operators to map information between the grid of each component. As these operators are often parts of long-term time integration schemes, their accuracy is of critical importance, so as not to introduce errors that accumulate over time and render the scheme unstable. Two requirements that are often imposed on remapping operators are that they are monotone, in the sense that no new extrema are created in the remapping process, and that they are consistent, so that the constant field is maintained across the remapping operation. While high order accuracy and monotonicity are often achieved through nonlinear operations such as slope-limiting, in this study, we describe a linear, second order monotone remapping scheme, and compare it to those that are currently in use in models such as the Earth System Modeling Framework (ESMF).

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MS25

Cyclic Ecosystems Subject to Climate Variability: Phase Tipping and Stochastic Resonance

Global warming is expected to lead to greater amplitudes and higher autocorrelation in climate variability. In this work, we explore how these changes could impact cyclic ecosystems, namely, predator-prey systems. Our analysis reveals a counter-intuitive behaviour, which we call phase tipping (or P-tipping), where the stable limit cycle persists, yet transitions to extinction occur from certain cycle phases. We use actual climate records from the boreal and deciduous-boreal forest in North America to show that tipping to extinction is possible under predicted changes in climate variability for the Canada lynx and snowshoe hare. Furthermore, we point out that there is an increasing tipping sensitivity to changes in climate variability at an intermediate noise level in the form of stochastic resonance. One noticeable implication of this phenomenon is that global warming leads to a higher likelihood of tipping events.

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MS25

Nonautonomous Dynamical Systems and Topological Tipping Points in the Climate Sciences

The dynamics of systems with time-dependent forcing or coefficients has become a matter of considerable interest in the last couple of decades in general and in the last dozen years or so in the climate sciences in particular (Ghil, 2019; Ghil & Lucarini, 2020; Ghil, 2021; Tel et al., 2021). We shall provide a general introduction to the topic and illustrate it with several climate-related examples. In the process of investigating in greater depth the properties of random attractors arising from multiplicative random perturbations of chaotic systems, Char et al. (2021) applied a novel method of topological data analysis, namely Branched Manifold Analysis through Homologies (BraMAH). They discovered abrupt changes in the homology groups of these time-evolving manifolds and labeled them topological tipping points (TTPs). Active research is proceeding on early warning signals for these TTPs. Perspectives for further applications of the concepts and methods of the theory of pullback and random attractors and of their tipping points to the climate sciences will conclude the talk.

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MS25

Rate-Induced Tipping in Reaction-Diffusion Problems: The Rise and Fall of Geographically Shifting Ecosystems

We introduce and analyse mathematical models that describe the spatial distributions of migratory species when subject to a geographically shifting habitat. These models are underpinned by reaction-diffusion equations that are heterogeneous in space and nonautonomous in time. To address this problem (as well as a wider class of problems), we propose a methodology that combines a compactification technique together with Lin's method for connecting heteroclinic orbits implemented in conjunction with numerical continuation. This allows for the transformation of a travelling-pulse problem into a heteroclinic orbit problem in the compactified system. Using our methodology, we identify and study two classes of tipping points in reaction-diffusion systems. Bifurcation-induced tipping causes the current state to become unstable when an environmental parameter goes through a critical level underpinned by a bifurcation of the autonomous system. Rate-induced tipping, the focus of this study, occurs when the slow components of the system change faster than some critical rate; this is underpinned by critical speeds of the moving habitat. Finally, we identify parameter boundaries for tipping points and determine how these boundaries depend on the size of the habitat, the speed of climate shifts, and dispersal rates of the migrating species.

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MS25

Rate and Noise Tipping Working in Concert

We present a theory for understanding tipping events in low-dimensional dynamical systems with additive noise and time-dependent parameters, whose interplay results in a large increase in the frequency of tipping. While rate-induced tipping does not require any random fluctuations within the system, the ramp parameter and added noise can conspire to cause tipping of the system below the critical rate. Building on the work of Ritchie and Sieber (2016), who considered rates close to the critical rate, we first consider a one-dimensional differential equation with additive noise and a ramp parameter. In this model, using the Fredlin-Wentzell theory, we show that there exists a heteroclinic connection in extended phase space between equilibria for all rates less than the critical rate. This heteroclinic orbit is a minimizer of the Freidlin-Wentzell functional and thus corresponds to the most probable path between these two points. We then extend this framework to show the existence of the most probable path for a fairly general class of functions. We construct this most probable path using geometric dynamical systems methods, as well as present numerical simulations for verification and visualization of this most probable path. We illustrate the utility of this framework by applying it to conceptual climate models where the ramp parameter corresponds to planetary warming.

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MS26

Sharp Spatial Transitions and the Predictive Power of Niche Models for Plankton in a Warming Ocean

Niche models derived using statistical machine learning approaches are increasingly used to predict how ecological communities will shift on a warming planet. Here, we argue that these models are more likely predictive if they, or their dependent variables, can independently explain population fluctuations across multiple distinct spatial-temporal scales. We apply this idea to the ocean, focusing on a well established niche model for the globally dominant phytoplankton species *Prochlorococcus*, exploring whether the dependent variables in this model, temperature and light, correlate with either temporal fluctuations from a long-term monitoring site or the spatial-temporal location of sharp transitions in the species' abundance. We find that local fluctuations in surface abundance from the Hawaii Ocean Time Series Station correlate weakly with changes in temperature and light. Spatial transitions also correlate weakly but do occur at temperatures greater than the experimentally measured viability temperature for this species. A two-state model based on this observation explains the majority of the variance contained in the original, but by definition has no predictive capability on abundance changes within the species range. This result reconciles recent work demonstrating that niche and global computational models for *Prochlorococcus* predict opposing trends as the ocean warms.

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MS26

Linking Plankton Size Spectra and Community Composition to Carbon Export and its Efficiency

The magnitude and efficiency of particulate carbon export from the ocean surface depends not only on net primary production (NPP) but also on how carbon is consumed, respired, and repackaged by organisms. We contend that several of these processes can be captured by the size spectrum of the plankton community. However, most global models have relatively simple food-web structures that are unable to generate plankton size-spectra. Moreover, the life-cycles of multicellular zooplankton are typically not resolved, restricting the ability of models to represent time-lags that are known to impact carbon export and its efficiency (pe-ratio). Here, we use a global mechanistic size-spectrum model of the marine plankton community to investigate how particulate export and pe-ratio relate to the community size spectrum, community composition, and time-lags between predators and prey. The model generates emergent food-webs with associated size distributions for organisms and detrital particles. We also implement the life-cycle of multicellular zooplankton (here represented by copepods). We find that carbon export correlates best with copepod biomass and trophic level, whereas the pe-ratio correlates best with the exponent of the size spectrum and sea surface temperature (SST). Community metrics performed better than NPP or SST for both deep export and pe-ratio. Time-lags between phytoplankton and copepods did not strongly affect export or pe-ratio.

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MS26

Cross-Scale Oceanographic Drivers of Human Activity on the Oceans

Forecasting human impacts on Earths biodiversity is key to preventing further losses of species and the key ecosystems services they provide. Of particular concern is the impact we are having on the oceans biodiversity through fishing. Here, we examine the cross-scale oceanographic drivers of spatial patterns of fishing. We utilize a variety of data: information on the spatial connectivity of marine populations driven by ocean currents, on convergence zones identified as Lagrangian Coherent Structures, as well as high frequency vessel location data. With these data we can identify the physical, biological and chemical drivers of the spatial patterns of fishing at multiple spatial and temporal scales. Doing so can help us identify improved approaches to spatial fisheries management, as well as approaches to conservation like the design of marine protected areas.

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MS26

A Unified Theory for Organic Matter Accumulation

Seemingly competing hypotheses have been proposed to explain organic matter accumulation in the ocean and other natural environments. Using a mechanistic model, we have developed a new theoretical framework that explains how organic matter predictably accumulates due to biochemical, ecological, and environmental factors, which subsumes previous hypotheses. The framework derives from the ecological dynamics of microorganisms, the dominant consumers of organic matter.

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MS27

Machine Learning Forecast of Conditional Statistics As Ensemble Members: A New Ensemble Forecast Algorithm for Complex Turbulent Systems

Ensemble forecast is important for complex turbulent systems. The traditional ensemble forecast replies on a Monte Carlo (MC) simulation of the given system. However, due to the curse of dimensionality, only a small number of ensembles is affordable in practice. Therefore, despite the reasonable skill in the ensemble mean, it is hard to characterize the entire probability density function (PDF), especially for non-Gaussian behavior and extreme events. In this talk, I will present a new ensemble forecast method. It has three steps. The first step involves a systematic decomposition of the target non-Gaussian PDF into a small number of Gaussian PDFs using a data assimilation method. The decomposition here is very different from the traditional kernel density estimation. Rigorous analysis shows that the new method avoids the curse of dimensionality. In the second step, we can write down the exact closed analytic formulae for the time evolution of the mean and covariance of each Gaussian component. This avoids sampling errors and is already much more reliable than the MC simulations. Finally, we build a neural network to approximate the most complicated part of the time evolution of the statistics, which further accelerates the computation. An information criterion is used as the loss function, which is shown to outweighs the traditional MSE loss. The method will be applied to some geophysical flows for numerical illustrations.

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MS27

Data Driven Representation of Un(der)resolved Processes in Atmospheric Models: A Case Study of Gravity Waves and the QBO

Gravity waves, or buoyancy waves, so named because their restoring force is the action of gravity on a stratified fluid, present a challenge to atmospheric modeling. They play an important role in the circulation by transporting momentum, but cannot be properly resolved in global models. Further, many of their sources, e.g., moist convection, are themselves not directly represented. Gravity wave impacts must therefore be approximated, or parameterized, based on the resolved flow. New observations have raised hope for a data driven approach to gravity wave parameterization. We first demonstrate the potential for machine learning to capture gravity wave momentum transport. We focus on a macroscopic effect of gravity waves on the circulation, the Quasi-Biennial Oscillation (QBO), a 28 month oscillation of jets in the tropical stratosphere. Neural network and regression tree approaches can successfully emulate an existing, physics based parameterization. Most critically, schemes trained on limited data successfully emulate out-of-sample conditions when coupled online with the model. We then turn to the question of calibrating data driven parameterizations to work with an imperfect atmospheric model (emphasizing that all models are imperfect), formulating a 1-D model of the QBO as a test bed. The simple 1-D model allows us to explore techniques to calibrate data drives schemes to compensate for biases in the resolve flow and gravity wave sources.

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MS27

Mesoscale Convective Systems in a Hierarchy of

Models

Mesoscale convective systems (MCSs) account for 50-70% of warm season precipitation in the central U.S. With high intensity rainfall covering large area, MCSs are also responsible for most of the slow-rising and hybrid floods in the U.S. east of the Rocky Mountains. MCSs develop under different environments featuring frontal systems and the Great Plains low-level jet providing a lifting mechanism and moist environment for their initiation. During summer, eastward propagating sub-synoptic perturbations are crucial for MCS initiation under unfavorable large-scale circulations. MCSs have been producing more intense precipitation and lasting longer in the last 35 years, motivating the need to understand how they may change in the future. However, MCSs are notoriously difficult to simulate, as even convection permitting simulations underestimate MCS number and precipitation in the central U.S., particularly during summer. Using a hierarchy of models including a Lagrangian parcel model, regional and global convection permitting models, global climate models with and without a superparameterization, and a tracer-enabled land surface model, we study MCSs, their large-scale environments, their role in land-atmosphere interactions, and the mechanisms of their response to global warming.

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MT1

Melancholia States in Climate Models

See session abstract.

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MT1

Bifurcation Analysis of Global Ocean Models

See session abstract.

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MT1

Equation-Free Bifurcation Analysis of Multi-Agent/Individual Simulations for Tipping Points

See session abstract.

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MT1

Applying Control to Find Unstable States

See session abstract.

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MT2

Statistical Methods for Analyzing Climate Extremes

See session abstract.

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