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IP1

Thin Film Fluid Dynamics Problems with Applications in Materials Science

Thin fluid films with free surfaces are ubiquitous in nature (e.g. a layer of rainwater on a rock face) and in a range of industrial applications (e.g. painting or coating processes). Flows of this kind are characterized by a separation in length scales, with the typical film height being small compared to the characteristic lateral length scale, which allows asymptotic long-wave methods to be used to simplify the problem and reduce it to a nonlinear parabolic partial differential equation (first-order in time, fourth-order in space) governing the evolution of the film height, h. Such flows can be especially interesting when the fluid has complex rheology, when it interacts with the underlying substrate, and/or when other external energy sources are involved in driving flow. We will discuss these flows, with a particular focus on pattern formation in nanoscale thin films of nematic liquid crystals (NLCs) that interact strongly with the substrate. If time permits we will also discuss other scenarios that this type of model can describe, such as the evolution of laser-irradiated metal films that, on melting, break up into droplets relevant for metallic nanoparticle manufacture. The governing PDEs are strongly nonlinear and may be stiff, hence to describe experimental-scale scenarios we implement a highly efficient numerical scheme on GPUs, finding excellent qualitative agreement with experimental results (where available).

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IP2

Liquid Crystal Polymeric Networks: Modeling, Approximation, and Computation

We discuss modeling, numerical analysis and computation of liquid crystal networks (LCNs). These materials couple a nematic liquid crystal with a rubbery material. When actuated with heat or light, the interaction of the liquid crystal with the rubber creates complex shapes. Thin bodies of LCNs are natural candidates for soft robotics applications. We start from the classical 3D trace energy formula and derive a reduced 2D membrane energy as the formal asymptotic limit of vanishing thickness and characterize the zero energy deformations. We design a sound numerical method and prove its Gamma convergence despite the strong nonlinearity and lack of convexity properties of the membrane energy. We present computations showing the geometric effects that arise from liquid crystal defects as well as computations of nonisometric origami within and beyond the theory. This work is joint with L. Bouck and S. Yang.

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IP3

Characterizations of Symmetric Polyconvexity and Applications in Geometrically Linear Theory of Elasticity

Energy minimization in the setting of the geometrically linear theory of elasticity typically involves relaxation theory and thus the notion of symmetric quasiconvexity. A sufficient condition for this is symmetric polyconvexity; a necessary condition is symmetric rank-one convexity. A characterization and deeper understanding of these notions and their relation is thus of fundamental interest. In this talk I will present related key results and show applications to martensitic phase transformations. This is in particular based on joint work with Omar Boussaid and Carolin Kreisbeck.

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IP4

Defects at Grain Boundaries: at the Frontiers of Variational Analysis for Material Defects

To Follow

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IP5

Integral Systems for Electron Kinetic Transport Mean Field Theory Problems Applied to Plasmas in Solid States and Soft Condensed Matter

We present an overview of kinetic transport systems for mean field theories arising in statistical mathematical physics phenomena. These systems model electron transport properties of dissipative nature by means of solving Vlasov-Boltzmann/Landau-Poisson, or Vlasov-Maxwell/Poisson. The dissipation mechanisms arises the dynamics mean field theories and particle interactions for the mixing of different species, usually modeled in plasmas, soft condensed matter and solid states. These type of systems can describe different phenomena, ranging from hot transport in nano-electronics with rough boundary conditions; coupled evolution of gaseous and condensed interactions in modeling Bose Einstein Condensation by the Quantum Boltzmann-Shroedinger system for braking of symmetry in soft condensed matter; to weak turbulence formation for electrostatic and highly magnetized plasmas, both in ergodic systems. We show a few examples and focus in their common points and differences. One novelty is the identification of system conserved quantities by focusing on the coupling mechanisms. This can be achieved by modeling the their system components, usually defined in different external domains, coercing their interactions through a dispersion relation and a resonance condition defining the conserved system quantities. As a consequence, one can identify weak formulations of such kinetic models, often view as their master or generating equations, which enables the development of unconditional conservative analytical and numerical schemes by Galerkin type methods. This property is of fundamental importance to obtain scheme stability and longtime behavior of analytical and computational solutions. This presentation collects work in collaboration with Ricardo Alonso, Jose Morales Escalante, Kun Huang, Minh Binh Tran, Michael Abdelmalik and Boris Briezman.

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IP6

Quantum-Accurate Large-Scale Atomistic Simulation of Materials with LAMMPS and FitSNAP*

Molecular dynamics (MD) is a powerful materials simulation approach whose accuracy is limited by the interatomic potential (IAP). The quest for improved accuracy has resulted in a decades-long growth in the complexity of IAPs, many of which are now implemented in the LAMMPS MD code[1]. Traditional physics-based IAPs are now being rapidly supplanted by machine-learning potentials (MLIAPs). The SNAP (Spectral Neighbor Analysis Potential) machine-learning approach is one example of this[2]. SNAP is formulated in terms of a set of general four-body descriptors that characterize the local neighborhood of each atom. The FitSNAP software[3], tightly integrated with LAMMPS, provides an automated methodology for generating accurate and robust application-specific MLIAPs. This approach has been used to develop potentials for diverse materials, including metal alloys, semiconductors, plasma-facing materials, and even magnetic materials such as iron. Each SNAP MLIAP is trained on quantum electronic structure calculations of energy, force, and stress for many small configurations of atoms. The resultant potentials enable high-fidelity large-scale MD simulations of these materials, yielding insight into their behavior on lengthscales and timescales unreachable by other methods. The relatively large computational cost of SNAP is offset by combining LAMMPS' spatial parallel algorithms with Kokkos-based hierarchical multithreading, enabling the efficient use of Exa-scale CPU and GPU platforms, allowing large-scale production simulations at 30 ns/day with millions to billions of atoms. Finally, I will discuss extensions of FitSNAP and LAMMPS to handle other MLIAPs, including neural network libraries and the more general Atomic Cluster Expansion descriptors. [1] Thompson et al., Comp. Phys. Comm., 271:108171, 2022. DOI 10.1016/j.cpc.2021.108171 [2] Thompson et al., J. Comp. Phys., 285:316, 2015. DOI 10.1016/j.jcp.2014.12.018 [3] Rohskopf et al., Journal of Open Source Software, 8: 5118, 2023. DOI 10.21105/joss.05118

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IP7

Advances in Massively Parallel Electronic Structure Calculations Based on High-Order Finite Difference Approaches

In this lecture, I will present recent advances in practical massively parallel electronic structure calculations based on high-order finite-difference approaches, as implemented in PARSEC (pseudopotential algorithm for real-space electronic structure calculations). I will first present the essentials of the method and explain its promise for large-scale applications. I will then focus on progress in grid representation, designed to minimize grid aliasing errors and optimize parallelization. Throughout, I will show practical examples ranging from structure optimization to molecular dynamics.

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IP8

Surrogate Modeling in Multiscale Computing

Multiscale modeling aims to describe the behavior of a complex system by combining models of the system's response at relevant scales. The approach has been remarkably successful in many areas of science and engineering, such as materials science, chemical engineering or climate modeling, and has yielded many high-fidelity models. Multiscale modeling is primarily a computational undertaking and the process of constructing and deploying multiscale computer models is now often referred to as multiscale computing. Yet, the success of multiscale computing is hindered by the staggering computational cost of at-scale models. In this talk, we chronicle our forays into multiscale computing. We start by describing a multiscale model of an energetic material in which both the equation-of-state and chemical decomposition information are obtained directly from lower-scale computer models. Even this relatively simple two-scale model proves to be computationally extremely expensive, leading us to explore the use of surrogate modeling to lower the cost of at-scale models. We examine a number of approaches for constructing surrogate models, and elaborate on their advantages and drawbacks. We also emphasize the need for incorporating dimensionality reduction into surrogate modeling and present an example of a surrogate model based on this principle. Finally, we chart a path forward and list some of the open problems in surrogate modeling in multiscale modeling/computing.

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IP9

A New Class of Numerical Methods with Computational Intelligence for Materials Processing and Layered Additive Manufacturing

Coupled thermo-chemo-mechanical phenomena involving fluid infused solids appear in many problems of scientific and engineering interests. Examples include thermochemical curing in advanced materials processing, reactive flows through porous deformable solids, and growth of soft biological tissues, to name a few. This talk focuses on the mathematical structure of new numerical methods that have embedded computational intelligence. Specifically, the Variational Multiscale Discontinuous Galerkin (VMDG) method is presented where multiscale decomposition of the unknown fields into coarse- and fine-scales leads to a hierarchically coupled system of equations. The coarse-scale equations describe physics at the global level while the fine-scale equations that operate on the residuals of the coarse system facilitate various modeling options to develop residual-based closure models. A systematic approach for variationally deriving analytical expressions for residual-based closure models is presented. These models represent missing physics which is variationally injected in the coarse-scale equations, thereby resulting in stabilized methods with enhanced accuracy properties. The proposed methods come equipped with a posteriori error estimator that can be exploited to investigate the accuracy of the solution during the complex phase evolution stages in continuous processing of materials. The constitutive relations for the solid-fluid system are developed in the context of mixture theory for multi-constituent materials. Evolving nonlinearities and coupled thermo-chemical effects give rise

to spatially localized phenomena that exhibit shear bands, steep gradients, and boundary and/or internal layers, and serve as good test cases to investigate the mathematical attributes of the method. The VMDG method is extended to the class of problems where interfaces traverse through the computational grids, giving rise to Immersed Methods for material deposition and processing in layered 3D printing. The mathematical constructs of the VMDG method also provide an avenue for data-driven discrepancy modeling wherein first-principles based models are augmented with variationally derived loss function. Several numerical test cases are presented that highlight the significance of enhanced stability and higher spatial accuracy in the modeling of the dynamic processes taking place during advanced materials manufacture.

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IP10

Boundary Defects in Liquid Crystals

We study the effect of "weak" and "strong" boundary conditions on the location and type of defects observed in a Landau de Gennes thin-film model for liquid crystals. We study both the minimizers of the associated Ginzburg-Landau energy as well as the Gamma limit when the correlation length tends to zero. A-priori estimates in case splay and bend moduli are included in the energy will also be presented. These represent joint works with S. Alama, L. van Brussel, A. Colinet and D. Stantejsky.

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IP11

Homogenization for Soft Composite Materials

Soft materials are materials that can undergo finite deformations under normal operating conditions. They include particle- and fiber-reinforced rubbers, thermoplastic and magnetorheological elastomers, polymer and metal foams, muscle and other biological tissues, as well as complex fluids, such as blood, toothpaste and other gels and even metals and rocks at high temperatures or rates of deformation. As a consequence of the finite deformations involved, their microstructure evolves with the deformation and their constitutive or rheological behavior can be highly nonlinear and anisotropic. This presents a challenge for the application of homogenization methods, which were originally developed to characterize the effective or homogenized constants of a composite, such as, for example, the Youngs modulus of an isotropic metal polycrystal. In this presentation, I will review various methods that have been developed to characterize the nonlinear multi-physics constitutive response of soft composites, as well as the evolution of the microstructure and the possible development of instabilities in such material systems.

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IP12

Origami Metamaterials

We study the geometric mechanics of origami assemblages and investigate how geometry affects behavior and properties. Understanding origami from a structural standpoint allows for conceptualizing and designing feasible applications across scales and disciplines. We review the basic mathematical rules of origami and use 3D-printed origami legos to illustrate those concepts. We then present a reduced-order-model, which consists of an improved bar-and-hinge model, to understand the nonlinear mechanics of non-rigid origami. We explore the stiffness of tubular origami and kirigami structures based on the Miura-ori folding pattern. A unique orientation for zipper coupling of rigidly foldable origami tubes substantially increases stiffness in higher order modes and permits only one flexible motion through which the structure can deploy. We couple compatible origami tubes into a variety of cellular assemblages that enhances mechanical characteristics and geometric versatility, leading to the design of structures and configurational metamaterials that can be deployed, stiffened, and tuned. We have designed, fabricated (using DLW, direct laser writing), and tested (in-situ SEM) this metamaterial at the micron-scale. This resulted not only in the smallest scale origami assembly, but also in a metamaterial with intriguing mechanical properties, such as anisotropy, reversible auxeticity, and large degree of shape recoverability. The presentation concludes with a vision toward the field of origami.

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IP13

Intelligentsia of Nano-Architected Hierarchical Materials

Creation of reconfigurable and multi-functional materials can be achieved by incorporating architecture into material design. In our research, we design and fabricate three-dimensional (3D) nano-architected materials that can exhibit superior and often tunable thermal, photonic, electrochemical, biochemical, and mechanical properties at extremely low mass densities (lighter than aerogels), which renders them useful and enabling in technological applications. Dominant properties of such meta-materials are driven by their multi-scale hierarchy: from characteristic material microstructure (atoms) to individual constituents (nanometers) to structural components (microns) to overall architectures (millimeters and above). Our research is focused on fabrication and synthesis of nano- and micro-architected materials using 3D lithography, nanofabrication, and additive manufacturing (AM) techniques, as well as on investigating their mechanical, biochemical, electrochemical, electromechanical, and thermal properties as a function of architecture, constituent materials, and microstructural detail. Additive manufacturing (AM) represents a set of processes that fabricate complex 3D structures using a layer-by-layer approach, with some advanced methods attaining nanometer resolution and the creation of unique, multifunctional materials and shapes derived from a photoinitiation-based chemical reaction of custom-synthesized resins and thermal post-processing. A type of AM, vat polymerization, has allowed for using hydrogels as precursors, and exploiting novel material proper-

ties, especially those that arise at the nano-scale and do not occur in conventional materials. The focus of this talk is on additive manufacturing via vat polymerization and function-containing chemical synthesis to create 3D nano- and micro-architected metals, ceramics, multifunctional metal oxides (nano-photonics, photocatalytic, piezoelectric, etc.), and metal-containing polymer complexes, etc., as well as demonstrate their potential in some real-use biomedical, protective, and sensing applications. I will describe how the choice of architecture, material, and external stimulus can elicit stimulus-responsive, reconfigurable, and multifunctional response.

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CP1

Long-Wave Behavior of Elastic Waves in Three-Layered Plates with Multifaceted Effects

This article focuses on studying the dispersion characteristics of three-layered sandwich plates in the long-wave, low-frequency spectrum to address potential engineering challenges related to their dynamic behavior and failure. Our study centers on a three-layered plate characterized by perfect layer bonding and external support from Winkler foundations. Furthermore, we explore the impact of a magnetic field, rotational forces, and viscous damping on the propagation of elastic waves within the low-frequency, long-wave regime. We particularly scrutinize the anti-plane shear motion of symmetric three-layered plates. We analyze dispersion relations by transforming partial differential equations into ordinary ones using a harmonic solution assumption. Our study covers dispersion relations for anti-symmetric and symmetric modes in symmetric structures, accounting for magnetic fields, viscous damping, and rotation. This results in relationships for cut-off frequencies, stresses, and displacements within each plate layer for both modes. Utilizing real-world data, we visually depict how Winkler foundation stiffness, magnetic field intensity, viscous damping, and rotation impact wave propagation in three-layered plates. These visuals provide a comprehensive understanding of their effects on wave dispersion in the low-frequency, long-wave regime.

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CP1

Analysis of Wave Scattering at the Common Interface of Piezoelectric Media Half-Spaces Under Surface/Interface Elasticity Theory

The study investigates the reflection and refraction phenomenon of shear horizontal waves at the interface between two piezoelectric media in the scope of surface/interface elasticity. In micro/nano smart structures such as Surface Acoustic Wave devices, where the ratio of the area of the surface/interface to the bulk is large, the produced field quantities are affected by surface/interface electromechanical properties. The Gurtin-Murdoch (1975) and Eremeyev (2016) approaches have been used to derive the surface strain energy density, surface stress tensor, and surface kinetic energy density accounting for the surface/interface energy. The expressions of the amplitudes of reflected and refracted wave have been derived analytically using the governing equations of a piezoelectric medium. Numerical simulations and graphical interpretations have been carried out to observe the effects of surface/interface elasticity on wave propagation. It has been found that the waves amplitude ratios are sensitive to the change in surface/interface elasticity parameters. The investigation may have possible applications in signal processing, transduction, and frequency shifting (a difference in the velocity of surface waves and controlling the selectivity of a filter compensation) of individual devices.

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CP1

Plasma-Piezo -Hygro-Thermal Wave in An Orthotropic Semiconductor under Photothermal Excitation Hygro-Thermal Theory.

Abstract: Purpose The purpose of this paper is to investigate the propagation and reflection of plasma-piezo-hygro-thermal waves in anisotropic medium. Design/methodology/approach The reflection of plane waves in piezo-electric anisotropic semiconductor were investigated in this study with reference to coupled hygro-thermo-elasticity. Research outcomes The reflection of plane waves from the stress free surface in piezo-electric-hygro-thermal orthotropic semiconducting medium results in six coupled quasi reflected waves namely longitudinal displacement, , thermal diffusion and moisture diffusion and shear vertical , electric potential and elasto-plasma . Expressions for the reflection coefficient are developed for the incidence plane wave. It is noted that these ratios are graphically displayed and are observed under the influence of coupled hygro-thermo-elasticity. Research limitations/implications There isn't much study on the model under consideration. No study has been made yet for piezo-electric semiconductor in coupled hygro-thermo-elasticity, according to the existing literature. The effect of coupling mechanical displacement, electric potential and the carrier density in the semiconducting medium under coupled hygro-thermo-elasticity is analyzed.

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CP2

Second Order Well Balanced Schemes for a Model of Granular Flow

We propose and analyse a discontinuous flux based, second order well balanced scheme for the 2×2 system of nonlinear partial differential equations proposed by Hadeler and Kuttler,and given by

$$\begin{aligned} u_t &= (1-\nabla u)v \quad \text{in} \quad \Omega \times (0,T] \\ v_t - \nabla.(v\nabla u) &= -(1-\nabla u)v + f \quad \text{in} \quad \Omega \times (0,T] \\ u(x,0) &= u_0(x), v(x,0) = v_0(x) \quad x \in \Omega \\ u(.,t) &= 0 \quad \text{in} \quad \partial\Omega \times (0,T]. \end{aligned} \tag{1}$$

It is known to model the dynamics of growing sandpiles

generated by a vertical source on a flat bounded rectangular table in multi-dimensions. The scheme is formed by carefully modifying the flux function locally by including source term as a part of the convection term. The well-balancedness of the scheme is preserved by modifying the limitation procedure which switches to first order near the steady state, and maintains the second order away from the steady state. The scheme is proven to be well-balanced in one dimension. It is also shown through the numerical experiments that the second order scheme reduces the finite time oscillations, takes less time iterations for achieving the steady state and gives sharper resolutions of the physical structure of the sandpile, as compared to the previously studies.

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CP2

Reconstruction of Grain Orientation Data Using U-Nets

Polycrystalline materials are composed of multiple crystal grain assemblies. The technique of electron-backscatter diffraction (EBSD), used in scanning electron microscopy (SEM), is applied to collect information about the orientation of these grains. Such data is vital for quantitatively analyzing and understanding the properties of the materials. Nevertheless, EBSD images often include numerous misoriented pixels that appear as noise and may also show regions where data is missing. Many algorithms widely used for reconstructing the grain orientation need tuning of algorithm-specific parameters. This aspect is not ideal for the users of these algorithms, as the parameter tuning may require a deep understanding of these methods. This talk will present our ongoing work that uses U-net, a convolutional neural network, to reconstruct the grain orientation data. Our approach is a significant step toward making the restoration of the grain orientation free of parameters and efficient. We will statistically compare our latest results with our previous work and other widely used methods.

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CP2

Two Case Studies of Grain Boundary Dynamics at the Atomic Scale and Challenges for Continuum Scale Modeling

Atomistic simulations continue to give insights into the complexity of grain boundary (GB) dynamics at the nanoscale. Continuum models are challenged to reasonably coarse grain atomistic complexity while furthering scientific insight. This talk will consider two case studies of GB dynamics across scales on the topics of GB-dislocation interactions and GB diffusion. Recent work decoupling the dependence of GB-dislocation interactions on GB structure will be described at the atomistic scale and on the coarse-grained scale of phase field dislocation dynamics. Recent insights into avalanche-like GB diffusion mechanisms will be discussed and open problems for continuum modeling presented.

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CP2

A Statistical Structure Description of Real Grain Boundaries

Among crystalline defects, grain boundaries are the most complex to characterize and study, largely due to their great structural variety. Although grain boundaries are simple to define in a continuum setting they are the common boundary shared by a pair of adjacent crystals - they are extremely challenging to define precisely, or even characterize, on the atomic scale. This is especially so in realistic systems far from their ground states. In this talk we introduce a robust statistical structural description of realistic grain boundaries. We show that this characterization is primarily determined by macroscopic degrees of freedom of a grain boundary, and is only minimally effected by factors such as internal stresses, thermal noise, differences in local density, the presence of defects, and variations in microscopic degrees of freedom. The proposed statistical structural characterization of grain boundaries is thus suitable for studying realistic non-ideal systems such as those described by thermodynamic ensembles.

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CP2

Image Processing and Analysis of Materials Microstructures with Machine Learning

Materials science aims at bridging the gap between materials elaboration processes and their macroscopic properties through an understanding of the key microstructural features. Scanning electron microscopy (SEM) is therefore one of the workhorses of materials scientists. Despite the importance of SEM image analysis, there does not yet exist a textbook that takes advantage of machine learning (ML) techniques. Publications on the SEM image analysis with ML for materials are also scarce. CNN, SVM, random forests and DL have been applied for feature extraction, image classification, segmentation and object detection, but the absence of high-quality datasets across material classes is a recurring limitation. The emphasis is also put on supervised rather than unsupervised techniques. The latter may be more relevant as they by-pass the labelling step and avoid spurious associations. In the EU-Project MatCHMaker, we build ML tools for automatic SEM images analysis of cements and solid oxide fuel cells. The k-Means and Gaussian mixtures models allowed us to extract the phase assemblage of cement pastes from SEM-BSE (BackScattered Electrons) and EDX (SEM Energy Dispersive X-Rays). The volume fraction of each phase is then injected into a multiscale micromechanical model to predict the elastic and compressive properties of mortars and concrete. The next step of our work focusses on image

uncertainty quantification.

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CP2

Does Elastic Stress Modify the Equilibrium Corner Angle?

We determine the effect of elastic stress on the equilibrium energy-minimizing corner angle for solids with highly anisotropic surface energy. In the absence of stress, the equilibrium corner angle is described by the Wulff shape. With stress, the Wulff shape is modified, and the corner generates an elastic singularity which in principle could modify the shape at the corner. The effect of elasticity on the corner angle has conflicting results in the literature. The motivation of our work is to resolve the contradiction between these results. We thus consider a void in a two-dimensional biaxially-stressed solid with anisotropic surface energy. We numerically determine the energy-minimizing shapes using a boundary-integral elasticity formulation and a spectral method for solving the nonlinear, nonlocal Euler-Lagrange equations for the void shape, focusing on the precise details of the elastic singularity in corner region and its influence on the energy-minimizing shape and corner angles. Our main finding is that elastic stress does not affect the precise corner angle, however, the stress singularity near a corner does cause an integrable singularity in the curvature near the corner that changes the macroscopic geometry of the shape and results in an apparent contact angle that is different from the no-stress corner angle [J. Mech Phys Solids, 167, art 105003 (2022)]

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CP3

A Phase-Field Fracture Model for Anisotropic Materials Under Compressive Loading

Regularized models of fracture, such as phase-field fracture models, are emerging as competitive approaches for realistic problems (e.g., heterogeneous materials, 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 standard 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. For addressing the contact of crack faces, we establish an effective crack energy density that gives the regularized phase-field crack the effective properties of an ideal sharp crack. On the basis of the crack, the QR decomposition of the deformation gradient tensor is applied, allowing for the identification of the crack deformation modes. By relaxing over those modes that do not incur energy costs, an effective energy is obtained with an unaltered response when the crack faces are closed and zero energy when they are open. Additionally, we extend our model to develop a homogenized fracture model of a material with anisotropy in the elasticity and fracture energy. This is achieved by incorporating anisotropy tensors in fracture energy and employing an anisotropic elasticity tensor. Subsequently, we evaluate the performance of our model by modeling homogenized crack growth in transversely isotropic rock samples subjected to compression.

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CP3

Phase-Field Modeling of Diffusion Bonding

Diffusion bonding is a critical process in materials science and engineering, enabling the joining of materials at a molecular level. Its significance lies in the ability to create strong, durable bonds between similar or dissimilar materials, crucial in industries ranging from aerospace to biomedical devices. However, accurately modeling diffusion bonding has posed challenges due to the complex interfacial behaviors involved. Conventional phase-field models typically allow interfaces to merge automatically upon contact, limiting their applicability in scenarios where distinct interfaces must be maintained until specific conditions are met. We develop a phase-field approach for diffusion bonding that modifies the kinetic evolution equation. Our approach introduces a temperature-dependent barrier, preventing automatic merging of interfaces until predefined thresholds are reached. This allows us to accurately simulate bonding processes, where interfaces need to remain distinct until reaching a predefined threshold.

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CP3

Perturbed Preconditioned Gradient Descent Method for Cahn-Hilliard Equation with Variable Mobility.

In the phase field models for applications from materials science such as the Cahn-Hilliard (CH) equation, the periodic boundary conditions are the most relevant and spectral methods are the workhorse for fast computations.

However, upon incorporating variable mobility, spectral methods are no longer useful because the variable mobility makes the fast Fourier transform of no use. In this talk, we propose what we call the perturbed preconditioned gradient descent method (PPGD) to overcome this difficulty. We prove convergence results for the convex version of the stationary CH equation. Then, We discuss its performance for the (non-convex) time dependent CH equation.

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CP3

Two-Dimensional Problem of An Elastic Matrix Containing Multiple Gurtin-Murdoch Material Surfaces Along Straight Segments

In this talk, we present the study of the plane strain problem of an infinite isotropic elastic medium subjected to far-field load and containing multiple Gurtin-Murdoch material surfaces arbitrarily located along straight segments. Each material segment represents a membrane of vanishing thickness characterized by its own elastic stiffness and residual surface tension. We provide a brief overview of the governing equations and boundary conditions for the problem, and present analytical integral representations for elastic fields everywhere in the material system in terms of unknown density functions. The problem is reduced to the system of coupled hypersingular boundary integral equations for the unknown density functions. Further, we provide the closed-form expressions for the stress intensity factors at the tips of the membranes. The numerical algorithm and several results of the numerical simulations will be presented to demonstrate the effectiveness of the proposed approach and study the influence of dimensionless parameters involved in the problem. The possible applications of our work are in modeling the local and overall properties of composite materials that utilize ultra-thin, stiff, and prestressed membranes as reinforcements.

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CP3

Phase-Field Thermomechanics of Dynamic Fracture

We study dynamic crack propagation and its interaction with thermal effects using a phase-field modeling approach. We develop a thermodynamically consistent free-energy-based formulation to study the thermomechanics of crack growth. We implement the formulation in a finite element framework and study the effect of thermal effects and dissipation on the evolution of cracks at high velocities.

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CP4

Analytic Solutions to the Two-Dimensional Inverse Problem of Deforming Nematic Elastomer Surfaces

A large catalog of thin materials and two-dimensional biophysical systems exhibit anisotropic length changes along embedded directions. One such class of materials are nematic liquid crystal elastomers, where local geometry changes are controlled by the nematic director field, and the so-called two-dimensional inverse problem consists of designing a director that after activation produces the desired surface geometry. The problem is known to be reducible to a system of non-linear, hyperbolic, locally integrable PDEs containing as source terms the surfaces' Gaussian curvature. We re-examine the set of equations defining the deformation from an analytic point of view in the sourceless case, which is genuinely linear. This allows for the derivation of a closed, exact integral solution for the director field in the space of parametric coordinates, written in terms of convolutions of an explicit kernel with suitably defined initial conditions. The implicit gauge freedom contained in the definition of the problem is made manifest in the PDEs. Additionally, for this sub-class of deformations, using a convenient gauge we derive a general classification scheme for all the solutions based on solutions of the Klein-Gordon equation. The form of the equations allows us to establish equivalencies between nematic elastomers and problems in plasticity theory, structural optimization, and the theory of constant principal strain mappings.

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CP4

An Optimized Species-Conserving Monte Carlo Method with Potential Applicability to High En-

tropy Alloys

We present a species-conserving Monte Carlo (MC) method, motivated by systems such as high-entropy alloys. Current fast local-structure MC methods do not conserve the net concentration of atomic species, or are inefficient for complex atomic systems. By coarse-graining the atomic lattice into clusters and developing a renormalized MC method that takes advantage of the local structure of the atoms, we are able to significantly reduce the number of iterations required for MC simulations to reach equilibrium. In addition, the structure of the method enables easy parallelizability for the future.

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CP4

Flexoelectricity in Thin Active Materials

Flexoelectricity is a phenomenon by which dielectric materials can exhibit spontaneous electrical polarization due to strain gradients. Unlike piezoelectricity, which is observed in materials with non-centrosymmetric crystal structures, flexoelectricity is observed in materials with centrosymmetry. In this talk, I will talk about recent work on modeling flexoelectricity in thin films grown on substrates. Calculations show that polarization is strongly dependent on film geometry and material constants. Recently a mechanism of flexoelectricity has also been proposed in soft materials. In the second part of my talk, I will talk about modeling flexoelectricity in active soft materials. Specifically, I will consider the problem of an active ribbon, and discuss the evolution of polarization during actuation.

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CP4

Modeling of Flexoelectric Composite Materials: Effective Properties Computation

Flexoelectricity is a phenomenon that describes the coupling between electric polarization and mechanical strain gradients in dielectric materials. It has potential applications in sensors, actuators, energy harvesting, nanoelectronics, and tissue self-restauration. However, the flexoelectric effect is usually weak in bulk materials and can be enhanced by creating composite structures with heterogeneities. In this paper, we propose an asymptotic homogenization method to compute the effective properties of flexoelectric composite materials with periodic microstructures. The process is based on separating scales and using asymptotic expansions to obtain the homogenized equations and the local problems. We apply the method for flexoelectric composite with complex geometrical shapes. We compare the results with those obtained by finite element simulations and show good agreement. We also analyze the influence of the electro-mechanical parameters on the effective flexoelectric coefficients and discuss the optimal design for maximizing the flexoelectric response.

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CP4

Statistical Mechanics of Breakdown in Dielectric Elastomers

Soft materials with electromechanical coupling have gained traction due to their suitability to be used in soft robots, energy harvesters, biomedical devices, etc. Dielectric Elastomers are one of such materials being used. One major drawback of these materials is that they often require high voltage to operate; which makes them susceptible to instabilities such as pull-in, wrinkling; and electromechanical failure such as dielectric breakdown. We propose a multiscale statistical mechanics analysis of polymer chains and networks to determine the contributing factors of these instabilities. We develop a self-consistent field-theoretic model that accounts for dipole-dipole interactions, and examine instabilities in this model.

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CP5

Multi-Species Rheological Model for Living Polymer Solutions

Applications of wormlike micelle surfactant (living polymer) solutions often require their significant shear thinning across a very wide range of shear rates. Viscosity and flow birefringence of surfactant solutions has been measured across 7 decades of shear rate and 5 decades of viscosity, at temperatures ranging from 20 °C to 60 °C. In this temperature range, the resting equilibrium state of these solutions varies between well-entangled coils at low temperature and short dilute semiflexible rods at high temperature, on account of the kinetics of breaking and combination reactions. Under stress, the scission reaction is accelerated and the average length decreases, and at high enough stress exhibits the short-dilute rod rheology. We have therefore developed a rheological model, based on modified living-Rolie-Poly entangled-polymer rheology and dilute reactive-rod rheology, with kinetic exchange between these states. This new model, whose parameters are deter-

mined from small-amplitude equilibrium measurements, finally accurately describes the transition in shear viscosity and alignment observed at high shear rates.

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CP5

Addressing Computational and Analytical Challenges Stemming from the In-Plane Fluidiy of Lipid Bilayer Membrane.

A semipermeable membrane encloses all cells called the *lipid bilayer membrane*, which protects the cell's organelles and genome. The membrane responds to external forces and changes shape. Within a continuum mechanics framework, these membranes' mechanics are modeled via the Helfrich model. Although this popular model has been well studied in the past few decades, it is plagued by formidable computational and analytical challenges stemming from its characteristic material symmetry, viz., "in-plane fluidity.' It is a model feature where the membrane lacks a well-defined reference configuration. A consequence of this symmetry is that the Euler-Lagrange equations of the Helfrich energy are underdetermined, and equilibrium solutions (when they exist) belong to an infinite dimensional equivalence class of solutions. The situation is particularly challenging for computations, with indeterminate degrees of freedom appearing as distortions of the finite element mesh and the presence of zero energy modes. This talk focuses on topologically spherical membranes and proposes a procedure that removes these degeneracies. We demonstrate how it can be applied to computations. Using global bifurcation theory techniques, we also show that the procedure can be used to prove the existence of solution branches rigorously.

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CP5

Stability for the Surface Diffusion Flow

We study the global existence and stability of surface diffusion flow (the normal velocity is given by the Laplacian of the mean curvature) of smooth boundaries of subsets of the n–dimensional flat torus. More precisely, we show that if a smooth set is "close enough' to a strictly stable critical set for the Area functional under a volume constraint, then the surface diffusion flow of its boundary hypersurface exists for all time and asymptotically converges to the boundary of a "translated' of the critical set. Our work generalizes to any dimension $n \in \mathbb{N}$ the result obtained in dimension $n = 3$ by Acerbi, Fusco, Julin and Morini (extending previous results for spheres of Escher, Mayer and Simonett, Wheeler and Elliott and Garcke).

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CP5

Median Filter Method for Wetting and Dewetting Dynamics with Anisotropic Surface Tension

The median filter scheme for motion by mean curvature in the two-phase setting turns out to be the natural level set version of threshold dynamics for the same evolution. Exploiting this precise connection between two different classes of algorithms for interfacial motion, we discuss extension of median filters to anisotropic (normal dependent) multiphase motion by mean curvature of networks of curves and surfaces, where each interface in the network can have a distinct, normal dependent surface tension and mobility. We demonstrate these new level set methods by simulating the wetting and dewetting of different substrates by particles that preserve their volume and have anisotropic surface tensions and mobilities.

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CP5

Consequences of Constitutive Choices in Soft and Thin Materials

Biopolymer gels and soft tissues are known to present rich nonlinear elastic responses, including strain-stiffening and a surprising tendency to develop a tensile stress perpendicular to the shearing direction (reverse Poynting effect). However, popular strain energies adopted for constitutive modeling fail to capture these responses, lead to universal relations that conflict with experimental data, and do not provide a satisfactory link with the mesoscale. For soft materials governed by quadratic energies, the choice of strain measure in which we expand the energy can be key to unlocking some of these behaviors. I will discuss that by adopting the Biot/Bell strain, instead of the usual strains based on Cauchy-Green deformation tensors, diverse nonlinear deformations can be captured, including a novel transition in the Poynting effect. Other overlooked consequences of the strain choice appear when deriving models for plates and shells. In fact, most models obtained from commonly employed energies present undesirable bending measures and behaviors, such as materials that stretch under a pure moment. I will explain how to avoid this contamination between bending and stretching, which is of importance in the study of buckling and defects on thin sheets. This talk contains contributions from J. A. Hanna and C. O. Horgan.

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CP6

Extending Local Solutions to the Smart Fabric Inverse Design Problem

Smart fabrics, comprising of filaments that can alter their lengths in response to environmental stimuli, offer a promising avenue for achieving complex and versatile shape-shifting objects. The inverse design problem is determining the distribution of filament responsiveness that will realize a specific target shape from an initially flat fabric. This problem is equivalent to constructing a suitable coordinate system on the target surface. Our study addresses this challenge by identifying the largest patch on a given target surface that can be formed from an initially flat fabric. Leveraging the Jacobi field formalism, we derive an analytic expression for critical points -locations where constructing the suitable coordinate system on the target surface fails. We present an algorithm that iteratively modifies the construction to extend its range and obtain the maximal domain coverable by a solution to the inverse design problem.

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CP6

n Adaptive Automated Process Control System utilizing a Predictive Modelling Approach

Process control plays an important role as it ensures the stability of processes and minimizes the influence of disruptions. In process engineering in particular, there are many complex processes that are difficult to regulate. Manually implemented, static control concepts are often cost-intensive and inflexible when systematic changes occur. An ideal control system should be able to adapt independently to the process requirements, to regulate the process as optimally as possible without prior knowledge of the system properties and to be transferable to different systems without much effort. The availability of higher computing power and advances in machine learning have led to asharp increase in interest in automated adaptable control systems which are based on historical process data. In this work, a control AI is developed that uses the Model Predictive Control (MPC) method to predict in real time the effects of different control strategies on a process over a certain time horizon and to identify the optimal strategy. An artificial neural network is trained continuously with a sliding time window, and with that is able to improve the prediction accuracy and thus the control accuracy over time and to adapt rapidly to dynamic changes in the system properties. The developed model was tested on a virtual proxy bioreactor system in various scenarios.

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CP6

Limiting Analysis of Optimal Control Problem for Stokes' System in an Oscillating Domain

In contemporary mathematical theory, limiting analysis is crucial for examining partial differential equations (PDEs), particularly in materials science, porous media studies, and structural engineering. Heterogeneous materials intricate nature poses computational challenges due to high costs or machine precision issues, necessitating a rigorous approach like limiting analysis. External factors drive homogenization exploration in optimal control problems constrained by dynamic PDEs. This study [1] focuses on limiting analysis of an optimal control problem constrained by the generalized stationary Stokes equation, featuring unidirectional oscillating coefficients in a pillar-type oscillating domain. We investigate the problems behavior by establishing optimal control characterization and conducting asymptotic analysis using the unfolding method [2]. Oscillating matrices in the Stokes equations and the cost function lead to an optimal control problem characterized by a perturbed tensor over the fixed domain in the limit. This can be further solved numerically. [1] S. Garg and B. C. Sardar, Homogenization of distributive optimal control problem governed by Stokes system in an oscillating domain, Asymptotic Analysis 136 (1):1-26, (2024). [2] D. Cioranescu, A. Damlamian, and G. Griso, Periodic unfolding and homogenization, C.R. Math. Acad. Sci. Paris 335 (1):99104, (2002).

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CP6

Machine Learning Driven Inverse Design of Metamaterials with Adaptable Force-Displacement Characteristics for Soft Robots

Developing materials with tailored nonlinear mechanical responses that can facilitate various functionalities remains challenging. Metamaterials have emerged as a promising solution for designing compliant materials not found in natural materials. This research focused on machine learning-based inverse design techniques, soft material analysis, and advanced manufacturing methods to optimize the force-displacement characteristics of metamaterials. Through finite element analysis on materials with various shapes and mechanical responses, we generated a comprehensive dataset of mechanical properties, which helped us understand the behavior of different geometry parameters under determined loading conditions. This dataset is then utilized to train a neural network that can predict the optimal geometric parameters needed to achieve the desired nonlinear mechanical response, based on the force-displacement outputs corresponding to different shapes. The metamaterials are designed to exhibit tunable nonlinear responses such as bi-stable, super-elastic, and constant force behavior, which are ideal for energy absorption, locking, and load-bearing applications by adjusting the shape parameters of the unit cell topology. The findings of this project will contribute to the potential of compliant mechanisms and the development of soft robotics, energy-absorbing devices, and wearable prosthetics with improved performance, comfort, and adaptability in diverse tasks and environments.

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CP6

Calibrating Complex Material Models: A Compar-

ative Analysis of Bayesian-Based, Optimization-Based and Neural Network-Based Approaches in the Presence of Uncertainty

Some materials significantly contribute to global carbon emissions. Specifically, steel production is a serious contributor, accounting for approximately 20 to 25% of industrial CO2 emissions [1]. Accurate predictions in this context are crucial but face various challenges in materials science, including costly experiments and involving computationally expensive models, all within uncertain environments. Kennedy and O′Hagan [2] introduced a Bayesian-based approach using Gaussian processes to calibrate hybrid models under uncertainty and predict with accurate uncertainty estimates. This study compares this Bayesian-based approach with numerical optimization-based, and neural network-based approaches. Real-world case studies, such as the prediction of steel creep behavior, enrich our discussion. 1. Clean Steel Partnership, Strategic Research and Innovation Agenda (SRIA) 2021
2. Kennedy, M.; O'Hagan, A. Bayesian calibration of computer models. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 2001, 63, 425–464.

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CP6

Definitive Screening Design-Based Regression Analysis to Study the Effects of Multiple Factors on Compressive Strength of Blended Cement Mortars

In concrete mixes, Portland cement has the highest share of carbon footprint. In this study, copper slag and limestone have been used to partially replace cement in a representative mortar system. The replacement results in a complex system with multiple factors affecting mechanical properties. Therefore, definitive screening design (DSD), a minimally-aliased Design of Experiment (DoE) technique, has been used to study the effects of factors, such as limestone-to-cement ratio, copper slag content, fineness of copper slag, cement type and water-to-binder ratio on the 2, 7, 28 day compressive strength and workability of the blended mortar mixtures with a sand-to-binder ratio of 3:1. As compared to traditional experimental designs like factorial, central composite, etc., DSD reduces the number of runs significantly. In the regression models generated for predicting compressive strength, there was no confounding of the main effects with any other main, interaction or quadratic effect. This was achieved with only 18 runs for 5 factors, while the traditional factorial design recommends 32 runs. It was possible to use 44.4 wt% of Portland cement (CEM I 52.5N) with 40 wt% copper slag and 15.6 wt% limestone (water-to-binder ratio 0.5) to obtain a blended cement corresponding to 32.5N strength class. Comparisons to reference mixes with inert materials are to be discussed further in the presentation.

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CP7

Symmetry Based Analysis of Buckling of Plate with Stiffened Edge

A non-linear system of partial differential equations with symmetries often exhibit bifurcations[D. H. Sattinger, Bifurcation and symmetry breaking in applied mathematics, Bull. Amer. Math. Sot. 3 779–819 (1980)]. In this research work, the symmetry based reduction [A. Vanderbauwhede, Local bifurcation and symmetry, Chapman and Hall, (1982)] is applied to the instabilities of a circular von-Kármán plate with stiffened boundary, which is treated as a curved rod, where the mismatch strain between the edge and the rest of the plate is treated as the bifurcation parameter. This problem is qualitatively motivated by applications in engineering and sciences, for example, composite structures, biological systems, etc. As part of the analysis, the nonlinear differential operator on a suitable Banach space is formulated using variational approach; then the null space of the linearized operator is constructed relative to the homogeneous deformation solution. After identifying the symmetry and its relevant subgroups for the operator, the reduced problem is formulated. Then, postbuckling analysis is carried out using the mathematical framework introduced by Healy[T. J. Healey,Symmetry and equivariance in nonlinear elastostatics I: Differential field equations, Arch. Rat. Mech. Anal. (1989)]. The semi-analytical results are verified using finite element method[Wohlever, J.C., Symmetry, nonlinear bifurcation analysis, and parallel computation, Cornell University (1996)].

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CP7

Higher Order Finite-Element Based Methods for Non-Collinear Magnetism and Spin-Orbit Coupling in Real-Space Pseudopotential Density Functional Theory

Spin-orbit coupling (SOC), a relativistic effect, is vital in active research areas such as spintronics, low-dimensional materials, and topological insulators. Pseudopotential Density Functional Theory (DFT), a widely used material simulation tool, has proven to be effective when extended to incorporate non-collinear magnetism and SOC effects. State-of-the art DFT codes either employ plane-wave basis restricting the simulation domains to be periodic, or atomic-orbital type basis which are not systematically convergent. Moreover, these basis sets do not exhibit good parallel scalability, severely limiting the range

of material systems. A promising alternative, the open-source code DFT-FE, employs a systematically convergent finite-element basis, exhibiting reduced computational prefactor and delayed onset of cubic scaling for larger system sizes. This study introduces a real-space formulation for non-collinear magnetism with SOC and presents an efficient, scalable, finite-element based implementation within DFT-FE. The methodology accommodates generic boundary conditions and is suitable for multinode CPU and GPU architectures. A generalized force approach is also proposed for evaluating atomic forces and unit-cell stresses in a unified computational framework. We demonstrate the efficiency of our implementation by studying the electronic properties of twisted bilayer transition metal dichalcogenides at low twist angles.

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CP7

Unlocking the Potential of Ab Initio Modelling of Materials: Real Space Finite-Element Based Methods for Projector Augmented Wave Formalism in Density Functional Theory

Gaining ab-initio insights into complex materials problems involving larger length-scales and longer time-scales demand enormous computational resources owing to the stringent accuracy requirements of density functional theory (DFT) calculations compounded with cubic scaling complexity of DFT with number of atoms. To address this, we introduce a local real-space formulation and an efficient finite-element-based implementation methodology to incorporate projector augmented wave (PAW) formalism in the DFT-FE framework on hybrid CPU-GPU architectures. We develop efficient HPC-centric implementation methodologies combining the ideas of low-rank perturbation of identity and mixed precision arithmetic in conjunction with Chebyshev Filtered subspace iteration approaches to solve the underlying FE discretized PAW generalized eigenproblem. We show that our framework (PAW-FE) facilitates a substantial reduction in the degrees of freedom in comparison to norm-conserving pseudopotentials for achieving the required chemical accuracy while accommodating generic boundary conditions, thereby enabling faster and accurate large-scale DFT simulations than possible today. Finally, we demonstrate the usefulness of PAW-FE on large-scale problems involving tens of thousands of electrons that cannot be effectively tackled using state-of-the-art plane-wave codes in the area of catalysis and energy storage.

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CP7

Geometric Rigidity for Incompatible Fields in the Multi-Well Case and An Application to Strain-Gradient Plasticity

We derive a quantitative rigidity estimate for a multiwell problem in nonlinear elasticity with dislocations. Precisely, we show that the L^{1^*}-distance of a possibly incompatible strain field β from a single well is controlled in terms of the L^{1^*}-distance from a finite set of wells, of curlβ, and of divβ. As an application, we derive a strain-gradient plasticity model as Γ-limit of a nonlinear finite dislocation model, containing a singular perturbation term accounting for the divergence of the strain field.

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CP8

Chydrodynamics of Wound Ballastics

Simulation of a human body from 20% gelatin and 80% water mixture is examined from wound ballistics point of view. Parameters such as incapacitation energy and temporary to permanent cavity size and tools of hydrodynamics have been employed to arrive at a model of human body similar to the one adopted by NATO. Calculations using equations of motion yield a value of 339 μs in which a temporary cavity with maximum size settles down to permanent cavity. This occurs for a 10mm size bullets and settle down to permanent cavity in case of 4 different bullets i.e. 5.45, 5.56, 7.62, 10 mm sizes. The obtained results are in excellent agreement with the body as right circular cylinder of 15 cm height & 10 cm diameter. An effort is made here in this work to present a sound theoretical base to parameters commonly used in wound ballistics from field experience discussed by Col Coats and Major Beyer. 2. Fackler, M.L, NATO Standard circa, IDR, 1988. 3. Fackler, M.L.and Malinowski, .J.A., "Ordnance gelatin for ballistic studies: Detrimental effect of excess heat used in gelatin preparation", The American Journal of Forensic Medicine and Pathology, 1988 Sep, 9 (3): 218–219. 4. Cooper,G.J and Ryan,J.M., "Interaction of penetrating missiles with tissues; some common misapprehensions and implications for Wound management", Br.J.Surg.1990, vol.77.June, 606–610.

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CP8

(Inviscid) Burgers in Conservation and Hamilton-Jacobi Form as Degenerate Elliptic Problems

A finite element approximation scheme for duality-based variational principles for P(O)DE systems is described. General classes of such systems, conservative as well as dissipative, are associated with dual variational principles. As examples, the approach is demonstrated on the hyperbolic inviscid Burgers, parabolic Burgers equations and their corresponding Hamilton-Jacobi equations (it has also been successfully demonstrated on the linear heat and transport equations, as well as nonlinear ODE systems). In the case of inviscid Burgers, the scheme picks up the ex-

pansion fan 'entropy' solution (as well as the 'shock' solution) for appropriate initial data, and we explain our understanding of why this must be so. The scheme essentially amounts to defining a robust and adapted change of variables, a dual-to-primal (DtP) mapping, that renders the Euler-Lagrange equations of the dual variational principles to be exactly the associated primal systems, on using the DtP change of variables. We show how the scheme transforms initial-value problems into well-set, space-time dual boundary-value problems (bvps). Such space-time bvps are then approximated by a common finite element strategy. The scheme associates a family of dual solutions with a single primal solution, demonstrating a form of 'gauge invariance.' This invariance also allows for causal primal problems to be solved by a non-causal technique.

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CP8

Efficient Koopman-Based Modeling with Random Fourier Features

Koopman operator theory [Mezic, *Nonlinear Dynamics*, 41:309-325 (2005)] is a powerful modeling approach for complex dynamical systems arising in physics, chemistry, materials science, and engineering. The idea is to leverage existing simulation data to learn a linear model that allows to predict expectation values of observable functions. Though the algorithm is quite simple, its underlying mathematical structure is very rich, and can be used for different purposes including control, coarse graining, or the identification of metastable states in complex molecules and materials [Noé and Clementi, *Current opinion in structural biology*, 43:141–147 (2017)]. A critical modeling decision in this context is the choice of a finite-dimensional basis set. Kernel methods have recently been shown to provide a powerful model class for Koopman learning, requiring only little prior information. The price to pay is that the dictionary size scales with the data size, leading to large-scale linear algebra problems. In this contribution [Nüske and Klus, *Journal of Chemical Physics*, 159:074105, (2023)], we demonstrate that stochastic low-rank approximations based on Random Fourier features lead to reduced linear algebra problems that can be solved at much lower cost. We also show that hyper-parameters of the kernel can be tuned efficiently based on physical principles, allowing for an effective identification of metastable states in molecular systems.

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CP8

Leveraging the Topology of a Liquid Crystal System to Identify Half Integer Strength Topological Defects

Existing computational techniques for identifying topological defects in particle-based simulations of liquid crystalline (LC) materials are based on Q-tensor theory, which can locate pronounced irregularities in local ordering; however, these methods do not account for global topological features of the system. Here, we describe a defect-detection algorithm suitable for use with mesogen-scale trajectory data, which assigns a unique vector to each particle, thereby defining the director field at the mesogen level and revealing the topology of the director field. We leverage the discontinuities in the assigned vector field to validate the existence, and identify the location(s) of the topological defects in the system, which are point defects in 2D LC assemblies and line defects in 3D LC assemblies. We exemplify the strengths of our methodology for various sample cases and compare its performance for defect detection on realistic geometries with respect to a commonplace technique based upon the scalar order parameter.

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CP8

Generating Rational Curves and Surfaces

This presentation targets the applications of computer aided geometric designs, in particular, we focus on generating a family of rational parametric curves and surfaces utilizing quaternions and dual quaternions as tools to represent rigid transformations. First, we construct a family of rational space curves via quaternion products of two generating curves. Then, we generate a family of rational surfaces in affine 3-space from three rational space curves by dual quaternion multiplication. Our approach of using dual quaternions to generate rational surfaces provides rational parametrizations for canal surfaces, the typical modeling surfaces in architecture and computer aided design that play an important role in geometric modeling and computing. Computational algorithms and illustrative graphics are included in this presentation.

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MS1

Infrastructure for Large-Scale Simulations Beyond Semilocal Dft

This talk summarizes our work on infrastructure for density functional theory simulations beyond the traditional accuracy limit of semilocal density functional theory for large-scale simulations. Within the FHI-aims code, a general-purpose, efficient all-electron electronic structure code, we show how to realize hybrid density functional theory simulations beyond 10,000 atoms for complex molecules and solids on current parallel CPU resources. The implementation relies on an accurate, local resolution of identity approach for the Coulomb operator, coupled with efficient load balancing that exploits the sparsity of all matrices involved, as well as the MPI-3 standard for shared memory arrays. Additionally, we rely on the ELPA eigenvalue solver in the ELSI infarastructure for parallel solutions of the DFT eigenvalue problem. In complex semiconductors, these techniques allow us to directly simulate defects and dopants in the dilute limit, while avoiding supercell arti-

facts in the simulations.

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MS1

Quantum Embedding Methods for Correlated Materials and Electron-Boson Coupled Systems

I will talk about an ab initio quantum chemistry framework for faithful simulations of correlated materials and electron-boson coupled systems. The first part includes the density matrix embedding theory (DMET) and its applications to high-temperature superconductors. The method allows for spin SU(2) and particle-number U(1) symmetry-breaking states such that the superconducting orders spontaneously emerge during the self-consistency. We directly computed the superconducting pairing order of several doped cuprate materials and structures. We found that we could correctly capture two well-known trends: the pressure effect, where the pairing order increases with intra-layer pressure, and the layer effect, where the pairing order varies with the number of copper-oxygen layers. In the second part of the talk, I will discuss a canonical transformation-based quantum embedding theory for electron-boson coupled problems. The method is applied to several electron-boson coupled systems, including the Hubbard-Holstein model and ab initio materials. In particular, we studied the modification of phase boundaries/reaction barriers via the formation of polarons or polaritons in an optical cavity. We show that the method gives accurate energies and observables comparable to exact diagonalization or DMRG calculations, and allows for large-scale simulations for quantum materials with modest computational cost.

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MS2

Reactive Binding of Solvent and Solute Molecules Forms a Solvation Shell That Pressurizes the Solution Due to Molar Volume Changes

When a solution is created as a mixture of a solvent and electrically neutral solute, an osmotic pressure is produced in the solution, which represents the pressure difference that would exist across a solute-impermeant membrane, between the solution and a pure solvent. Equating the chemical potential of the solvent across the membrane produces vant Hoffs law in the limit of dilute solutions, which fails to produce accurate results for macromolecular species such as polymers. Instead, we propose that the osmotic pressure represents the superposition of two effects: (a) vant Hoffs law, and (b) solvation shell pressure. When an electrically neutral polymer is mixed with a solvent such as water, whose molecules consist of electric dipoles, a mutual attraction is produced between charge distributions along the polymer length and the electric dipoles of the solvent. This electrical attraction creates a solvation shell around the polymer, which may change its molar volume. We propose to model this charge attraction as a chemical reaction that transforms the solute + solvent mixture into a solvated solute + solvent mixture. The molar volume of the solute reactant is less than that of the solvated solute product, causing an additional tendency of the mixture to swell (and thus, pressurize when the mixture is constrained within the walls of a container). We expect that this modeling approach can resolve a classical conundrum in the field of physical chemistry.

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MS2

Embryogenesis Understood Via Strain Mapping

Embryogenesis in almost any organism involves a series of morphological transformations. In this work, we aim to understand the dynamics of embryogenesis on the scale of the whole embryo: this requires quantifying strain tensors, which rigorously describe the differences between the deformed configurations taken on by local clusters of cells at time instants of observation and their reference configuration at an initial time. We present a systematic strategy for computing such tensors from the local dynamics of cell clusters, which are chosen across the embryo from several regions whose morphogenetic fate is central to viable gastrulation. Our approach is based on constructing graphs of neighboring cells to extract the local strain using incremental deformation gradients. However, our methods do not depend on computing spatial derivatives. Therefore they are gradient-free, and more robust to noise than naive gradient-based methods. As an application of our approach, we demonstrate a systematic connection between Drosophila gastrulation kinematics at the cell and whole embryo scales.

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MS2

Computing Growth-Induced Elastic Deformations from Energy Minimization

Based on a discretized energy formulation, I will present a novel numerical method to solve growth-induced finite elastic deformation coupled with free boundaries. In the context of constrained-growth or differential-growth induced pattern formations, previous numerical methods can generate specific simulations, but are limited to provide theoretical understanding of the numerical results. When a new shape state emerges in the numerical simulation, little is known if such a transition is subcritical or supercritical, and if multiple locally stable states exist. I will apply the new method to provide such details in shape formations such as wrinkles, creases, and ridges in a bilayer problem.

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MS2

Mechanics of Remodeling

A large-deformation formulation of the mechanics of remodeling is presented. Remodeling is a material evolution that is mass and volume-preserving. The governing equations of remodeling solids are derived using a two-potential approach and the Lagrange-d'Alembert principle. We study a particular remodeling of fiber-reinforced solids in which the fiber orientation is time-dependent in the reference configuration. We define an additional remodeling

energy, which is motivated by the energy spent in living systems to remodel to enhance stiffness in the direction of loading. We consider the examples of a solid reinforced with either one or two families of reorienting fibers and derive their remodeling equations. We study three examples of material remodeling, namely finite extensions and torsion of solid circular cylinders. We consider both displacement and force-control loadings. It is observed that during remodeling, there is a competition between the action of the internal strain energy function and the remodeling energy (governed by the motivation to provide additional stiffness or strength). For a given material, a remodeling process dominated by strain energy works to align fibers in a direction that minimizes strain energy. On the other hand, a remodeling process dominated by the remodeling energy aligns fibers in the direction of the maximum principal strain according to a constitutive choice.

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MS3

Hyperbolic Metasurfaces

In this talk, I discuss our recent efforts in the context of nano-optics, photonics and phononics, with a special emphasis on extreme wave-matter interactions enabled by polaritonic material responses coupled to metasurfaces. I will discuss our recent theoretical and experimental results in the context of hyperbolic wave propagation, spanning multiple domains, from nano-optics and polaritonics to radio-waves and mechanical waves. I will discuss the general implications of hyperbolic dispersion to enhance light-matter interactions over broad bandwidths and collimate waves well below the diffraction limit. In addition, our results map surface wave propagation to non-Euclidean spaces, connecting to relevant problems in applied math, e.g., funny billiards and airplane boarding optimization, and feed back these concepts to new designs for sub-diffractive imaging devices.

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MS3

Chirality in Metamaterial Design

Metamaterials and composite structures can manipulate waves, screen particular parts of the domain, and focus fields, currents, and waves in desirable directions. The talk deals with the robust design of metamaterials and optimal composite structures. Forming anisotropic composite zones and using materials of different chirality allows us to create designs that are stable to perturbations of the structure and applied excitations. We consider edge states in topological insulators, particularly in gyroscopic metamaterials, and examine various types of lattices of gyroscopes connected by springs. Depending on the lattice structure and frequency of the applied excitation, the lattice might exhibit different chiral edge modes characterized by the corresponding Chern number and propagating only around the domain's boundary. We consider an extension to the lattices on surfaces and nonorientable manifolds such as a Moebius strip.

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MS3

Limits to Nonreciprocity in Three-Dimensional Composite Materials

In the last few years, nonreciprocal systems have seen a surge of interest, which is at least partly due to their importance for many practical applications including, e.g., optical isolators and circulators. Mathematically, nonreciprocal effects are characterized by an antisymmetric contribution to the tensor describing the material properties. One way of tailoring the nonreciprocal behavior of a material to a specific need is to introduce a microscopic structure, thereby obtaining a composite material. In general, it is well known that the effective properties of composite materials can go well beyond those of their constituent materials. This raises the question as to what the limits of the effective nonreciprocal behavior of composite materials are. Here, we report on new corresponding bounds that were derived using the quasistatic approximation and assuming that there is no resonance. Notably, our bounds are much tighter than those that were previously known. In many cases, our bounds are even attained or at least are almost attained by laminate microstructures. In regard to enhancements, we found that while some quantities associated with the nonreciprocal behavior (e.g., the effective Hall coefficient) can be enhanced, this does not hold true for most quantities for which an enhancement would be desirable for practical applications. To obtain useful enhancements, one should therefore consider composites for which at least one of our assumptions does not hold true.

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MS3

Acoustic Metamaterials with Rotating Components

The exploration of acoustic wave propagation in moving media has garnered considerable interest due to its potential for diverse applications. This presentation delves into our recent advancements in understanding acoustic wave behavior within spinning fluids, such as air or water. The theoretical foundation of these advancements is rooted in the Mie scattering framework, which incorporates the rotational motion into the wave equation and boundary conditions within the linear regime and demonstrates distinctive scattering features. Three examples will be presented. The first example introduces a generalized Scattering Cancellation Theory(SCT), aiming at concealing spinning objects from static observers. Leveraging rotating shells with varying angular velocities, our work expands the scope of SCT,

bridging the gap towards its practical application involving moving objects. In the second example, we explore the intriguing dynamics of a spinning cylindrical column of fluid immersed in a static fluid environment. This investigation uncovers the inherent spin angular momentum, probing torque and force behaviors in evanescent acoustic fields. Notably, despite lacking an imaginary part associated with intrinsic absorption, the resulting discontinuity induces unconventional sound scattering, exemplified by a negative radiation force. The third example delves into the acoustic analog of an optical fiber, presenting a novel perspective based on rotational principles.

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MS4

A Local Variational Principle for Fracture

The problem of including body loads in variational fracture, the question of understanding what phase-field fracture, as implemented, is approximating, and the goal of restricting the part of the total elastic energy that competes with fracture surface energy, have motivated formulating a local variational principle for fracture. We describe such a variational principle, which is satisfied by all global and local energy minimizers, and which can be used to formulate variational models for fracture with body and boundary loads.

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MS4

On Rigidity for Differential Inclusions into Nowhere Elliptic Curves in 2x2 Matrices

After surveying results on differential inclusions we will state a regularity/rigidity result for differential inclusions into a class of nowhere elliptic connected closed curves in 2x2 matrices. This result generalizes our previous result for the special case of a nowhere elliptic closed curve (that arises in the study of the Aviles Giga conjecture) to a somewhat general class of nowhere elliptic curves. The methods of the proof are from the theory of the Aviles Giga functional and from scalar conservation laws. The main proof ideas will be motivated and sketched in broad outline.

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MS4

Defect Formation in Microfluidic Channels

Flow-induced deformations of nematic liquid crystals in confinement are ubiquitous, both in passive systems when driven by external agents and in active systems under the collective motion of their particles. We study nematics confined to microfluidic channels, in both types of systems, with a view of analyzing defects actualized as domain walls. We work within a reduced Beris-Edwards framework which leads to a system of nonlinear and coupled differential equations. Our analytical and numerical results highlight the universality of order reconstruction solutions, characterized by distinct orientational sub-domains that are separated by domain walls.

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MS4

Asymtotics of Anisotropic Stokeslets in Nematic Liquid Crystal Flows

Stokeslets are solutions of the Stokes flow with a singular source term. They can be used as building blocks to construct solutions with distributed force and also to analyze the interactions between moving particles in a fluid. In this talk, we investigate such an object in a liquid crystal environment which necessarily produces anisotropic effects. We start from the Beris-Edwards model for nematic liquid crystal flows and consider the asymptotic regime (strong elastic effect and small particle) so that the far-field behavior of the Stokeslets can be clearly revealed.

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MS5

Frequency Analysis of Optomechanical Networks for Physical Information Processing

Nonlinear dynamics are a pervasive phenomenon in natural and synthetic mechanical systems, which can be leveraged for control of elastic wave propagation and programming of complex input-output mappings. A mechanical system with high dimensionality and nonlinear dynamics can perform information processing on the physical stimuli that act upon the system. The enriched signal contains both nonlinear transformations as well as memory of the original input, which can emulate recurrent neural network mappings using the training framework of reservoir computing (RC). In this study, we develop a spectral projection method to characterize this relationship between system nonlinearity and reservoir computing performance, and evaluate it in an optomechanical system. This analysis partitions the dimensionality increase of the signal among its frequencies, distinguishing between the strengths of the linear and various classes of nonlinear responses. The nonlinear springs in the network produce bilinear force-displacement responses. Elastomeric optical fibers coupled to the springs bend with spring compression, producing a nonlinear optical transmission vs displacement due to Snells law. This work demonstrates the benefit of combining different physical nonlinearities and develops greater insight into the connection between the nonlinearity and

computing performance in RC systems.

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MS5

Nanoscale Origami and its Free Energy Landscapes

The multistable energy landscapes of origami have proven useful for deployable structures, mechanical information, and energy storage. There has been recent interest in applying origami principles to 2D materials in order to design a wide array of nanoscale devices. However, to properly understand the behavior of these origami-based nanodevices, one must consider the interplay of the geometric mechanics of origami with thermal fluctuations, steric repulsion, van der Waals attraction, and other molecular-scale phenomena. Here we develop a model for the statistical mechanics of a single fold in a nanosheet by drawing inspiration from past work on entropic pressure between biological membranes. The statistical mechanics model is then used to inform fold and interfacial free energies of a broader nanoscale origami structure. The free energy landscape and multistability of nanoscale origamis are explored with a particular emphasis on the influences of crease pattern, size, and temperature.

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MS5

Vitrimers Nanocomposites: Thermomechanical 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 this unique material's self-healing, shape memory, and shape reconfigurability properties, aiming toward 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 that adding 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, illustrating a healing efficiency of $\approx 70\%$ 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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MS5

Statistical Physics-Inspired Metamaterials

Coupled bistable nodes enable complex, programmable mechanical behavior across many different metamaterial systems. Here, we describe a system in which bistable nodes are created by locally dilating a surface at a regular array of lattice sites. When the dilation is sufficiently large, the site will buckle either above or below the surface. An interaction between neighboring buckled sites is generated via the difference in the elastic energy of different deformation patterns. We show that this material mimics a simple model for a phase transition called an Ising model. By making this connection, we are able to understand preferred states, stability, and tunability. We discuss how statistical physics can guide our efforts to design and operate metamaterials more broadly, especially in noisy environments.

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MS6

Machine Learning for Multi-Scale Modeling of Materials: Simulation and Design

Materials systems have long been both understood and modeled from multiple scales. This talk will highlight how utilizing such hierarchical structures with machine learning can provide novel capabilities in molecular dynamics (MD) simulation and materials design. I will first discuss our works on MD acceleration by (1) decomposing an ab initio potential into fast and slow components coupled with multi-scale integration algorithms; and (2) learning a coarse-grained dynamics propagator that directly predicts long-time coarse-grained future states with multi-scale graph neural networks. These methods can speed up the simulation by a factor of 3x to 1000x while maintaining relevant levels of accuracy. The second part of the talk introduces crystal diffusion models that can generate novel crystal structures by learning from a materials data distribution. The diffusion model can be extended to highly complex metal-organic frameworks with a coarse-grained representation based on structural building blocks. This new approach in generative modeling opens a new paradigm in property-driven inverse design.

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MS6

Representation-Space Generative Models for Periodic Materials Design

Generative models hold the promise of significantly expediting the materials design process when compared to traditional human-guided or rule-based methodologies. However, effectively generating high-quality periodic structures of materials on limited but diverse datasets remains an ongoing challenge. We describe a novel approach for periodic structure generation which fully respect the intrinsic symmetries, periodicity, and invariances of the structure space. Namely, we utilize differentiable, physics-based, structural descriptors which can describe periodic systems and satisfy the necessary invariances. In conjunction with a suitable generative model, this approach generates new materials within this descriptor or representation space and reconstruction is then performed on these representations using gradient-based optimization to recover the corresponding Cartesian positions of the crystal structure. This approach differs significantly from current methods by generating materials in the representation space, rather than in the Cartesian space, and the model training process can be greatly simplified. We show this approach is able to provide competitive performance on established benchmarks compared to current state-of-the-art methods.

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MS6

Shallow Ensembles: Simple, Scalable and Size-Extensive Uncertainty Estimates for Atomistic Modelling

Statistical learning algorithms provide a generally-applicable framework to sidestep time-consuming experiments, or accurate physics-based modeling, but they introduce a further source of error on top of the intrinsic limitations of the experimental or theoretical setup. Uncertainty estimation is essential to quantify this error, and make application of data-centric approaches more trustworthy. To ensure that uncertainty quantification is used widely, one should aim for algorithms that are reasonably accurate, but also easy to implement and apply. In particular, including uncertainty quantification on top of an existing model should be straightforward, and add minimal computational overhead. Furthermore, it should be easy to process the outputs of one or more machine-learning models, propagating uncertainty over further computational steps. We compare several well-established uncertainty quantification frameworks against these requirements, and propose a practical approach, which we dub shallow ensemble propagation, that provides a good compromise between ease of use and accuracy. We present applications to the field of atomistic machine learning for chemistry and materials, which provides striking examples of the importance of using a formulation that allows to propagate errors without making strong assumptions on the correlations between different predictions of the model.

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MS6

Unifying Views on the Extrapolation Power of Machine Learning Potentials and Materials Thermodynamics

Recent advances in machine learning (ML) interatomic potentials (IPs) allow density functional theory (DFT) calculations to be bypassed with models that balance high accuracy and relatively low computational cost. However, MLIPs can be unreliable in regions of the configuration space not represented in the training data, which often hinders their use as universal predictors when modeling high-complexity systems. In this talk, I will describe how understanding robust generalization in ML provides unifying views in materials thermodynamics and ML-driven simulations. First, I will demonstrate how extrapolation in atomistic systems can be rigorously defined in a model-free approach, thus without surrogate metrics such as variance of predictions, and connect this concept with statistical thermodynamics. Then, I will describe how deep learning theory can be used to improve the generalization of MLIPs. These results are used to model several problems in materials simulation, from phase transformations in bulk materials to combinatorial spaces in surface catalysis. In combination with automated workflows for combinatorial data generation, robustness in ML models can help drive the field towards the development of universal MLIPs towards length and time scales not accessible by ground truth calculations.

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MS7

Nonlocal Optimal Design of Conductive Domains in the Vanishing Material Limit: A Nonlocal Basis Pursuit Problem

We consider the problem of optimal distribution of a limited amount of conductive material in systems governed by local and non-local scalar diffusion laws. Of particular interest for these problems is the study of the limiting case, which appears when the amount of available material is

driven to zero. Such a limiting process is of both theoretical and practical interest and continues to be a subject of active study. In the local case, the limiting optimization problem is convex and has a well understood basis pursuit structure. Still this local problem is quite challenging both analytically and numerically because it is posed in the space of vector-valued Radon measures. With this in mind we focus on identifying the vanishing material limit for the corresponding nonlocal optimal design problem. Similarly to the local case, the resulting nonlocal problem is convex and has the basis pursuit structure in terms of nonlocal antisymmetric two-point fluxes. In stark contrast with the local case, the nonlocal problem admits solutions in Lebesgue spaces with mixed exponents. When the nonlocal interaction horizon is driven to zero, the "vanishing material limit' nonlocal problems provide a one-sided estimate for the corresponding local measure-valued optimal design problem.

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MS7

Symmetry Results for Sets with Ordered Nonlocal Mean Curvature

It is well known that, in $\mathbb{R}^n$, a boundaryless C^2-surface with constant mean curvature must be a sphere. Li and Nirenberg studied the problem where instead the mean curvature is assumed to be monotone (ordered) in a given direction ν. Under certain geometric assumptions, they showed there must be a hyperplane orthogonal to ν across which the surface is symmetric. Thus, if the mean curvature is ordered in all directions, the surface is a sphere. I will present the analogous result where the curvature is measured with a nonlocal operator and the surface is the boundary of an open set.

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MS7

Finite Difference Method for Variable-Order Laplacian

We propose a simple and easy-to-implement finite difference method for the multi-dimensional fractional Laplacian of variable order. We analyze the convergence of the discrete operator in the Barron space and apply the finite difference approximation in the numerical solution for some nonlocal partial differential equations(PDEs). Moreover, we present the efficient solver with quasi-linear complexity for the fast evaluation of the nonlocal and singular operator and associated fractional PDEs. Numerical examples show the accuracy and efficiency of our method.

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MS7

Some Shape Optimization Problems Involving the Regional Fractional Laplacian

I will describe some shape optimization problems involving or inspired by the regional fractional Laplacian, related to optimal constants in certain Faber-Krahn, Sobolev, or Hardy-type inequalities. This talk will be loosely based on joint work with Tianling Jin and Jingang Xiong.

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MS8

Goal Oriented Optimal Design of Infinite-Dimensional Bayesian Inverse Problems

We consider optimal sensor placement for Bayesian inverse problems governed by partial differential equations with infinite-dimensional inversion parameters. Working within the framework of optimal experimental design (OED), we consider the case where we seek sensor placements that minimize the uncertainty in a prediction or goal quantity of interest (QoI). The prediction quantity is a nonlinear function of the inversion parameters that are being estimated. To address this, we propose a goal-oriented OED (gOED) approach that uses a quadratic approximation of the parameter-to-prediction mapping to obtain a measure of posterior uncertainty in the prediction QoI. We focus on linear inverse problems in which the prediction is a nonlinear functional of the inversion parameters. We seek to find sensor placements that result in minimized posterior variance of the prediction QoI. In this context, and under the assumption of Gaussian prior and noise models, we derive a closed-form expression for the gOED objective. We also discuss efficient and accurate computational approaches for computing the gOED objective and its optimization. We illustrate the proposed approach in model inverse problems governed by an advection-diffusion equation.

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MS8

Optimization-Based Frequentist Confidence Intervals for Functionals in Constrained Inverse Problems: Resolving the Burrus Conjecture

We introduce an optimization-based framework to construct confidence intervals for functionals in constrained inverse problems, ensuring valid one-at-a-time frequentist coverage guarantees. Our method builds upon the now-called strict bounds intervals which offer ways to directly incorporate any side information about parameters during inference without introducing external biases. By tying these intervals to an inversion of a constrained likelihood

ratio test, we translate interval coverage guarantees into type-I error control, and characterize the resulting interval via solutions of optimization problems. Along the way, we refute the Burrus conjecture. Our framework provides a novel approach to analyze the conjecture and construct a counterexample by employing a stochastic dominance argument, which we also use to disprove a general form of the conjecture. We illustrate our framework with several numerical examples and provide directions for extensions beyond the Rust-Burrus method for non-linear, non-Gaussian settings with general constraints.

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MS8

Riemannian Probabilistic Presentation of Model Ensembles, with Applications in Atomistic and Continuum Simulations

In this work, we propose a new probabilistic framework that enables the seamless integration of model-form uncertainties in computational materials science. We specifically focus on a multi-model setting where a collection of model proposals, built using either domain knowledge or (e.g., approximation-theory- or machine-learning-based) surrogates, is available. The approach relies on a stochastic reduced-order model involving a randomized projection operator. A probabilistic model is specifically constructed on the tangent space to the manifold defining the approximation subspace, using Riemannian operators. This formulation offers key advantages, including a simple and interpretable low-dimensional parameterization, the ability to constraint the mean on the underlying manifold, and ease of implementation and propagation through multiscale operators. Applications are finally presented to demonstrate the relevance of the method, including molecular dynamics simulations and phase-field simulations for brittle fracture.

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MS8

Quantification and Propagation of Material Uncertainties Across Multiple Scales

The macroscopic properties of materials and structures that we observe and exploit in engineering applications result from complex interactions between physics at multiple length and time scales: electronic, atomistic, defects, domains, etc. Multiscale modeling seeks to understand the interactions between these physics across scales. However, assessing such interactions can be challenging due to the complex nature of material properties and the prohibitive computational cost of integral calculations. This talk will focus on how to quantify the propagation of material uncertainties across multiple scales. To this end, we exploit the multiscale and hierarchical nature of material response and develop a framework to quantify the overall uncertainty of material response induced by the uncertainties at finer scales without the need for integral calculations. Specifically, we bound the uncertainty at each scale and then combine the partial uncertainties in a way that provides a bound on the overall or integral uncertainty. As a result, the bound provides a conservative estimate on the uncertainty. Importantly, this approach does not require integral calculations that are prohibitively expensive. Finally, we will present the applications of the developed framework, including the ballistic impact of magnesium alloys, the hyper-velocity impact of ceramics, and the collapse of mechanical octet metamaterials.

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MS10

Stochastic Mass Transport - Beyond the Optimality Conditions

Traditionally, stochastic mass transport is studied as an optimization problem. The goal is to push forward a given source measure to a target measure in a way that minimizes distances. Due to Caffarelli, a prominent result in Euclidean spaces establishes the Lipschitz regularity of these optimal transport maps in some specific cases. Lipschitz continuity allows the transfer of analytic properties of the source measure to an a priori complicated target, and Caffarellis result has proven to be widely influential.In this talk, we will explore extensions of Caffarellis theorem to various settings. Our main observation is that the optimality conditions mentioned above are not necessary for most applications. We shall thus introduce a general construction of transport maps, based on semigroup interpolation, and analyze its Lipschitz constant via stochastic calculus of variations techniques. In particular, we will go beyond the Euclidean setting and consider Riemannian manifolds as well as infinite-dimensional spaces. Interestingly, these types of problems relate to some modern numerical applications, which we shall also discuss.

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MS11

Slip and Twinning in Bravais Lattices

A unified treatment of slip and twinning in Bravais lattices is given, focussing on the case of cubic symmetry, and using the Ericksen energy well formulation, so that interfaces correspond to rank-one connections between the infinitely many crystallographically equivalent energy wells. Twins are defined to be such rank-one connections involving a nontrivial reflection of the lattice across some plane. The slips and twins minimizing shear magnitude for cubic lattices are rigorously calculated, and the conjugates of these and other slips analyzed. It is observed that all rank-one connections between the energy wells for the dual of a Bravais lattice can be obtained explicitly from those for the original lattice, so that in particular the rank-one connections for fcc can be obtained explicitly from those for bcc.

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MS13

Eulerian Modeling of Surface Growth: Chemo-Mechanical Instabilities

Surface growth, i.e., the addition or removal of mass from the boundary of a solid body, causes morphological instabilities in a wide range of processes, including the growth of biological tissues and electrodeposition in batteries. In this study, a thermodynamically consistent Eulerian chemo-mechanical model is developed, which bypasses the difficulties of definition of an evolving reference configuration for a growing solid matrix. Coupled with the phase field approach, a finite element numerical model in a fixed computational domain with a fixed discretization is developed to numerically study geometrical and kinetical complexities that arise in morphological instabilities. This novel framework is used to study residual stresses and unstable growth of finite bodies formed due to the non-uniformity of growth.

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MS13

Mechanics of Surface Growth: Investigations of Stability and Residual Stress Formation

Motivated by experiments on dendritic actin networks exhibiting surface growth, we address the problem of its stability. We choose as a simple, reference geometry a biaxially stretched half plane growing at its boundary. Actin is modelled as a neo-Hookean material. A kinetic relation is assumed between growth velocity and a driving force for growth dependent on stress and chemical potential. The stability problem is formulated and results discussed for different loading and boundary conditions. Connections are drawn with Biot's 1963 surface instability threshold. The proposed approach is extended to encompass the effect of surface tension on surface growth. Current, still ongoing research is applying the above framework to the surface growth of cylindrical vessels where interconnections between growth and residual stress formation are expected to arise. In addition to the theoretical interest of the proposed approach, we hope these results can provide a useful reference for experiments and numerical simulations.

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MS14

Shape Optimization of Microstructures Governed by Maxwells Equations

We describe a class of shape optimization problems for optical metamaterials comprised of periodic microscale inclusions composed of a dielectric, low-dimensional material suspended in a non-magnetic bulk dielectric. The shape optimization approach is based on a homogenization theory for time-harmonic Maxwell's equations that describes effective material parameters for the propagation of electromagnetic waves through the metamaterial. The control parameter of the optimization is a deformation field representing the deviation of the microscale geometry from a reference configuration of the cell problem. This allows for describing the homogenized effective permittivity tensor as a function of the deformation field. We show that the underlying deformed cell problem is well-posed and regular. This, in turn, proves that the shape optimization problem is well-posed. In addition, a numerical scheme is formulated that utilizes an adjoint formulation with either gradient descent or BFGS as optimization algorithms. The developed algorithm is tested numerically on a number of prototypical shape optimization problems with a prescribed effective permittivity tensor as the target.

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MS14

Anomalous Frozen Evanescent Phonons

Frozen evanescent phonons are eigensolutions of periodic elasticity problem with zero eigenfrequency. The corresponding Bloch wavenumbers are complex-valued, with the imaginary (real) part determining the spatial decaying length (oscillation period) of the eigensolutions. Mostly, frozen evanescent phonons are overlooked due to extremely rapid decaying over one or two unit cells. Here, we demonstrate anomalous frozen evanescent phonons with large decaying length in mechanical metamaterials. They are

connected to local minimums of phonon dispersion bands in the complex wavenumber space through the Cauchy-Riemann equations. Their decaying length scales inversely to the square root of the minimum frequency, and thus can be arbitrarily large at sufficiently small minimum frequency. For finite-size samples, the static solutions are linear combinations of different frozen evanescent phonons. Interferences of these frozen evanescent modes can lead to anomalous interesting behaviors, including the violation of Saint Venants principle, strong dependence of effective stiffness on system size, sensitivity to boundary condition. Theory and experiment are in excellent agreement. The revealed connection between unusual static and dispersion bands allows to engineer large characteristic decay lengths in static problem. The study can also be extended to other waves, including acoustics, optics and matter waves.

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MS14

Completely Monotone Functions in Nmr

A standard model in NMR represents the magnetization induced by a resonant pulse excitation of nuclear spins of whater molecules as a multiexponential signal, whose exponents describe the diffusion coefficients of isolated tissue compartments, and whose coefficients correspond to their volume fractions. The question of identifying these parameters from experimental measurements leads us to investigate the degree of well-posedness of this problem, which exhibits power law transition to ill-posedness characteristic of "sloppy problems", whose model manifold has an exponential "ribbon" structure. In this talk the power law govering the loss of relative precision as one moves away from the interval containing the experimental data is identified explicitly.

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MS14

Spectral Theory for Slow Light in 1D Nonreciprocal Photonic Crystals

For one-dimensional (1D) photonic crystals (PCs) with passive lossless nondispersive media, Maxwells equations for time-harmonic electromagnetic fields become, under separation of variables, linear periodic differential-algebraic equations (DAEs) in canonical form. In this talk, we discuss how the electrodynamics of 1D PCs is reduced to studying the spectral theory (with frequency as the spectral parameter) of the associated minimal and maximal differential-algebraic operators of these DAEs. My recent results (with Bader Alshammari) will be presented on the self-adjointness of the maximal operator and its eigenvalues. We use this eigenvalue problem to highlight the differences in the spectral theory of canonical DAEs vs ODEs. To motivative the need for this spectral theory, we also discuss how it applies to my previous work (with Stephen Shipman) on scattering problems involving slow and frozen light when a defect is introduced into such photonic crystals.

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MS15

Defects and Geometry in Shapeshifting Liquid Crystal Systems

Liquid crystals are complex fluids that flow but possess orientational order and consequently exhibit anisotropic properties including elasticity, surface tension and electromagnetic response. When dispersed as droplets—known as tactoids—in a host fluid, they may form droplet shapes other than spherical solutions as observed in isotropic fluids. The configuration of a liquid crystal tactoid may be predicted by an energy minimization principle including the various physical effects. They are an exemplar of a broader class of *shape-order* problems whereby the optimization is to be performed with respect to embedded fields describing the spatially varying order and the shape of the domain. Our approach to discretizing and solving these problems with finite elements is presented, as are other examples of shapeshifting in soft materials.

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MS15

Ferroelectric Phases in Liquid Crystals

We will present some analytical and computational results on the modeling and simulation of polar smectic A ferroelectric phases formed by rigid bent-core molecules. This is joint work with Carlos Garca-Cervera and Sookyung Joo.

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MS15

A Study of the Non-Isothermal Allen-Cahn Equations

In the first part of the talk, we propose a mathematical framework modeling non-isothermal phase field models. The framework is based on a coupling between non-equilibrium thermodynamics and an energetic variational approach for the mechanical parts of the system. Applying this framework to the Ginzburg-Landau energy we obtain

a non-isothermal Allen-Cahn system. In the second part of the talk, we will show the well-posedness of the system and study its limit as the interphase thickness ε goes to zero. Using a formal asymptotic expansion we are able to recover the two-phase Stefan problem in the limit.

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MS15

Existence of Axisymmetric Solutions to the Ericksen-Leslie System in Dimension Three

In this talk, I will discuss the simplified axisymmetric Ericksen-Leslie system in dimension three, and present the existence of global weak solutions for any axisymmetric initial data with finite energy. I will also indicate the weak compactness theorem among weak solutions of the axisymmetric Ericksen-Leslie system. This is a joint work with Joshua Kortum.

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MS16

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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MS16

Soft Intelligent Materials with Liquid Metal and Liquid Crystal Elastomer

Combining soft materials with fluids into multifunctional systems has been an area of interest ranging from functionalized gels to soft microfluidics. Liquid metal (LM) alloys like eutectic gallium-indium (EGaIn) have emerged as a popular fluids for use in biphasic material systems due to their low viscosity and high electrical and thermal conductivity. Applications include stretchable electrical circuits, soft thermal interface materials, and highly deformable batteries and energy harvesting transducers. New shape reconfigurable capabilities emerge when incorporating LM fluidics into a shape memory or self-healing material. In this talk, I will present recent approaches to create transforming materials and structures by combining EGaIn liquid metal alloys with liquid crystal elastomer (LCE) or a self-healing organogel. This includes a percolating network of microscale EGaIn droplets suspended in an LCE or organogel matrix as well as thin-film LCE strips with an EGaIn coating. The low viscosity of the EGaIn allows the surrounding material to maintain its elastic, shape memory, and self-healing properties while also enabling high electrical conductivity and response to electrical stimulation. Where possible, I will show how these material systems can be examined mathematically using a variety of statistical and homogenization techniques. In addition to presenting recent efforts in modeling, I will also propose several open questions for possible future study.

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MS16

Programmed Growth in Engineered Living Materials

The growth of multicellular organisms is a process akin to additive manufacturing, where cellular proliferation and mechanical boundary conditions, amongst other factors, drive morphogenesis. Engineers have limited ability to engineer morphogenesis to manufacture goods or to reconfigure materials comprised of biomass. In this talk, a method that uses biological processes to grow and regrow engineered living materials into desired geometries will be discussed. This process can be applied to composites of living bacteria and yeast embedded within synthetic hydrogels. For example, we will describe composites of Saccharomyces cerevisiae and magnetic particles within a hydrogel matrix. The reconfigurable manufacturing process relies on the growth of living cells, magnetic forces, and elastic recovery of the hydrogel. The engineered living materials then adopts a form in an external magnetic field. Yeast within the material proliferate, resulting in $259 \pm 14\%$ volume expansion. Yeast proliferation fixes the magnetic deformation, even when the magnetic field is removed. The shape fixity can be up to $99.3 \pm 0.3\%$. The grown material can recover up to $73.9 \pm 1.9\%$ of the original form by removing yeast cell walls. The directed growth and recovery process can be repeated at least five times. This work enables engineered living materials to be processed and reprocessed into user-defined geometries without external material deposition.

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MS16

Buckling in Aircraft Structures

This presentation will discuss buckling and postbuckling of primary airplane structures (wing and fuselage). We will discuss impact of buckling design criteria on weight (qualitatively) and also illustrate typical buckling checks performed for sizing using both hand-calcs and detailed

Finite Element Models (FEM).

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MS17

Machine Learning for Metadynamic Acceleration in Molecular Host-Guest Interaction Prediction

With the advent of nanotechnology and the perspective of atomic-precision engineering the holy grail of material scientists has become the ability to design, in silico, materials with target properties for functionality objectives. Recently, the improvement in deep learning and generative methods has open the possibility to boost the discovery of new materials [1]. This is possible by a direct structure-to-property prediction, by coupling with experimental characterization data or by improving numerical models making them more efficient. However, compared to other fields, i.e. image and language analysis, material science offers smaller databases for training. Despite that, the rich underlining physical and chemical structure could be leveraged to guide the construction of meaningful latent spaces. This can be achieved providing some priors (physical or mathematical) which guide the model to correctly learn the target space and avoid unphysical solutions. In this talk, I will present several attempts to use transfer learning and latent space manipulation to accelerate numerical models and make more efficient predictions using domain adaptation, contrastive learning and beta-variational autoencoders [2, 3]. [1] F Mayr et al.; The Journal of Physical Chemistry Letters 13 (8), 1940-1951 (2022). [2] G Siddiqui et al.; ChemistryA European Journal, e202302375 (2023). [3] M Rinderle et al.; The Journal of Physical Chemistry C 124 (32), 17733-17743 (2020).

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MS17

Generative Methods for Design of Microstructures for Organic Electronics Applications

We explore the application of generative AI methods for the design of microstructures, concentrating particularly on two- and three-phase microstructures prevalent in organic electronics. Our approach involves the development of a novel framework that combines Variational Auto Encoders with Latent Diffusion models. We show that this framework is able to create a context-aware latent representation of the microstructure space, which allows straightforward mapping to both process and property. A key aspect of our method is its capability to reconstruct and design microstructures that adhere to user-specified traits. This includes not only structural motifs but also certain property features that are application specific. We demonstrate the versatility of our approach through both 2D and 3D examples, showcasing its efficacy in handling complex microstructural designs. Furthermore, we extend our investigation to encompass the manufacturability aspects of the designed microstructures. This includes assessing how these microstructures can be realistically produced, considering the constraints and practicalities of manufacturing processes. By integrating manufacturability considerations into our framework, we bridge the gap between theoretical design and practical application, paving the way for more feasible and efficient production of advanced microstructures in the field of organic electronics.

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MS17

Diamondback: Diffusion-Denoising Autoregressive Model for Non-Deterministic Backmapping of Biomolecules

Coarse-grained molecular models of proteins permit access to length and time scales unattainable by all-atom models and enable the simulation of important processes that occur on long time scales. Backmapping is the process of restoring the all-atom details to coarse-grained molecular representations in order to recover atomistic-level insight. Conventional backmapping approaches rely on deterministic heuristics to generate initial all-atom structures and and apply energy relaxation, which can be computational expensive and cause deviations from realistic sidechains distributions. Recently, data-driven approaches have demonstrated great promise in furnishing trainable models to efficiently perform backmapping on individual protein systems. In this work, we report a novel backmapping approach based on autoregressive denoising diffusion probability models to restore all-atom details to simulations represented only by C-alpha coordinates. As an inherently transferable and local model, it is scalable to proteins of arbitrary size with linear scaling. We train the model on 65k proteins and demonstrate state-of-the-art performance on large proteins from the Protein Data Bank in addition to molecular dynamics trajectories. Furthermore, we demonstrate that fine-tuning the transferable model on a given system can further improve performance in recapitulating protein-specific sidechain distributions. We make the backmapping tool available as a free, open source Python package.

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MS17

Data-Driven Coarse-Graining Without Data

Coarse-graining (CG) in molecular dynamics has become a significant tool in overcoming the spatiotemporal limitations of all-atom models in computational simulations of materials. Relevant data-driven techniques follow two, generally separate, steps by first generating all-atom simulation data and subsequently fitting the appropriate CG model. The first step relies either on very long molecular

dynamics (MD) simulations, which visit all modes in the configurational space, or enhanced sampling techniques, which use collective variables (CVs) to accelerate sampling and barrier hopping. The discovery of CVs, however, relies on physical insight or, again, on data obtained from very long MD simulations. Apart from the physical insight that CG models provide, this chicken-and-egg problem hampers their utility in predictive tasks. We present an alternative formulation that unifies the steps above and does not require any MD runs. Instead, the interatomic potential and force field are inquired at configurations sampled from an appropriate generative model that attempts to learn a lower-dimensional, coarse-grained representation of the all-atom ensemble. Once trained, the model can generate unbiased, one-shot equilibrium samples from the Boltzmann distribution at different temperatures. We demonstrate the efficacy and performance of the probabilistic, generative model proposed in various synthetic and benchmark problems, such as the alanine dipeptide.

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MS18

Study of Some Nonlocal Operators

In this talk, we will discuss some useful properties of a nonlocal operator which is 'nonlocal' version of Monge-Ampere operator. This particular nonlocal version was introduced by Caffarelli-Silvestre. We will discuss about the viscosity solutions (sub-solution and super-solution) of this Monge-Ampere operator.

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MS18

Asymptotic Behaviors For The Compressible Euler System With Nonlinear Velocity Alignment.

In this talk we will explore various alignment models and their practical applications. Our primary focus will center on the pressureless compressible Euler system, specifically highlighting a family of nonlinear velocity alignment models. This system serves as a nonlinear extension of the well-known Euler-alignment system found in collective dynamics. During our exploration, we will demonstrate the emergence of crucial asymptotic phenomena within the system, primarily centered around alignment and flocking behaviors. To provide a more comprehensive understanding, we will investigate various forms of nonlinearity and nonlocal communication protocols, which, in turn, give rise to a diverse range of distinctive asymptotic behaviors.

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MS18

Eringen's Model Via Linearization of Nonlocal Hyperelasticity

Nonlocal models have received a lot of attention in the last two decades. One of their main motivations is peridynamics, a new description of Solid Mechanics proposed by Stewart Silling aiming to englobe in a single model elasticity and singularity phenomena. Another prolific case of nonlocal problems is that of fractional derivatives, such as the fractional gradient or Laplacian. It was shown in previous works that a framework inspired by both aforementioned motivations is suitable for nonlocal hyperelasticity. In this talk we will study its linearization from its Euler-Lagrange equations. Then we will also see the existence and uniqueness of solution and finally that the resulting linear model actually coincides with Eringens model for the right choice of the kernel. Eringens model is a rather popular model in the engineering community, where the stress tensor from the classical case is substituted by a nonlocal one, concretely through averaging the former one with a particular kernel. If time permits, a glimpse of new results in the same framework will be provided.

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MS18

Nonlocal Equations on the Boundary

Abstract: We will discuss regularity for a problem involving a fractional Dirichlet-to-Neumann operator associated to harmonic functions. In particular, we will define fractional powers of the normal derivative, compatible Sobolev spaces, and consider various examples. We will further look at the extension problem characterization to obtain various estimates. This is joint work with Luis Caffarelli (UT Austin) and Pablo Ral Stinga (Iowa State University)

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MS19

Random Persistence Diagram Generator for Materials

We will present a random persistence diagram generator (RPDG) method that generates a sequence of random persistence diagrams from the ones produced by the data. RPDG is underpinned by a model based on pairwise interacting point processes and a reversible jump Markov chain Monte Carlo (RJ-MCMC) algorithm. A first example, which is based on a synthetic dataset, will demonstrate the efficacy of RPDG and provides a comparison with another method for sampling PDs. A second example will demonstrate the utility of RPDG to solve a materials science problem given a real dataset of small sample size.

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MS19

Learning Dynamics with Random Features

A common challenge in modelling, at all scales, is how to learn an evolution law from time series data, allowing for prediction. Classical approaches have involved mathematical modeling with differential equations. This has

been extended to the neural ODEs and PDEs, which incorporate data into fitting generalized right hand sides to the evolution equations with neural nets fo various architectures. Here, we make use of recently developed adaptive random Fourier feature methods to learn near optimal approximations in Fourier space, representing our evolution map, directly, in terms of trigonometric activation functions within a shallow neural network. This talk will present the method, its theoretical basis, our progress in learning dynamics, and highlight outstanding questions and future directions of activity. This is joint work with P. Plechac and J. Knap, along with graduate students.

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MS19

Generative Diffusion Learning for Parametric Partial Differential Equations

Randomness and uncertainty are inherent parts of science and engineering. Understanding and quantifying the propagation of uncertainty in physical systems enables reliable decision making with known levels of confidence. In this talk, we introduce a class of generative models that learn the solution operator for parameter-dependent partial differential equations (PDE) from a possibly noisy dataset. We propose a novel probabilistic formulation of the operator learning problem based on recently developed generative denoising diffusion probabilistic models (DDPM) in which the solution operator for the PDE is represented by a class of conditional distributions. In comparison to existing deterministic methods, the probabilistic formulation combined with DDPM allows for an automatic quantification of confidence intervals for the learned solutions. We perform numerical benchmarks to demonstrate that the proposed method achieves high accuracy with a quantified uncertainty and is able to learn the solutions even when applied to data sets with noisy outputs.

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MS20

Variational Modeling of Stress-Driven Rearrangement Instabilities

Variational models in the context of the theory of stress driven rearrangement instabilities are introduced in order to describe the morphology of crystalline materials under stress due to the boundary interaction with other adjacent materials. The existence and regularity of energy minimizers is discussed in various settings, from two to higher dimensions, and in the framework of a two-phase free-boundary problem by letting free also the contact interface with the other materials, both in its coherent and incoherent portions.

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MS20

On Polyconvex Energy Densities with Prescribed Elastic Constants

In variational models based on nonlinear elasticity, the elastic energy density play a major role. These density functions are often assumed to be polyconvex and frame invariant. Furthermore, they should respect material symmetries and reproduce the linear elastic constants of the material. In this talk, I will discuss recent advances in the analytical construction of such elastic energy densities.

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MS21

Machine Learned ACE Interatomic Potentials for 2D Materials

Machine learned interatomic potentials (MLIPs) have become a reliable method to achieve computational speedup over Density Functional Theory (DFT) methods for large systems. While DFT methods are already more efficient than quantum many-body methods, the computational cost of running on large systems of more than a couple hundred atoms is still prohibitive. MLIPs trained on DFT data offer a way to efficiently extend DFT's accuracy to the larger systems frequently encountered in the field of 2D materials when simulating moiré systems. The Atomic Cluster Expansion (ACE) method in particular provides a basis of isometry and permutation invariant functions for machine learning to fit. This has a benefit over directly using machine learning on basis functions without this symmetry as the resulting potentials may not exhibit physically accurate symmetries outside of the training data set. 2D materials have been an area of intense research recently due to their ease of fabrication and suitability as a platform for exploring unusual physical phenomena like superconductivity. Of particular interest is using machine learning to fit an ACE potential for twisted bilayer graphene, though the same set of steps can be used for other 2D materials and heterocrystals. We present an initial application to the mechanical relaxation in twisted bilayer graphene.

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MS21

Large-Scale First-Principles Calculations of Excited State Properties of Quantum Materials

First-principles investigations of excited state properties of materials are instrumental for the interpretation of spectroscopic experimental results and for the prediction of new functionalities. Here, we focus on spin defects in semiconductors, and we present large-scale calculations of excited state properties obtained with time-dependent density functional theory (TDDFT), including the atomic geometry optimization of excited state potential energy surfaces. Our large-scale calculations are enabled by a recent implementation of TDDFT with analytical forces in the West code (https://west-code.org/). By using a GPU-accelerated code and controlled numerical approximations, we show that TDDFT calculations with hybrid functionals are feasible for systems comprising thousands of atoms, thus enabling detailed studies of excited-state geometries and finite-size effects of a wide range of spin defects of interest to quantum technologies. *This work was supported by the Midwest Integrated Center for Computational Materials (MICCoM) as part of the Computational Materials Science Program funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences (DOE-BES).

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MS22

How Mechanobiology of Ligand-Binding in Cell Membranes is Mediated by Viscosity and Remodeling

This work deals with the co-localization of rafts during ligand-binding of active transmembrane proteins (e.g. GPCRs-G Protein Coupled receptors). The latter reside within the cell membrane, and they are responsive to chemically affine ligands. The resulting signaling, such as the production of cAMP-cyclic Adenosine Mono Phosphate, is known to be generated by GPCRs through their conformational changes and simultaneous remodeling. This process is enhanced by raft co-localization, as the involved proteins find the right environment for their activation on those sites. Physiological levels of cAMP are known to be maintained by MRPs-Multidrugs Resistant Proteins, playing the role of regulators in such dynamics. Thanks to the confining work that lipids surrounding GPCRs and MRPs exert on one another, both proteins kinetics and their diffusion are coupled with the deformation of the hosting membrane. While predicting that rafts formation is triggered by ligand-binding, a recent work was unable to provide insights on the experimentally observed raft coalescence. This is analyzed here through a suitable energetics and kinetics of the phase transition of the involved species. The coupling between the balance of forces and the interspecific kinetics governing both species, and membrane viscosity shows diffusive-induced membrane remodeling and rafts coalescence, enhancing the size of active receptors sites.

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MS22

Elastic-viscoplastic shells with growth: an Eulerian formulation

A constrained Cosserat-type shell theory is presented with a free energy that depends on elastic deformations of the shell material and elastic measures of the mean and of the Gaussian curvatures. These elastic measures are determined by remodeling evolution equations and the resultant forces and couples are determined by thermodynamically consistent hyperelastic constitutive equations. Some analytical solutions are presented for a shell with special symmetry.

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MS23

Characterization of Directional and Total Band Gaps in Spatio-Temporal Laminates

We are interested in the band diagrams of a special cate-

gory of time-modulated composites called space-time laminates. These are standard one-dimensional spatial laminates in which the pattern of material properties moves at a constant speed, via an external mechanism. These materials are raising increasing interest in the engineering and physics community as they break reciprocity: a wave traveling through them in one direction cannot travel in the opposite direction. This results in the associated dispersion diagram presenting directional band gaps, ranges of frequencies at which waves cannot propagate only from the right or only from the left. For material design, it is of paramount importance to be able to identify for which frequencies one has total band gaps (the wave cannot propagate regardless of the direction of propagation) and for which one has directional band gaps. In this talk, we will show that the frequency spectrum of two-component space-time laminates admits a universal structure which is independent of the geometry of the laminate as well as the specific material properties. This is achieved by mapping the band diagram on a torus and using compactness arguments. Furthermore, the maximal width, the expected width, and the density of the band gaps (total and directional) in the spectrum are derived.

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MS23

Guiding Stress : From Pentamodes to Cable Webs to Masonry Structures

Pentamode materials are a class of materials that are useful for guiding stress. In particular, they have been proposed for acoustic cloaking by guiding stress around objects, and have been physically constructed. A key feature of pentamode materials is that each vertex in the material is the junction of 4 double cone elements. Thus the tension in one element determines the tension in the other elements, and by extension uniquely determines the stress in the entire metamaterial. Here we show how this key feature can be extended to discrete wire networks under tension supporting forces at the terminal nodes and which may have internal nodes where no forces are applied. In usual wire or cable networks, such as in a bridge or bicycle wheel, one distributes the forces by adjusting the tension in the wires. Here our discrete networks provide an alternative way of distributing the forces through the geometry of the network. We extend such a problem to compression-only 'strut nets' subjected to fixed and variable nodal loads. These systems provide discrete element models of masonry bodies. In particular, we solve the two-dimensional problem where one wants the strut net to avoid a given set of obstacles, and also allow some of the forces to be reactive ones. This is joint work with Ada Amendola, Guy Bouchitté, Andrej Cherkaev, Antonio Fortunato, Fernando Fraternali, Ornella Mattei, and Pierre Seppecher.

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MS23

Bessmertnyi Realizations of Effective Tensors for Metamaterial Synthesis: Conjectures and Counterexamples

We discuss the representability and analytic characterization of effective tensors for isotropic n-phase composites using a Hilbert space approach. The key properties of such tensors is that they are homogeneous degree-1 rational Herglotz-Nevanlinna functions of n complex variables. Recently, M. Bessmertnyi (in a preprint posted to arXiv) claimed to characterize any such rational function as being in the Bessmertnyi class because each partial Wronskian associated with it has a polynomial sum-of-squares representation. Unfortunately, we discovered that a certain lemma of his (attempting to rehabilitate a similar claim by T. Koga in 1968), that he uses in the proof of this theorem, is false. We show this by constructing a counterexample (which also provides a counterexample, as we will show, to the result of T. Koga) that utilizes the stability properties of the basis generating polynomial to the Vmos matroid. These properties have been shown, over a decade, by several authors investigating matroids with the half-plane property and generalizations of the Lax Conjecture for hyperbolic polynomials. In this talk, we provide an overview of how these necessary properties for the counterexample were proved, such as being a homogeneous multiaffine stable polynomial and the existence of a certain real nonnegative polynomial that can not be written as a polynomial sum-of-squares (SOS). This talk is joint work with Aaron Welters.

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MS23

Negative Stiffness and How It Can Help Us in Wave Manipulation

We conduct an in-depth analysis of methods and components for realizing actual and frequency-independent negative stiffness in mechanical and vibro-elastic metamaterials. Examples include networks of rotating disks, pendulum arrays, and bi-stable architectures. The advantages and special features of each system will be investigated with a strong focus on controlling wave propagations in architected solids.

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MS24

Can Large Defects Generate Target Patterns in Oscillatory Media?

We study the existence of target patterns in oscillatory media with weak local coupling and in the presence of a heterogeneity, or defect. We model these systems using a viscous eikonal equation posed on the plane, and represent the heterogeneity as a perturbation. In contrast to previous results we consider large defects, which we describe using a function with slow algebraic decay, i.e. $g \sim \mathrm{O}(1/|x|^m)$ for $m \in (1, 2]$. We prove that these defects are able to generate target patterns and that, just as in the case of strongly localized impurities, their frequency is small beyond all orders of the small parameter describing their strength. Our analysis consists of finding two approximations to target pattern solutions, one which is valid at intermediate scales and a second one which is valid in the far field. By matching the intermediate and far field approximations we then determine the frequency of the pattern that is selected by the system.

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MS24

Select Stories of Solitary Wave Interactions with Material Defects: from Continuum Sine-Gordon Kinks to Discrete Granular Breathers

In the present talk we will consider two examples of the interaction of solitary waves with defect-based inhomogeneities stemming, respectively, from continuum and discrete nonlinear dynamical systems of relevance to materials science. Our first example will consist of the well-known sine-Gordon model in which we will consider a kink-like excitation and its interaction with a material defect both in the context of a 1d setting and in that of a higher dimensional version of the model. In the latter the kink will become a line soliton deformed at the inhomogeneity, for which we derive an effective lower-dimensional description of its dynamics. Notice that both the Hamiltonian and the damped-driven variants of the model will be discussed. Our second example will stem from the discrete realm of granular crystals, where we will see how the presence of heterogeneities has a dramatic impact on the different type of coherent structures, including traveling waves and breathers. Importantly, in the latter case, we will also explore some case examples of connecting with experimental results.

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MS24

Variational and Machine-Learning Approaches to Investigating Defects in Striped Phases

Within an appropriate range of the stress parameter, the 2D Swift-Hohenberg (SH) PDE admits stationary straight roll solutions on the plane, where the wavenumber of the rolls is a parameter of the PDE. When confined to a finite domain, SH wants to form straight rolls locally with this preferred wave number, but the orientations of the rolls can vary significantly across the domain. As the system evolves, one sees patches of stripes of different orientations meet and meld within the interior of the domain, forming point and line defects. Canonically, SH is viewed as a model of convection rolls, where the microscopic field being evolved is the vertically averaged temperature. However, away from defects, a local wave vector is well defined, and evolves slowly relative to the microscopic field. Starting with the SH energy, a macroscopic PDE in terms of the wave vector may be derived. This PDE is known as the Regularized Cross Newell equation (RCN). This talk will cover properties of the RCN energy, minimizers that exhibit well-known point and line defects, and an open challenge in using the RCN framework to describe a particular transition observed in an elliptical cylinder. I will also cover efforts to extract wave vector fields from the microscopic data, as well as the application of SINDy-like methods to fit PDEs in terms of the wave vector to the microscopic data.

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MS24

Sea Slugs to Soft Robots: Computation, Discrete Geometry, and Soft Mechanics in Non-Euclidean Elasticity

Why are there intricate, self-similar wrinkles along the edges of growing leaves, blooming flowers, torn plastic sheets, and frilly sea slugs? I will describe how these complex and exquisite patterns are governed by interacting non-smooth geometric defects in the material. Characterizing and analyzing these defects using discrete differential geometry can uncover insights into the elastic behavior and properties underlying the morphogenesis of leaves and flowers, the biomechanics of sea slugs, and how one might design and actuate soft robots.

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MS25

Tight Bounds on the Quality Factor of Two-Phase Quasistatic Metamaterial Resonators and Optimal

Microstructure Designs

Resonances in materials have led to many exciting properties and applications in nano-photonics and optics. A famous example of material resonance is the "Lycurgus cup", which is a 4th century Roman drinking cup made of glass with fine particles of gold suspended in it. The resonances of the gold particles at optical wavelengths cause it to appear either red or green depending on where the light shines from. By making the gold particles hollow one can shift the resonant frequency, even into the infrared where nanoshells have proved significant in destroying cancer cells. So, it is of great interest to know what are the limits to which they can be tuned. The bandwidth of the resonances in materials is an important feature which is commonly characterized by using the Q-factor. We present tight bounds correlating the peak absorption with the Q-factor of two-phase quasi-static metamaterials evaluated at a given peak frequency by introducing an alternative definition for the Q-factor in terms of the complex effective permittivity of the composite material. Optimal metamaterial microstructure designs achieving points on the bounds are presented. The most interesting optimal microstructure is a limiting case of doubly coated ellipsoids that attains points on the lower bound. We also obtain bounds on Q for three dimensional, isotropic, and fixed volume fraction two-phase quasi-static metamaterials and particle clusters with an isotropic polarizability.

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MS25

Statistical Mechanics of Functional Soft Matter

The existing approaches for polarizable polymers are either unable to account for the nonlocal dipole-dipole interactions or have been restricted to the case of weak anisotropy of the monomer polarizability. Here, we formulate a general approach based on the framework of statistical field theory to account for the nonlocal nature of the dipolar interactions without any restrictions on the anisotropy or nonlinearity of the polarizability of the monomer. We found that the nonlocal dipolar interactions increase, over the case where dipole-dipole interactions are neglected, the magnitudes of the polarization and electric field by orders of magnitude as well as significantly change their spatial distributions. We show that a dielectric polymer chain, constrained at both ends, undergoes sharp chain collapse when exposed to a strong external electric field due to nonlocal dipole-dipole interactions. We study the trend of the critical electric field required for chain collapse with chain stretch and the orientation of the applied electric field. We further augment the model to additionally account for the nonlocal excluded volume repulsive interactions among polymer segments. We show that at higher excluded volumes, the induced dipoles flip their directions due to the interplay between repulsive excluded volume interactions and attractive dipole-dipole interactions.

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MS25

Dissipative Shock Waves in Metamaterials

Porous meta-materials with both regular and random microstructure are of intense research interest today due to their interesting dynamical properties, including but not limited to, their acoustic band structure, shock absorption properties, and fracture toughness. Some of these materials can exist in a rarefied or densified state depending on the state of stress, and recover their original configuration after a cycle of loading and unloading. Many aspects of their mechanical behavior can be captured using a continuum theory of phase transitions. In this talk, impact problems on such materials are explored and it is shown that solutions with shocks, phase boundaries and fans are possible. The fan solutions which arise in decompressive impact problems have not received much attention in the literature and may be regarded as a novel contribution of this work. The shocks considered here are dissipative. The dissipation manifests as rapid oscillations behind the shock front; the origin of such Dissipative Shock Wave (DSW) solutions in discrete lattices will be discussed. An approximate solution to the continuum version of the discrete problem will be constructed by first adding a strain-gradient term to the constitutive law and then looking for traveling wave solutions in terms of elliptic functions.

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MS25

Responses Made-to-Order: Molecularly Encoded Multifunctionality in Liquid Crystalline Elastomers

The coupling of molecular order to mechanical responses has presented liquid crystalline elastomers (LCE) as an attractive platform to program shape change by architecting orientationally patterned microstructural domains. Furthermore, their ability to generate actuation profiles and work-contents that compare or exceed natural mammalian muscles enables the ability to power shape change in composite structures that couple LCE with suspensory elements. This is also key to powering multimaterial designs that characterize soft robotics. LCE artificial muscles have evolved beyond their thermotropic responses. Photoactive materials that use photoisomerization to disrupt molecular order have enabled freeform light-drive microrobots, actuators and shape morphing structures. 3D printable molecular order has unlocked design spaces beyond the flat formfactors. Emerging directions in LCE assimilate electromechanical and ionic moieties in their backbone. This presents a framework to customize multiresponsive freeforms, where ion gradients, photo and thermomechanical responses interplay to enable actuation that the structure can self-sense. The ability to custom order responses with embodied control and autonomy can enable their utilization in new applications that include biomechanically active devices, where freeform responsiveness in self-contained compact volumes is a key design constraint.

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MS26

Deep Molecular Modeling with Experimental and Simulation Data Fusion

Molecular modeling has become a cornerstone of many disciplines, including material science. However, the quality of predictions critically depends on the employed model

that defines particle interactions. A class of models with tremendous success in recent years are neural network (NN) potentials due to their flexibility and capacity to learn many-body interactions. In this talk, I will present the current state-of-the-art in deep molecular modeling. I will discuss the ongoing challenge of accurate and sufficiently broad training datasets and our approach to alleviating this issue by combining experimental and simulation data sources. Furthermore, I will demonstrate how scalable Bayesian methods can be used to accurately quantify the uncertainty of MD simulation predictions. I will showcase the effectiveness of these approaches for various test case materials.

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MS27

Comparing Two Nonlocal Biharmonic Operators with Clamped Boundary Conditions

Nonlocal operators are advantageous choices in modeling due to their flexibility in handling discontinuities. The biharmonic operator appears in many models including deformations of beams and plates. The nonlocal biharmonic operator can be formulated in at least two ways: utilizing a fourth difference operator or iterating the nonlocal Laplacian. In this talk we discuss some similarities and differences between the two operators, as well as discuss nonlocal clamped boundary conditions.

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MS27

Asymptotic Mean Value Formulas for Nonlinear Equations

In recent years there has been an increasing interest in whether a mean value property, known to characterize harmonic functions, can be extended in some weak form to solutions of nonlinear equations. This question has been partially motivated by the surprising connection between Random Tug-of-War games and the normalized p-Laplacian discovered some years ago by Peres et al., where a nonlinear asymptotic mean value property for solutions of a PDE is related to a dynamic programming principle for an appropriate game. In this talk we discuss asymptotic mean value formulas for a class of nonlinear second-order equations that includes the classical Monge-Ampre and k-Hessian equations among other examples.

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MS27

Some Recent Results on the 1-D Fractional Spectral Problems Involving Different Types of Fractional Derivatives

In this presentation, we will introduce some recent results of elliptic-type for 1-D fractional spectral problem

$$\begin{cases} D_{a+}^{\alpha} D_{b-}^{\beta} u = \lambda u, x \in \Omega = (a,b) \\ u(a) = u(b) = 0.0 \leq \alpha, \beta \leq 1, 1 < \alpha + \beta \leq 2, \end{cases}$$

where D_{a+}^{α} and D_{b-}^{β} denote the left- and right-sided R-L fractional derivatives. We will also propose some open questions and conjecture on the distribution of the eigenvalues.

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MS28

Convergence Rates for Machine Learned Random Feature Neural Network Approximations in Molecular Dynamics

Random feature neural network approximations of the potential in Hamiltonians systems yield approximations of molecular dynamics correlation observables that has the expected error $\mathcal{O}\big((\frac{1}{K}+\frac{1}{\sqrt{J}})^{1/2}\big)$, for networks with K nodes using J data points, provided the Hessians of the potential and the observables are bounded. The loss function is based on the least squares error of the potential and regularizations, with the data points sampled from the Gibbs density. The proof uses a new derivation of the generalization error for random feature networks that does not apply the Rademacher or related complexities.

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MS28

Data-Driven Surrogate Modeling and Sensitivity Analysis for Particle-In-Cell Simulations of Plasma-Material Interactions

Plasma-material interactions in magnetic fusion devices are dominated by processes involving impacts of energetic ions on the wall, leading to impurity sputtering, ion implantation, particle reflection, and more. All such processes are functions of both the energy and angle of the impacting ions. In this talk, we will present a data-driven strategy for effective construction of a surrogate model in high-dimensional parameter space for the ion energy-angle distribution (IEAD) output of Particle-In-Cell (PIC) simulations of plasma-material interactions. The methodology is based on a bin-by-bin least-squares fitting of the IEAD in the parameter space. The fitting is performed in a transformed coordinate system to normalize the IEAD, and it employs sparse grids for sampling the parameter space to overcome sampling challenges in high dimensions. The surrogate model is significantly cheaper computationally than direct PIC simulations yet maintains high fidelity to them, providing a fast emulator for those simulations. We will

demonstrate the use of the surrogate model for sensitivity analysis by characterizing the dependence of the ion impact angle and energy moments on the physical parameters.

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MS28

Efficient Computation of Transport Coefficients via a Control Variate Method

In molecular dynamics, transport coefficients measure the sensitivity of the invariant probability measure of the stochastic dynamics at hand with respect to some perturbations. They are typically computed using either the linear response of nonequilibrium dynamics, or the Green-Kubo formula. The estimators for both approaches have extremely high variance, which motivates the study of variance reduction techniques for computing transport coefficients. We present an alternative approach, called the "transient subtraction technique" (inspired from early work by Ciccotti and Jaccucci in 1975), which amounts to simulating a transient dynamics, from which we subtract a sensibly coupled equilibrium trajectory, resulting in an estimator with smaller variance. In this talk, we present the mathematical formulation of the transient subtraction technique, give various error estimates on the bias and variance of the associated estimator, and demonstrate the relevance of the method through numerical illustrations for various systems.

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MS32

Hierarchical Decomposition Scheme for Non-Equilibrium Quantum Systems

The Kadanoff Baym equations are a set of coupled non-linear differential equations that describe the time-dependence of non-equilibrium Green's functions. These Green's functions are important objects because they give us access to all one-body observables. Solving these equations in full scales cubically with the number of timesteps, which prohibits long time propagation of the equations. Many methods have been proposed for circumventing this cubic scaling, many of which rely on uncontrolled approximations to the equations of motion. Recently, there has been success in decreasing the scaling of these equations by utilizing hierarchical decomposition methods. This method compresses the Green's function away from the diagonal in order to drastically reduce the amount of memory used as well as the computation time. We have implemented this scheme for multi-orbital models as well as for high order integrators. We show results for the compressibility as well as the speed-up in computation time for realistic molecular systems.

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MS32

Compressed Quantum Dynamics for Multiorbital Materials

The nonequilibrium evolution in quantum many-body systems is accompanied by a complexity growth that prevents the exploration of long-time dynamics. We will present a numerical scheme based on nonequilibrium field theory, where we tackle the problem by compressing the evolution. The advance is based on the observation that nonequilibrium Greens functions have a hierarchical low-rank structure, making it highly compressible. For practical application to real-world scenarios, particularly in addressing multiorbital problems, we present an efficient representation of matrix-valued Green's functions. We illustrate the practical advantages of scheme through various examples, shedding light on previously inaccessible facets of nonequilibrium dynamics. The first example explores photodoped superconductors using time-dependent Dynamical mean-field theory. Our findings reveal a phenomenon termed chirping, wherein amplitude mode softens as the system approaches the dynamical critical point. We demonstrate the measurement of this chirping phenomenon through optical pump-probe experiments. The second example applies the formalism on current-induced phase transition in transition metal chalcogenites. These materials serve as promising platforms for inducing Bose-Einstein condensation of excitons and we elucidate strategies for engineering coupling to the bath, manipulating the density of states, and optimizing driving protocols to achieve optimal steady-state condensation.

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MS32

On the Unimportance of Memory for the Time Non-Local Components of the Kadanoff-Baym Equations

The Kadanoff-Baym equations(KBE) offer a theoretically exact approach for propagating Green's functions under the action of a time-dependent Hamiltonian. The dependence of these equations on the time-nonlocal self-energy (corresponding to memory effects) means that the KBEs are prohibitively expensive to solve in most scenarios. The generalized Kadanoff-Baym ansatz in turn neglects certain memory effects and reduces the numerical scaling from cubic to linear in the number of time steps in the propagation. In this talk, we investigate the validity of the approximation made in the derivation of the GKBA. We provide arguments and numerical evidence that the neglected terms are typically orders of magnitude smaller than the terms that are left. Furthermore, we provide a mathematical proof that bounds the neglected terms further reinforcing that these terms are typically small in comparison to terms that are kept in the GKBA. We test our arguments for several models, including different non-equilibrium excitations, filling fractions, system sizes, and different forms of the Hamiltonian with a variable range of interactions. In almost all cases the observation remains the same. For systems that are well captured by a particular self-energy at equilibrium, the quantities derived from the density matrix are well captured by the GKBA.

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MS32

RNN for Solving the Kadanoff-Baym Equation

The Kadanoff-Baym equation (KBE) serves as the foundational equation of motion for nonequilibrium Green's functions. As a system of integro-differential equations (IDEs), the conventional numerical solver for the KBE demands computational resources scaling at $O(N^3)$, where N represents the total time steps. This computational intensity becomes particularly burdensome for large-scale quantum many-body systems during long-time simulations. In this talk, we will show that recurrent neural networks (RNNs) can be used to learn the functional mapping between Green's function and the collision integral (the integral component of the IDE), which facilitates a fast numerical solver for the KBE with a computational cost scaling as of $O(N)$. We will show applications of this new machine-learning algorithm in different quantum many-body systems and discuss its strengths and weaknesses.

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MS33

From Bubbles, Balloons, and Beads, to Morphomechanical Structures

The canonical rod – objects with two dimensions much smaller than a third – provides the basic unit of engineered structures around us. However, using deformable rods with controllable shapes and strength to accomplish complex tasks primarily remains the handiwork of biology. For example an octopus arm, elephant trunk, or human arm operates with extreme flexibility, precision, and robustness. Here, we take lessons from thin-film manufacturing, insect wings, and traditional bead-weaving to fabricate rods with controllable shape, size, and stiffness. The focus of this talk is to develop a framework to understand the mechanics and consequently the design for these synthetic morphing rods. I then explore how to use these structures - independently and in unison - to create soft robotics, deplorable structures, and functional materials.

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MS33

Programmable Metastructures From Combinatorial Stable States

Reconfigurable structures, soft materials, and metamaterials have introduced opportunities for mechanical computation, control complexity reduction, and shape programmability. Recently, hierarchical multistable metastructures composed of patterned arrays of bistable units have been shown to exhibit multiple energy minima, unit activation path dependency, and influence of local prestress in its global shape. As each unit cell can be reversibly inverted, multiple global stable states are achieved. In contrast to many systems where the number of stable states scales exponentially ($\sim 2^N$) with the number of bistable units, N, this substrate's response offers a combinatorically large ($\sim N!$) design space reminiscent of geometrically frustrated condensed matter phases. The high degeneracy and distinct stable shapes provide a vast design space. We present the modeling, design, and applications of the combinatorically large stable states of hierarchically multistable metastructures. We explore interrelations between units and their spatial arrangement in our metastructures's global shape using reduced order and finite element models, enabling us to target desired configurations. We further examine the role of interactions between units in generating geometric frustration, and its role in optimal multistability design strategies. This work opens a route for the fast design of soft reconfigurable structures that morph and have mechanically embodied computation.

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MS33

Emergence of Spatio-Temporal Patterns in Out-of-Equilibrium Dynamic Networks

A large majority of soft biological materials are made of molecular networks with changing topology, allowing to accommodate growth, remodeling, and self-healing over time. These networks exhibit a myriad of new physics (flow, elastic deformation, self-healing, programmability, actuation, ...) that can be controlled by the nature of the constituents, their topology as well as bond dynamics. This presentation will discuss a statistical mechanics framework to understand the trajectories of these networks and their complex emerging response, including elasticity, viscoelasticity and self-healing. We will then focus on active networks, whose bond dynamics is out of equilibrium. For this, we take the example of a biological network made by Solenopsis invicta

(better known as fire ants) that can actively heal defects and exhibit treadmilling dynamics, a behavior that is reminiscent of that of the actin cytoskeleton. We finally show that these dynamics culminate with the networks ability to exhibit morphogenesis with the stochastic emergence and retraction of long protrusions on the networks boundary. These out-of-equilibrium networks can therefore inspire the design of decentralized, autonomous transforming materials, and synthetic swarms.

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MS34

Combining Predictive Machine Learning and Causal Models for Functional Materials Design

Every key facet of physical sciences including design of materials description to estimation of structure-property relationships to process optimizations, have experienced tremendous growth in utilization of data-driven machine learning models in the past decade. There exists plenty of studies to encode complex graphs, symbolic representations, invariances, and positional embeddings in these models for targeted design. However, the intrinsically inbuilt correlative nature of ML models does not capture the causal hypothesis-driven nature of physical sciences. This presentation will focus on how causal ML models and hypotheses-driven active learning can be exploited in combination with materials representation to extract governing fundamental atomistic mechanisms with direct ties to experimental observables for a variety of systems such as perovskite oxides, molecular ferroelectrics, and two-dimensional materials. Acknowledgments: This research is sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy.

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MS34

Physics Informed Neural Networks for Modeling Elastic Fields of Continuously Distributed Dislocations

We develop a physics-informed machine learning framework for finite deformation static dislocation mechanics. The framework is built upon finite deformation (Mesoscale) Field Dislocation Mechanics theory that fundamentally accounts for polar/excess dislocations at the mesoscale. We demonstrate the use of framework to compute static finite deformation stress fields of arbitrary dislocation distributions in finite bodies with elastic anisotropy under different boundary conditions.

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MS34

Neural Operator Accelerated Inverse Design for Heterogeneous Materials

Multifunctional metasurfaces bear promise for the embodiment of cutting-edge multiscale devices that support miniaturization and customization. However, their inverse design remain largely under-explored, due to the difficulties associated with the vast input space and the complicated trade-off across the multiple functionalities of interest. Pursuing to build an automatic design support, we present a next-generation data-driven design framework that is dedicated to multifunctional systems. At the heart of the framework is an implicit Fourier neural operator (IFNO), which offers fields-to-field predictions over field-type pairs of a meta-atom and designable stimulus. Based on IFNO, we formulate an inverse problem for multifunctional systems and present gradient-based multitask concurrent optimization that offers a set of Pareto-optimal architecture-stimulus pairs. To validate the proposed framework, we consider light-by-light programmable plasmonic nanoantenna arrays as a case study, whose inverse design involves heterogeneous plasmonic fields subject to opaque long-range interactions and vast design space jointly formed by a quasi-freeform supercell, maneuverable incident phase distribution, and possibly conflicting on-demand functionalities. Accommodating all the challenges without a-priori simplifications, the proposed framework shows the potential to propel the future advancements of multifunctional multiscale architectures.

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MS35

An Immersogeomertic Framwork for Fluid-Peridynamic Shell Coupling

In this work, we develop and analyze an immersogeometric method for computational fluidshell interaction that is capable of modeling large elasto-plastic deformations and fracture in thin-walled structures. In particular, we employ a correspondence-based peridynamics formulation to describe the shell kinematics, together with a bond-associative damage correspondence modeling approach to use classical failure criteria at the bond level. Then, the peridynamic shell model is discretized with an asymptotically compatible meshfree approximation scheme. On the fluid side, a divergence-conforming B-spline fluid discretization is employed, with the influence from the structure side as a forcing term. This force has the interpretation of a Lagrange multiplier field supplemented by penalty forces, and the the FSI kinematic constraints are then enforced in an augmented Lagrangian formulation. Because of the non-matching fluid and structure discretizations used, our framework readily enables the simulation of brittle and ductile fracture and its coupling with fluid. Lastly, we numerically demonstrate the efficacy of the coupling framework by demonstrating its asymptotic convergence to the local solution and its capability to capture

crack initiation and growth in FSI problems

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MS35

Interior Sobolev Regularity Estimates for Solutions of Strongly Coupled Linear Systems of Peridynamic-Type

We extend the Calderon-Zygmund theory for nonlocal equations to strongly coupled system of linear nonlocal equations $\mathcal{L}_A^s u = f$, where the operator $\mathcal{L}_A^s$ is formally given by

$$\mathcal{L}_A^s u = \int_{\mathbb{R}^n} \frac{A(x,y)}{|x-y|^{n+2s}} \frac{(x-y)\otimes(x-y)}{|x-y|^2}(u(x)-u(y))dy.$$

For $0 < s < 1$ and $A : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ taken to be symmetric and serving as a variable coefficient for the operator, the system under consideration is the fractional version of the classical Navier-Lame linearized elasticity system. Our regularity result states that if $A(\cdot, y)$ is uniformly Holder continuous and $\inf_{x\in\mathbb{R}^n} A(x,x) > 0$, then for $f \in L^p_{loc}$, for $p \geq 2$, the solution vector $u \in H^{2s-\delta}_{loc}$ for some $\delta \in (0, s)$. This is a joint work with A. Schikorra and S. Yeepo.

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MS35

Fractal and Fractional Order Effects in Modeling Complex Viscoelasticity of Soft Materials

In this talk we evaluate the differences in predicting nonlinear viscoelasticity using both fractal and fractional order time derivatives. It is well known that the non-local fractional Caputo derivative has certain advantages in predicting viscoelasticity in soft materials that cannot easily be predicted using integer order operators. In addition, local fractal operators are also superior to integer order operators in their predictive behavior. Under constant loading rates, the Caputo and fractal derivatives are shown to be equivalent up to a pre-factor. However, these operators are different for other functions. In this work, we experimentally test elastomers under steady loading, creep, and sinusoidal loading. The experimental data is compared to the local fractal and nonlocal fractal operators using Bayesian uncertainty quantification. We give guidance to which operator provides better predictions of complex viscoelasticity over a much broader range of operating conditions than has previously been given.

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MS35

Upscaling Random Media with Peridynamics

In modeling heterogeneous solids, it is often necessary to use smoothed, upscaled variables rather than attempting to resolve all the small-scale features in full detail. The evolution laws followed by these upscaled variables generally involve nonlocal interactions. A coarse graining method to be described in this talk maps the small-scale interactions in the original heterogeneous system into peridynamic bond forces at the larger length scale. These coarse-grained forces can be used to calibrate a peridynamic material model suitable for use with the upscaled equations of motion. With this technique, upscaled peridynamic descriptions of random media are found to accurately reproduce the response of the original system. Because the upscaled model is heterogeneous, it accounts for mesoscale variations in the statistics of the small-scale model. This provides an advantage over assigning a single set of effective properties that do not account for such variations. It is demonstrated in this talk that the method exhibits acceptable convergence properties as the spacing between coarse-grained degrees of freedom is reduced. Extensions to fracture modeling will be discussed.

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MS36

Grain Interface Functional Design to Create Damage Resistance in Polycrystalline Metallic Materials

Even though polycrystalline metallic materials are ubiquitous in daily life, when and where metallic structural components damage and fail is difficult to predict, which generally leads to overdesign. One form of damage ductile damage takes place in materials which are easily plastically deformed by formation of voids and localized shear bands. The initiation of these voids are strongly influenced by the internal constitution of the aggregate composite made up of single crystals comprising the polycrystalline metal. Ductile damage generally includes the processes of void nucleation, growth, and coalescence in addition to localized shear banding. High-purity refractory body-centered cubic tantalum has been selected as the model material due to its potential for extreme environment use. This material is known to form voids predominantly at grain boundaries and will be the focal point of material design through advanced manufacturing processes. The material design process will include the highly interactive elements of nano, micro and macro-scale experiments at varying strain rates and temperatures, molecular dynamics simulations, thermodynamically consistent plasticity and theory development, micro-scale polycrystal simulations, macro-scale damage simulations for component design, and machine-learning uncertainty quantification/assessment for self-consistent consolidation of large

experimental and simulation datasets to guide material design and manufacturing process.

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MS36

Bloch Waves in High Contrast Electromagnetic Crystals

Analytic representation formulas and power series are developed describing the band structure inside non-magnetic periodic photonic three-dimensional crystals made from high dielec- tric contrast inclusions. Central to this approach is the identification and utilization of a resonance spectrum for quasiperiodic source-free modes. These modes are used to represent solution oper- ators associated with electromagnetic and acoustic waves inside periodic high contrast media. A convergent power series for the Bloch wave spectrum is recovered from the representation formulas. Explicit conditions on the contrast are found that provide lower bounds on the convergence radius. These conditions are sufficient for the separation of spectral branches of the dispersion relation for any fixed quasi-momentum.

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MS36

Microstructure by Design, Integrating Grain Growth Experiments, Data Analytics, Simulation, and Theory

Cellular networks are ubiquitous in nature. Many technologically useful materials arise as polycrystalline microstructures, composed of a myriad of small monocrystalline cells or grains, separated by interfaces, or grain boundaries. Grain boundaries play an essential role in determining the properties of materials across a wide range of scales. During grain growth (also termed coarsening), an initially random grain boundary arrangement reaches a steady state that is strongly correlated to the interfacial energy density. Thus, to develop a predictive and prescriptive theory, an investigation of a broad range of statistical measures for microstructure evolution during grain growth in polycrystalline materials is needed. In this talk, we will discuss recent progress in modeling, simulation, analysis, data analysis, and experiments of the evolution of the grain boundary network in polycrystalline materials.

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MS37

Microstructure Entropy for Predicting Materials Performance

Microstructure analysis is a critical part of many technologically important problems. Mesoscopic characteristics of grain structures related to grain size, morphology, microstructure entropy, location/form of defects as well as other metrics play a role in the coarsening processes and impact the way materials react to deformation. In this talk we will review some of the recent advances related to modeling microstructure behavior through the lens of fatigue and additive manufacturing applications. In particular, we will highlight the role of misorientation entropy as an essential concept underlying some of the recently developed PDE, machine learning and dimension reduction techniques aimed at predicting materials failure, modeling growth and optimizing processing parameters.

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MS37

Two-Dimensional Foams and Coagulation Equations with Reaction Costs

A three-dimensional soap foam can be compressed between two plates to form a two-dimensional collection of cells with boundaries having the structure of a 3-regular geometric graph. Typically, the foam is allowed to coarsen over several hours through gas diffusion between walls. However, we will focus on another coarsening method which ruptures edges through applying heat, resulting in drastically different network statistics from those found in coarsening by diffusion. In particular, the rupturing process quickly produces large and irregularly shaped cells. In this talk, we will outline physical experiments performed to create the rupturing process, and also associated image processing used for generating network datasets. The results of these experiments are compared with a mean-field computational model. The fundamental topological reaction, tracking the numbers of sides gained and lost in cells neighboring a rupturing edge, is similar to the discrete Smoluchowski coagulation equation for coalescing particles with a multiplicative collision kernel. We will analyze a family of such coagulation equations with a "reaction cost", meaning that after each reaction one or several particles are removed from the product. Under certain initial conditions, reaction costs can prevent the formation of a massive cluster, or gel, which is well-known to be found in coagulation models with multiplicative kernels.

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MS37

Advanced Manufacturing Qualification through Multiscale Multiphysics Modeling, Validation, Reduced-Order Modeling, and Process-informed Optimization

Advanced manufacturing (AM) techniques are revolutionizing industries by enabling efficient production of complex components. However, ensuring AM process reliability and part quality presents significant challenges. Computational tools show promise in elucidating the process-structure-property-performance (PSPP) correlation for AM. This talk highlights recent research conducted at Idaho National Laboratory to qualify AM materials and processes via synergistic integration of multiscale multiphysics modeling, validation, reduced-order modeling, and process-informed optimization. This talk will emphasize multiscale multiphysics modeling and validation of AM processes such as laser powder bed fusion (LPBF), directed energy deposition (DED), and electric field-assisted sintering (EFAS). Reduced-order models are developed using data-driven methods to address computational complexity. Recent advancements in process-informed material design and optimization leverage insights from validated models to optimize manufacturing processes. This entire work is based on the open-source Multiphysics Object-Oriented Simulation Environment (MOOSE) and its specialized application for AM (the MOOSE Application Library for Advanced Manufacturing Utilities, MALAMUTE). The combined development of multiscale multiphysics models, reduced-order models, and process-informed optimization carries great potential for improving and qualifying AM materials and processes.

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MS38

An Inverse Problem in Mean Field Game from Partial Boundary Measurement

In this work, we consider a novel inverse problem in mean-field games (MFG). We aim to recover the MFG model parameters that govern the underlying interactions among the population based on a limited set of noisy partial observations of the population dynamics under the limited aperture. Due to its severe ill-posedness, obtaining a good quality reconstruction is very difficult. Nonetheless, it is vital to recover the model parameters stably and efficiently in order to uncover the underlying causes for population dynamics for practical needs. Our work focuses on the simultaneous recovery of running cost and interaction energy in the MFG equations from a finite number of boundary measurements of population profile and boundary movement. To achieve this goal, we formalize the inverse problem as a constrained optimization problem of a least squares residual functional under suitable norms with L1 regularization. We then develop a fast and robust operator splitting algorithm to solve the optimization using techniques including harmonic extensions, three-operator splitting scheme, and primal-dual hybrid gradient method. Numerical experiments illustrate the effectiveness and robustness of the algorithm. This is a joint work with Samy W. Fung (Colorado School of Mines), Siting Liu (UCLA), Levon Nurbekyan (Emory University), and Stanley J. Osher (UCLA)

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MS38

Rate of Convergence in Periodic Homogenization for Convex Hamilton-Jacobi Equations with Multiscales

In practice, a wide range of problems encompasses both macroscale and microscale variables. However, our primary interest often lies in understanding the macroscale behavior. To achieve this, we employ a process known as homogenization, which aims to average out the microscale behavior. In this talk, my main focus will be on examining the rate of convergence in homogenization for convex Hamilton-Jacobi equations with multiscales. Specifically, I will demonstrate that for the Cauchy problem, the rate of convergence is $O(\sqrt{\epsilon})$, and the power of ϵ is optimal. This is a joint work with Jiwoong Jang.

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MS38

Accelerate Sampling Using Birth-Death Dynamics

I will discuss the birth-death dynamics for sampling multimodal probability distributions, which is the spherical Hellinger gradient flow of relative entropy. The advantage of the birth-death dynamics is that, unlike any local dynamics such as Langevin dynamics, it allows global movement of mass directly from one mode to another, without the difficulty of going through low probability regions. We prove that the birth death dynamics converges to the unique invariant measure with a uniform rate under some mild conditions, showing its potential of overcoming metastability. We will also show that on torus, the kernelized dynamics, which is used for numerical simulation, Gamma-converges to the idealized dynamics as the kernel bandwidth shrinks to zero.

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MS39

Introduction to Theory for Ductile Damage of Metallic Materials

Accurately representing porosity-based ductile damage in polycrystalline metallic materials remains a significant challenge and will be reviewed for this mini-symposium. There are also mathematical instabilities which are typically encountered with incremental damage model formulations. Traditional deterministic forecast utilizing continuum-based physical models generally lack in representing the statistics of structural evolution during material deformation and conditions for formation of a damage field. A macro-scale damage model, which accounts for elastic compressibility, material deformation rate-dependence and micro-inertial effects, will be presented and simulations of experiments discussed. An elasto-viscoplastic single-crystal model will be presented which accounts for the motion asymmetry of screw dislocations in Ta and experimental simulations will be compared with experiments. Results of polycrystal calculations using synthetic microstructure models built upon the specific Ta material used for this study will be presented. This provides local-scale stress conditions for porosity initiation within the polycrystalline network. Results suggest that the von Mises stress and triaxiality at the grain boundaries and the grain boundary triple lines are highly variable, but the variability is diminished with distance to the grain center. Non-Gaussian distributions of micro-scale response variables are consistently observed.

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MS39

Crystal Plasticity Finite Element Simulations of Nanoindentation and Tension for Yielding of Ta Crystals

In this work, we performed experiments and corresponding crystal plasticity finite element (CPFE) simulations of nanoindentation to determine yield stress under indentation of fifteen Ta single crystals randomly distributed in the orientation space. Moreover, simple tension simulations were performed for the same crystals to study the differences in tensile versus indentation yielding. Ratios of the indentation to tensile yield stress were found to vary with crystal orientation in the range from 2.4 to 3. The simulations allowed us to reveal underlying deformation mechanisms accommodating the yielding. It is found that more crystallographic glid mechanisms activate under indentation than tension owing to the more complex state of stress and strain in indentation than in tension. Finally, the model was used to predict the initial hardening slopes for several crystals. Comparisons of the measured and simulated indentation stressstrain curves demonstrated the versatility of the model. The modeling framework, simulation setups, results, and several insights from the results will be presented and discussed in this paper.

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MS39

The Mathematics and Dynamics of Cavitation in Nonlinear Solids

Here we examine the mathematics of cavitation and subsequent dynamic void growth response in a number of nonlinear materials including dislocation-starved metals, dislocation-rich metals, and soft gels. Moreover, the mathematics and dynamics of cavitation are presented for several cavity growth mechanisms, e.g. spherically-symmetric isotropic plasticity of the matrix, dislocation emission, and vacancy aggregation. The implications of dislocation kinetics and substructure evolution on cavitation and dynamic void growth are discussed. In particular, we account for the combined effects of relativistic dislocation drag and an evolving mobile dislocation density on the dynamics of void growth. We compare these effects to the constraints imposed by micro-inertia and discuss the conditions under which each mechanism governs the rate of void growth. The consequences of these constraints may be seen in a number of experimental observations associated with dynamic tensile failure, including the extreme

rate-sensitivity of spall strength observed in laser shock experiments, an apparent anomalous temperature dependence of spall strength, and some particular features of void size distributions on spall surfaces.

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MS40

Semiclassical Limits for Twisted Semiconductors

Twisted semiconductors, more precisely twisted TMDs, have received a lot of attention recently since they exhibited the fractional quantum Hall effect in the absence of a magnetic field. I will review the mathematical theory of such twisted TMD structures and show how semiclassical methods can shed light on these otherwise analytically intractable models describing these materials. This is joint work with Mengxuan Yang.

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MS40

Metamaterial Properties of Thin Networks

Thin graph-convergent networks are modelled by ODEs on metric graphs. The corresponding convergence is established in [O. Post, Spectral Analysis on Graph-Like Spaces, 2012], the matching conditions at the graph vertices depending on the asymptotic behaviour of the ratio of vertex and edge volumes of the network. The possibility of metamaterial-type behaviour in quantum graphs, and in particular the negative refraction, has been shown numerically in [T. Lawrie, G. Tanner, D. Chronopoulos, A quantum graph approach to metamaterial design, 2022]. In this talk, I will demonstrate a class of periodic thin networks in the so-called resonant case in which the negative group velocity and, by implication, the negative refraction can be obtained quantitatively in explicitly computed frequency bands. This requires both an alternative approach to the asymptotic analysis of thin networks, see [K. Cherednichenko, Y. Ershova, A.V. Kiselev, Norm-resolvent convergence for Neumann Laplacians on manifolds thinning to graphs, 2022, arXiv: 2205.04397], and the in-depth study of Rayleigh-to-Mie transitional scattering regimes, see, e.g., [K. Cherednichenko, Y. Ershova, A. Kiselev, V. Ryzhov, L. Silva, Asymptotic analysis of operator families and applications to resonant media, 2023]. Alongside analytic results, I will also show some numerics. The talk is based on joint work with K. Cherednichenko and A. V. Kiselev (Bath, UK).

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MS40

Wave Propagation in Unbounded Hyperbolic Metamaterials

Hyperbolic metamaterials are artificial materials with unusual properties for wave propagation. They are typically constructed as periodic structures, e.g. as alternating layers of metals and dielectrics. Upon the formal application of the homogenization process, time-harmonic wave propagation in hyperbolic metamaterials is described by homogeneous hyperbolic PDEs, as opposed to elliptic ones in classical cases. Dispersion curves in such media have a form of hyperbolae, hence the name 'hyperbolic.' Materials with similar properties exist in nature, e.g. cold plasma (cf. [Poddubny et al., Nature 2013]). Closed boundary-value problems for such PDEs are typically ill-posed (cf. [John, J. Amer. Math. Assoc., 1941]). Surprisingly, the free space problem for the Klein-Gordon equation $\partial_y^2 u - \partial_x^2 u + \omega^2 u = 0$ can be rendered well-posed in an appropriately chosen functional framework (weighted Sobolev space with anisotropic weights), provided with a well-designed radiation condition. We discuss this question and present some numerical experiments illustrating our findings; see [Ciarlet, Kachanovska, SIMA 2022]. Time permits, we will delve into the ongoing work. We will explore the Bloch homogenization technique to discuss why the homogenization process succeeds in the free space case and fails in the presence of boundaries. We will also address the question of how the limiting model should be rectified in cases where boundary conditions are present.

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MS40

Two-Scale Cut-and-Projection Convergence for Quasiperiodic Monotone Operators

The cut-and-project method is used to map a quasiperiodic monotone operator onto a corresponding periodic monotone operator in a higher dimensional spatial space. We consider a real valued matrix $\mathbf{R}$ with m rows and n columns ($n < m$), such that $\mathbf{R}^T\mathbf{k} \neq \mathbf{0}$ for all non-zero vectors $\mathbf{k}$ with m integer components. The homogenized problem is obtained as the limit system using the cut-and-projection convergence of the original monotone partial differential operator for a bounded sequence u_ε in $W_0^{1,p}(\Omega)$, where $1 < p < \infty$ and Ω is a bounded open subset in $\mathbb{R}^n$ with Lipschitz boundary. Corrector results are presented and the ill posedness if the periodic local equation in higher dimension is discussed.

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MS41

Hierarchical Self-Assembly at Equilibrium

A persistent theme in studies of programmable self-assembly is designing building blocks to ensure a target state is both thermodynamically stable and kinetically accessible. One system where this tradeoff plays out is in addressable self-assembly, where each building block is distinct and has a specific location in the target structure at temperatures where the target structure is stable, kinetics favours disordered aggregates. One can overcome this tradeoff using nonequilibrium protocols, such as by varying temperature, leading to spectacular progress experimentally for example using DNA bricks. However, such protocols require energy input and they typically waste most of the input material. Here, we introduce a model system for addressable self-assembly to show that particle interaction energies can be designed so that multiple copies of a target structure assemble at equilibrium, with low kinetic barriers, and with little wasted material. The energies are designed by hand to encourage a hierarchical form of assembly, but the success of this approach shows there could be barrier-free pathways to self-assembly in more complex systems that have yet to be discovered.

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MS41

Rational Design of Multipolymorph Materials

Biology provides numerous examples of multicomponent mixtures that self-organize into multiple distinct structures, or polymorphs. This mechanism relies on the ability of biomolecular systems to establish complex phase diagrams by tuning the interactions among the various species in a heterogeneous mixture. Assembling a specific structure then requires control over the dynamics of a seeded nucleation and growth process. In an effort to reproduce this behavior in synthetic systems, I will describe recent theoretical and computational advances towards the goal of designing fully programmable multipolymorph materials. I will first discuss optimization algorithms for designing mixtures that can self-organize into prescribed phases. I will then discuss how nucleation and growth pathways govern polymorph selection in multiphase systems. Taken together, these design rules provide a deeper understanding of the limits of multipolymorph organization in biological systems and establish practical strategies for engineering fully programmable multipolymorph materials.

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MS41

Inverse Design with Differentiable Patchy Particles

Technologies ranging from clean energy devices to plant-based meat and printable organs would be transformed by the rapid design of complex functional materials. Towards the goal of readily designing functional materials, researchers have investigated a wide array of materials components. On one end of the spectrum, exciting results have emerged from inverse design of materials with simple, spherical components. However, the simplicity of these components has restricted the design space of possible materials. In contrast, materials composed of highly complex components have demonstrated rich functional properties, but the complexity of the components of these systems hinders inverse design approaches. In this talk, we introduce a novel model system that strikes a balance between component complexity and design feasibility: differentiable patchy particles. We showcase the model by demonstrating control over complex functional behavior, including self-limited assembly. Our approach opens new avenues for the direct design of materials with tailored functionalities by expanding the scope of materials we can reliably design.

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MS41

Programming Interaction and Assembly with Magnetic Handshake Materials

Biological materials gain complexity from the programmable nature of their components. To manufacture materials with comparable complexity synthetically, we need to create building blocks with low crosstalk so that they only bind to their desired partners. Canonically, these building blocks are made using DNA strands or proteins to achieve specificity. Here we propose a new materials platform, termed Magnetic Handshake Materials, in which we program interactions through designing magnetic dipole patterns. This is a completely synthetic platform, enabled by magnetic printing technology, which is easier to both model theoretically and control experimentally. In this talk, I will give an overview of the development of the Magnetic Handshake Materials platform. I will start with discussing the theoretical foundations of how we model and design specific interactions using an information theory based framework. I will then talk about how we utilize the anisotropic nature of magnetic dipoles to design energy landscapes, leading to materials assembly and properties design. Lastly, I will briefly touch on the experimental advancement of the system, showcasing potential future applications.

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MS43

From the Mathematical Structure of Quantum Response Functions to Better Numerical Algorithms Projection and Extension Technique

Response functions of quantum systems, such as electron Green's functions, magnetic, or charge susceptibilities, describe the response of a system to an external perturbation. They are the central objects of interest in field theories and quantum computing and measured directly in experiment. Response functions are intrinsically causal. In equilibrium and steady-state systems, they correspond to a positive spectral function in the frequency domain. This talk will show that response functions define an inner product on a Hilbert space and thereby induce a positive definite function. The properties of this function can be used to reduce noise in measured data and, in equilibrium and steady state, to construct positive definite extensions for data known on finite time intervals, which are then guaranteed to correspond to positive spectra. Applications to

interacting quantum systems for data obtained in imaginary time and in real time will be presented.

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MS43

Convergence of Lindblad Equations

The use of Lindblad equations to prepare thermal and ground states have received increasing amount of attention in quantum computing, yet there have been not many analytical results regarding its convergence rate. In this talk, we will discuss some recent progress in analytical understanding of equilibration mechanism of Lindblad equation, drawing connections with the study of classical dynamics.

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MS43

Light-Controlled Many-Body Entanglement in Quantum Materials

The rapidly evolving quantum material science calls for precise and predictive control of collective electronic properties beyond the classical realm. In this talk, I will discuss the application of time-resolved resonant inelastic x-ray scattering (trRIXS) in the characterization and ultrafast control of entangled quantum states in correlated materials. By trRIXS, we find that the instantaneous short-range paramagnon excitations can be manipulated by pulsed laser in a predictive manner, following the Floquet theory in the center of the pulse. These light-engineered spin fluctuations exhibit many-body entanglement. The entanglement depth of the transient state can be witnessed by the quantum Fisher information and quantified by trRIXS snapshots via a self-consistent iteration. Here, we use a cuprate chain as an example to show the possibility of enhancing many-body entanglement using an ultrafast laser pulse.

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MS43

Dynamic Mode Decomposition of Nonequilibrium Green's Function for Quantum Many-Body Systems

Simulating quantum many-body systems away from equilibrium is computationally challenging. To make it easier, a practical way is to examine the Green's function based on the many-body perturbation theory. However, the KBEs which describe the dynamics of the two-time non-equilibrium Green's function (NEGF) form a set of coupled nonlinear integro-differential equations difficult to solve. In fact, to propagate the system until time T, typical numerical methods will take $O(T^3)$ computational time. To deal with this problem, I applied DMD, which is a data-driven model order reduction technique, to simulate the long-time dynamics of the NEGF by using snapshots computed within a small time window. This technique was first applied to the time-diagonal of the two-time Green's function, and then to the off-diagonal elements by decomposing the Green's function into a number of one-time functions. The effectiveness of DMD is demonstrated on a two-band Hubbard model system. In the equilibrium limit, the DMD analysis yields results that are consistent with those produced from a linear response analysis. In the nonequilibrium case, the extrapolated dynamics produced by DMD is more accurate than a special Fourier extrapolation scheme. A potential pitfall of the standard DMD method comes from the insufficient spatial/momentum resolution of the discretization scheme. For the model system, this problem can be overcome by using a variant of DMD known as the higher order DMD (HODMD).

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MS44

Not-So-Planar Kirigami: Experimental Challenges and Opportunities

As research on mechanical metamaterials is booming, planar kirigami patterns are one of theoreticians' favorite toy problems, owing to their relatively-simple kinematics. Yet, for experimentalists, making planar kirigami that actually remain planar when actuated is far from simple, and fabrication/testing challenges are particularly significant when the actuation or the design cause these patterns not to follow pure mechanism motions. In this talk, I will illustrate the challenges we encountered when kirigami are: i) too elastic to behave mechanistically, ii) too energetic and iii) too non-periodic to remain planar. I will also demonstrate that interesting functionalities emerge if we actually embrace planar kirigami's tendency to be not-so-planar.

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MS44

A Unified Framework for Learning Energy Landscape of Textile Metamaterials

Textile-based metamaterials have become widely used in engineering applications ranging from wearable sensors, health monitoring devices to soft robotics. The richness exhibited in their energy landscapes, which can be manipulated for functionality such as localized compliance, calls for a systematic learning framework. We propose a systematic way to construct fibrous networks with varying segment length, local curvature and topology based on a yarn representation. Using a first-principles computational model based on Lagrangian mechanics, we determine their mechanical behaviors through sampling along multiple loading curves, in order to construct their strain energy landscapes. We first show that a wide range of energy states can be achieved by varying the representative textile structures. Then, we extract mechanical property such as anisotropy from these informative landscapes. Last, we guide the design of textile-based metamaterials through proposing spatially textured structures to achieve tailored mechanical responses.

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MS44

A Computational Model for Wrinkling and Crumpling in Thin Sheets

From cell membranes to tectonic plates, crumpling is the result of geometric incompatibility between a thin sheet and external confinement. Its been shown that crumpling statistics progress predictably, and crumpling occurs when planar facets of a sheet fragment into smaller facets. This progression is a robust function of the geometric confinement parameter and the number of compression cycles the sheet undergoes. This fragmentation model, however, has only been analyzed in the specific context of axially compressed sheets. Through simulations and comparison to experimental data, we demonstrate that the fragmentation model for crumpling applies to thin sheets crumpled via several different confinement geometries, including radial compression and cylindrical twisting. This suggests crumpling could be described universally if the correct confinement parameter can be identified.

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MS44

Discrete Breathers in a Mechanical Metamaterial

We consider a previously experimentally realized discrete model that describes a mechanical metamaterial consisting of a chain of pairs of rigid units connected by flexible hinges. Upon analyzing the linear band structure of the model, we identify parameter regimes in which this system may possess discrete breather solutions with frequencies inside the gap between optical and acoustic dispersion bands. We compute numerically exact solutions of this type for several different parameter regimes and investigate their properties and stability. Our findings demonstrate that upon appropriate parameter tuning within experimentally tractable ranges, the system exhibits a plethora of discrete breathers, with multiple branches of solutions that feature period-doubling and symmetry-breaking bifurcations, in addition to other mechanisms of stability change such as saddle-center and Hamiltonian Hopf bifurcations. The relevant stability analysis is corroborated by direct numerical computations examining the dynamical properties of the system and paving the way for potential further experimental exploration of this rich nonlinear dynamical lattice setting.

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MS45

Capturing Discontinuities Using Physics-Informed Neural Networks

Physics informed neural networks (PINNs) have emerged as a powerful tool to provide robust and accurate approximations of solutions to partial differential equations (PDEs). However, PINNs face serious difficulties and challenges when trying to approximate PDEs with dominant hyperbolic character. This research focuses on the development of a physics informed deep learning framework to approximate solutions to nonlinear PDEs that can develop shocks or discontinuities without any a-priori knowledge of the solution or the location of the discontinuities. The work takes motivation from finite element method that solves for solution values at nodes in the discretized domain and use these nodal values to obtain a globally defined solution field. Built on the rigorous mathematical foundations of the discontinuous Galerkin method, the framework naturally handles imposition of boundary conditions (Neumann/Dirichlet), entropy conditions, and regularity requirements. Several numerical experiments and validation with analytical solutions demonstrate the accuracy, robustness, and effectiveness of the proposed framework.

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MS45

A Strategy for Selecting Optimal Predictive Neural Network Surrogate Models

This work presents a framework, known as Occam-Plausibility Algorithm (OPAL), for systematic validation

and selection of Bayesian Neural Network (BNN) surrogate model of complex physical model. OPAL integrates various components, including the prediction pyramid for signifying the scenarios for generating training and validation data sets, hierarchical Bayesian inference for parameter and hyper-parameter determination, and the notion of model plausibility for adaptive selection of the BNN architecture. The validated and selected BNN model delivers sufficiently accurate computational prediction of the key quantities of interest (QoI) with quantified uncertainty, given the synthetic data from physics-based model. In this work, we demonstrate the application of OPAL in the context of predicting the mechanical response of silica aerogel porous material, governed by a physics-based model at the pore scale. Our results illustrate that the proposed validation and architecture selection procedures significantly enhance the BNN surrogate model's ability to extrapolate predictions beyond the domain sizes accessible to the physics-based model. This advancement greatly facilitates quantification of uncertainty in large-scale physics-based models and has broader implications for the accurate modeling of complex physical systems.

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MS45

Solving the Poisson Equation with Neural Networks with Special Attention to Boundary Values

Partial differential equations are the natural language in which force balances in material science are formulated. Following their success in data science, neural networks have made inroads in scientific computing as solvers for PDEs. A classical question in theory and numerics is: If the data of a problem can be represented by a certain function class, what can we say about the solution? We study the simplest example of harmonic functions on the unit square with boundary values given by a shallow neural network and prove both positive and negative results on approximating the solution by neural networks.

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MS46

Compactness Results for a Dirichlet Energy of Nonlocal Gradient with Applications

We prove two compactness results for function spaces with finite Dirichlet energy of half-space nonlocal gradients. In each of these results, we provide sufficient conditions on a sequence of kernel functions that guarantee the asymptotic compact embedding of the associated nonlocal function spaces into the class of square-integrable functions. Moreover, we will demonstrate that the sequence of nonlocal function spaces converges in an appropriate sense to a limiting function space. As an application, we prove uniform Poincar-type inequalities for sequence of half-space gradient operators. We also apply the compactness result to demonstrate the convergence of appropriately parametrized nonlocal heterogeneous anisotropic diffusion problems. We will construct asymptotically compatible schemes for these type of problems. Another application concerns the convergence and robust discretization of a nonlocal optimal control problem.

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MS46

Efficient Optimization-Based Quadrature for Variational Discretization of Nonlocal Problems

Casting nonlocal problems in variational form and discretizing them with the finite element (FE) method facilitates the use of nonlocal vector calculus to prove well-posedeness, convergence, and stability of such schemes. However, nonlocal weak problems involve the computation of a double-integral, which is computationally expensive and presents several challenges. In particular, the inner integral of the variational form associated with the stiffness matrix is defined over the intersections of FE mesh elements with a ball of radius δ. Identifying and parameterizing these intersections is a nontrivial computational geometry problem. We propose a quadrature technique where the inner integration is performed using quadrature points distributed over the full ball, without regard for how it intersects elements, and weights are computed with the generalized moving least squares method. This circumvents the computation of element-ball intersections. We consider 1D and 2D implementations of piecewise linear continuous FE approximations, focusing on the case where the element size h and the nonlocal radius δ are proportional. Our method is asymptotically compatible in the limit of both h and δ going to zero and features at least first-order convergence in the L^2 norm, for both uniform and nonuniform grids. Numerical tests also indicate that, even for nonuniform grids, second-order convergence can be observed over a substantial pre-asymptotic regime.

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MS46

Variations on a Theme: Two Existence Theorems For Nonlocal Variational Problems

Nonlocal derivatives are integral operators that can play a

modeling role similar to derivatives. These nonlocal operators satisfy an analog of integration by parts and converge to the classical derivative as the nonlocality shrinks. As integral operators, the domain of a nonlocal derivative is a much larger function space than the classical derivative. This makes them useful tools for studying systems with low regularity, such as fracture dynamics studied in peridynamics. Motivated by recent advances in peridynamics and the success of variational methods in the classical theory of elasticity, we study a class of variational problems where a nonlocal derivative with integrable kernel takes the place of the classical derivative. We show that, in practice, there are two primary cases of interest, depending on the assumed properties of the kernel. In both cases, we establish existence of minimizers for the nonlocal variational problem. We'll conclude with Young's Tacking Problem: an example of a local functional that lacks a minimizer, but whose nonlocal analog is well-posed with a smooth solution.

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MS46

Asymptotically Compatible Discretization Schemes for Nonlinear Nonlocal Models

We present a study on asymptotically compatible discretizations for a class of nonlinear problems. The generic analytical framework uses variational convergence, or Gamma-convergence, rather than the strong convergence of operators. We apply this program to obtain asymptotically compatible discretizations of a class of nonlocal variational problems with classically-defined, local boundary constraints through heterogeneous localization at the boundary. Along the way, we present recent analytical results for this nonlocal model that allow us to apply the general AC framework.

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MS47

Uncovering Mechanisms of Grain Boundary Migration in Polycrystals for Predictive Simulations of Grain Growth

3D x-ray diffraction microscopy provides a new opportunity to investigate a fundamental behavior in materials processing: grain growth. Curvature is considered the common driving force for grain boundary motion in all polycrystals. However, models and simulations derived from curvature-based motion cannot predict irregular, albeit commonly observed, grain growth behavior. To build better predictive models, we need to employ new tools to understand what governs local migration. Traditional grain growth studies use destructive characterization methods that do not allow the same grains to be tracked over time in 3D. With x-ray diffraction microcopy, the internal structure of inorganic materials can now be captured non-destructively to provide details of how materials evolve during processing. Here, we will show recent experimental observations in metals and ceramics that show the significance of anisotropic grain boundary energy on its migration. These results will be compared to simulations that incorporate anisotropic grain boundary properties to evaluate the mechanisms governing local grain boundary motion. These observations can help us understand how to design microstructures and build better predictive grain growth models.

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MS47

Iterative Design and Fabrication of Hyperuniform-Inspired Materials for Targeted Mechanical and Transport Properties

Micro-lattice and nano-lattice structures are an exciting class of materials with better strength-to-weight and stiffness-to-weight ratios than bulk solids. We aim to develop novel approaches to design a new class of disordered lattice materials that are inspired by the special transport properties, e.g., heat transfer and diffusion, of the so-called hyperuniform structures. Hyperuniform materials may nominally be described as materials with minimal density variation as the length scale increases. In addition to creating additive manufacturing techniques to produce, and experimental designs to measure transport through, the lattice structures, we will also create new modeling approaches, such as network analysis to create design heuristics and higher-order stochastic spatial-averaging techniques to account for microscale heterogeneity. This talk will present an overview of our approach and preliminary results.

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MS47

Simulation-Informed Models for Amorphous Metal Additive Manufacturing

Additive manufacturing of amorphous metals is a potentially transformative technology for printing three-dimensional parts with superior strength and toughness. Since amorphous metals solidify without adopting a crystal structure, they do not form crystalline defects that can limit part performance. While the high cooling rates associated with using a laser to deposit metal on a surface are favorable for avoiding crystallization, the scanning of the laser can lead to subsequent crystallization and variations in properties from one location to another. These issues currently limit the technique to small scale and specialty parts. This collaborative DMREF project will address these limitations through a combination of experiment, simulation, and data fusion. Machine learning will be used to quantify key order parameters suitable for predicting mechanical properties from nanometer-resolution electron nanodiffraction and atomistic simulation data. The research team will build simulation-informed models, continuum numerical tools that will capture how processing gives rise to the strength and toughness of the resulting materials. Validation will be achieved by direct comparison to ex situ and in situ mechanical testing.

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MS48

Multiscale Entropic Approach to Materials Degradation

Degradation of metals in general and fatigue of metals specifically rely heavily on empiricism with little to no theoretical underpinning. The challenge in developing a unified theory of metals fatigue stems from the fact that fatigue is a multiscale phenomenon with irreversible slips occurring at nanoscale to crack initiation at micro/mesoscale grains to fracture at part scale. The span of length scale over which fatigue of metals evolves with number of cycles renders any theoretical development challenging. Entropy is a truly multiscale concept that plays a central role both in information theory and in thermodynamics. In this talk we will discuss recent advances in fatigue damage prediction revealing the potential of employing thermodynamic principles to assess damage accumulation without resorting to traditional empirical models. Multiscale nature of thermodynamic entropy, from grain scale fatigue damage accumulation to macroscale part failure, will be discussed.

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MS48

On Median Filters for Motion by Mean Curvature

The median filter scheme is an elegant, monotone discretization of the level set formulation of motion by mean curvature (an evolution that arises in many applications, including materials science and image processing). It turns out to be connected, in a completely precise way, to another class of numerical methods for the same evolution: threshold dynamics. In particular, median filters evolve every upper level set of their initial condition by threshold dynamics. In other words, they are the natural level set versions of threshold dynamics algorithms. Exploiting this connection, we revisit median filters in light of recent progress on the threshold dynamics method. We give a variational formulation of, and exhibit a Lyapunov function for, median filters, resulting in energy based unconditional stability properties. The connection also yields analogues of median filters in the multiphase setting of mean curvature flow of networks. These new multiphase level set methods do not require frequent redistancing, and can accommodate a wide range of surface tensions.

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MS48

Microstructural Evolution in 3D: An Existence Result

Microstructural coarsening is a network of grains separated by interfaces, facets, that evolve by generalized curvature. The facets meet along curves that come together at points. Systems of this nature consist of many nonlinear PDE'S with their boundary conditions. Here we explore the local in time existence for a configuration, perhaps the simplest, close to a known equilibrium configuration. We discuss our progress, pitfalls, and difficulties in demonstrating the PDE formulation.

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MS48

Suitability of Microstructure Representations for Machine Learning

The microstructure is the internal structure of a polycrystalline material at the micron scale, is comprised of domains known as grains with associated orientations, and governs many material properties. Machine learning inputs for microstructure classification and prediction tasks should reflect both grain geometry and orientation. We compare the performance of convolutional neural networks trained on 2D microstructure images augmented with four different vectorized representations of crystallographic information. This is joint work with Tyrus Berry, Jeremy Mason, Dylan Miley, and Shrunal Pothagoni.

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MS49

Some Computational Methods for Reaction-Diffusion Type Equations

We propose an easy-to-implement iterative method for resolving the implicit (or semi-implicit) schemes arising in reaction-diffusion (RD) type equations. In our treatment, we formulate the nonlinear time implicit scheme on the space-time domain as a min-max saddle point problem and then apply the primal-dual hybrid gradient (PDHG) method. Suitable preconditioners are applied to accelerate the convergence of our algorithm under different circumstances. We provide conditions that guarantee the convergence of our method for various types of RD-type equations with Lipschitz reaction terms. We discuss how the hyperparameters of the algorithm are chosen in order to achieve efficient performance. Several numerical examples as well as comparisons with commonly used numerical methods will be demonstrated to verify the effectiveness and the accuracy of our method.

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MS49

Projected-Transport Gradient Flows for Sampling

To obtain gradient flows that can be approximated in high dimensions we introduce the projected Wasserstein distance where the space of velocities has been restricted to have low complexity. We will show some of the basic properties of the distance and the corresponding gradient flows. Application towards interacting particle methods for sampling will also be discussed.

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MS49

Structure-Preserving Numerical Discretization to Fokker-Planck Equations

Fokker-Planck-type equations have wide applications in physics, biology, and materials science. Mathematically, these equations can be viewed as a specific type of gradient flow associated with a particular energy functional and dissipation potential. In this talk, I will explore various numerical discretization techniques for solving Fokker-Planck-type equations. These techniques include particle methods and neural network-based approaches, which are developed directly from the variational formulation of these equations. Additionally, I will discuss the applications of these methods in machine learning and biology.

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MS50

A Modified Void Nucleation and Growth Model (mnag) for Understanding and Predicting Damage Evolution in Bcc Ta

This work investigates the nucleation and evolution of spall-induced void damage in magnesium of varying microstructure, using an in-situ, absorption contrast imaging approach. Damage and failure in ductile metals is characterized by nucleation, growth, and coalescence of voids. The underlying mechanisms and kinetics that control void nucleation and growth have been linked to material microstructure, but the specific controlling mechanisms associated with these processes are not understood or predicted. Our experimental results establish that microstructure plays a significant role in damage onset and evolution. Different primary failure mechanisms are activated depending on the sample microstructure, which we demonstrate leads to a clear difference in void shape and propagation which are not captured by traditional spall measurement approaches. Damage prediction models make simplifying assumptions regarding the growth rate, shape, and distribution of voids which do not fully capture damage evolution intricacies. Here, we show that high resolution, in-situ data is needed to fully understand the onset and evolution of damage, as well as its relationship with sample microstructure. Furthermore, we show for the first time the direct measurement of experimental void growth rates. The insights provided by our work can be applied to the refinement of existing analytical damage models and the development of new, superior damage models.

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MS50

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

Our NSF-DMREF project seeks to fundamentally change how we approach the design and manufacture of materials by controlling both defect/feature character and internal stress state to achieve a 30% reduction in accumulated damage. Our interdisciplinary approach to developing advanced damage-resistant materials is validating mod-

els, statistical analysis, uncertainty reduction, and computational simulations through characterization and high-throughput multi-scale deformation techniques at the extremes. Our initial efforts describe the utility of spherical nanoindentation stress-strain curves in order to characterize the local mechanical behavior within individual grains of Ta (our model BCC refractory material) and near grain boundaries of polycrystalline Ta samples. Using a series of examples, we demonstrate the capabilities of our data analysis procedures in a) characterizing the local indentation yield strengths in individual grains of deformed polycrystalline metallic samples and relating them to increases in the local slip resistances, b) correlating the stored energy differences of individual grains to their Taylor factors as a function of imposed cold work, and c) understanding the role of interfaces such as grain boundaries in the deformation of a multi-phase polycrystalline sample.

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MS50

Dynamic Strength of Materials under High Pressures Using Pressure Shear Plate Experiments

Developing advanced materials with desired mechanical properties requires a fundamental understanding of the physics of the deformation and failure behavior of materials over a wide range of lengths and time scales. Strength measurement at high dynamic pressures is critical for space shielding, hypersonic vehicles, and armor protection applications. However, the experimental techniques to investigate the strength of materials at high pressures are limited. This talk will present the recent advancements in pressure shear plate impact (PSPI) technique to study the material behavior at high dynamic pressures involving shock waves. The high-pressure PSPI experiments provide a unique methodology for extracting the complete stress-strain behavior of materials at pressures approaching 50 GPa. The results from experiments on oxygen-free high conductivity (OFHC) copper at pressures ranging from 10 to 43 GPa and strain rates of 100000 /s will be presented. A strong pressure hardening strength is observed in copper, which cannot be explained using the shear modulus scaling conventionally used in materials models. The atomistic mechanisms responsible for pressure-dependent strength are explored using molecular dynamics simulations.

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MS51

Coupled Cluster Greens Function Formulations in Reduced-Dimensionality Spaces

The double unitary coupled cluster (DUCC) ansatz, an extension of the sub-system embedding sub-algebras coupled cluster (SES-CC) formalism, allows one to include dynamical (outside the active space) correlation effects in a complete active space effective Hamiltonian. In contrast to the standard single-reference SES-CC theory, the unitary CC approach results in a Hermitian form of the effective Hamiltonian, which has been promising for quantum computing applications, among others. This presentation will review the DUCC theory, including time-dependent and quantum flow extensions. We will demonstrate that the effective Hamiltonians obtained with the downfolding procedure based on the DUCC ansatz can be used in the context of Green's function coupled cluster (GFCC) formalism to calculate spectral functions of molecular systems. This combined approach (DUCC-GFCC) provides a significant reduction of numerical effort and good agreement with the corresponding all-orbital GFCC methods in energy windows consistent with the choice of active space.

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MS51

Simulating Open Quantum Systems using Hamiltonian Simulations

The Lindblad quantum master equation is a fundamental tool in studying the dynamics of a quantum system interacting with quantum baths. Unlike the time-dependent Schrdinger equation, the Lindblad equation accounts for the effects of an environment on a quantum system by incorporating non-Hermitian operators that depict dissipative processes and jump operators that characterize environment noise. We present a novel method to simulate the Lindblad equation, drawing on the relationship between Lindblad dynamics, stochastic Schrdinger equations, and Hamiltonian simulations. By introducing extra ancilla qubits, we derive a sequence of unitary dynamics in an enlarged Hilbert space that can approximate the Lindblad dynamics up to an arbitrarily high order. Compared to classical algorithms, the quantum algorithm is much more efficient in terms of how the complexity depends on the spatial dimension.

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MS51

Quench Dynamics with Time-Dependent Selected

Configuration Interaction Method

Describing electron dynamics in the presence of strong electron correlation poses a challenging methodological problem. In this work, we have attempted to develop such methods, where for the strong correlation, we have considered a selected CI method, namely Adaptive Sampling Configuration Interaction (ASCI) as implemented in Q-Chem [N. M. Tubman J. Chem. Phys. 145, 044112 (2016)]. We have then applied this method to study the real-time relaxation dynamics of the fermionic systems subjected to a quench.

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MS51

Real-Time Simulation of Spin Chains in An Open Quantum System

We study the real-time simulation of open quantum systems, where the system is modeled by a spin chain, with each spin associated with its own harmonic bath. Our method couples the inchworm method for the spin-boson model and the modular path integral method for spin systems. In general, computation of path integrals will suffer from the numerical sign problem, which means the oscillation of the integrand, leading to strong cancellations during the integration, requires an unacceptably large number of samples to achieve accurate results. In our work, the methodology of "partial summations" is applied to alleviate the numerical sign problem. Both the inchworm method and the modular path integral method are developed based on such an idea, and we have tweaked both methods to make them work seamlessly with each other. Our method will then be coupled with the transfer tensor method with representations using tensor trains to improve the efficiency.

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MS52

Design of Origami Structures with Curved Tiles Between the Creases

An efficient way to introduce elastic energy that can bias an origami structure toward desiredshapes is to allow curved tiles between the creases. (Think: a Frank Gehry building that folds upspontaneously from a flat sheet.) Isometric bending of the tiles then supplies the energy. The h^3 scalingof the energy of thin sheets (h =thickness) spans a broad energy range, that is also consistent with a singleorigami design. And with a given design, different tiles can have different values of h. Even a single tile canhave differing values of your h. In this lecture we present a theory and systematic design methods for quite generalcurved-tile origami structures that can be folded from a flat sheet. Unlike the standard approach to origamidesign (which is Eulerian), we find it useful to develop Lagrangian methods. A group orbit method using discreteisometry groups enables the design of complex structures from simple calculations. Along the way, we make some speculative remarks about the relation of our results to a) buckling and imperfection sensitivity, and b) the structures of some sea and land creatures.

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MS52

Phase-Field Damage Modeling and Simulation of Paper Folding

Origami is the ancient Japanese art of folding paper into intricate shape. One of the main challenges of origami is to determine the fold pattern so as to approximate a given target surface. We follow a previous approach of [Bartels et al, 2022] by modeling the folding of a thin elastic sheet as a two-dimensional piecewise nonlinear Kirchhoff plate bending model with a continuity condition on the fold set. We reformulate this problem in the framework of special functions of bounded variation SBV, and propose to use a phase-field damage model to approximate the solutions of this problem. We prove that the approximation Γ-converges to its sharp interface counter-part. This allows us to reproduce previous numerical results but also to compute the creation of fold curves from previously undamaged domains, which is a novelty.

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MS52

Derivation of an Effective Plate Theory for Parallelogram Origami from Bar and Hinge Elasticity

Periodic origami patterns made with repeating unit cells of creases and panels can bend and twist in complex ways. In principle, such soft modes of deformation admit a simplified asymptotic description in the limit of a large number of cells. Starting from a bar and hinge model for the elastic energy of a generic four parallelogram panel origami pattern, we derive a complete set of geometric compatibility conditions identifying the patterns soft modes in this limit. The compatibility equations form a system of partial differential equations constraining the actuation of the origami's creases (a scalar angle field) and the relative rotations of its unit cells (a pair of skew tensor fields). We show that every solution of the compatibility equations admits a well-defined soft mode – a sequence of origami deformations with finite bending energy and negligible stretching. We also show that the limiting energy of these sequences is a plate-like theory for parallelogram origami patterns with an explicit coarse-grained quadratic energy depending on the gradient of the crease-actuation and the relative rotations of the cells. Finally, we illustrate our theory in the context of two well-known origami designs: the Miura and Eggbox patterns. General soft modes captured by our theory involve a rich nonlinear interplay between actuation, bending and twisting, determined by the underlying crease

geometry.

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MS52

Complex Patterns of Stress and Strain in Mechanism-Based Metamaterials

Mechanical metamaterials designed around a zero-energy nonlinear pathway of deformation, known as a mechanism, have repeatedly challenged the conventional picture of elasticity. However, rather than activating this mechanism uniformly, generic loading conditions produce spatially complex patterns of strain and stress even at low energies. Here we present a unified theoretical framework for such deformations, showing that the presence of a uniform mechanism in a two-dimensional structure yields a new pattern of responses that differs dramatically from conventional elasticity. Our formalism reveals a mathematical duality between these stress-free strains, which we term "sheared analytic modes" and the supported spatial profiles of stress. These modes undergo a transition from bulk periodic response to evanescent surface response as the Poisson's ratio of the mechanism is tuned through zero, an exceptional point. We suggest a first application of these unusual response properties as a switchable signal amplifier and filter for use in mechanical circuitry and computation.

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MS53

Accelerated Materials Innovation Using High-Throughput Experiments and Ai/ml Tools

The dramatic acceleration of the materials innovation cycles is contingent on the development and implementation of high throughput strategies in both experimentation and physics-based simulations, and their seamless integration using the emergent AI/ML toolsets. This talk presents recent advances made in the presenters research group, including: (i) a novel information gain-driven Bayesian ML framework that identifies the next best step in materials innovation (i.e., the next experiment and/or physics-based simulation to be performed) that maximizes the expected information gain towards a specified target (e.g., optimized combination of material properties, refinement of a material constitutive response), (ii) computationally efficient versatile microstructure image analyses and statistical quantification tools, (iii) formulation of reduced-order process-structure-property models that enable comprehensive inverse solutions needed in materials design (e.g., identifying specific compositions and/or process histories that will produce a desired combination of material properties), and (iv) high throughput experimental protocols for multi-resolution (spatial resolutions in the range of 50 nm to 500 microns) mechanical characterization of heterogeneous materials in small volumes (e.g., individual phase constituents in multiphase material samples, thin coatings or layers in a multilayered sample). These recent advances will be illustrated with multiple case studies.

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MS53

Geometry-Driven Surrogate Modeling of Complex Physical Systems

Differential geometry, a mathematical field renowned for its applications in understanding dynamical systems, finds new relevance in the domain of surrogate modeling for these systems. Surrogate modeling aims to approximate simulated data while mitigating computational expense. In this study, we explore the significant benefits of incorporating principles from differential geometry into the development of novel surrogate models for complex physical systems. Central to our approach is the utilization of Diffusion Maps, a powerful tool that discovers the intrinsic geometry of data manifolds and naturally captures the underlying dynamics, nonlinearities, and interdependencies paramount to the study of physical systems. To illustrate the potential of our method, we apply it to the chemical kinetics modeling of RDX decomposition. Our results showcase the considerable improvements in accuracy, robustness, and interpretability of our approach, underscoring its potential to revolutionize the modeling and understanding of complex physical systems.

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MS53

Modeling Process Structure Property Relationships in Mo Thin Films from Multi-Modal Data Using Machine Learning

We discuss a multi-modal machine learning (ML) approach to study process-structure mapping of thin films fabricated using physical vapor deposition (PVD). Thin films play a significant role in the semiconductor industry. Hence, there is an interest in fabricating thin films with desirable properties that can improve the efficiency of semiconductor devices. However, trial-and-error approaches to find optimum processing conditions for materials with desirable properties can be slow and costly. Data science models can accelerate material discovery by first fitting them to capture relationships between process conditions and material structure/properties and then using them to find optimal process conditions that are expected to result in desirable properties. To enhance the accuracy and confidence of these models, they must be trained on sufficient data sizes and multiple data modalities. We present a multi-modal ML approach that predicts structural information of Mo thin films from PVD process conditions. The construction employs an ML model to learn a joint latent representation of the multi-modal microstructure data and another ML model to learn a mapping from process parameters to this joint latent space. The predicted latent representation can be mapped back to the original data space. We will discuss this machinery's design and performance and explore

its utility as a process-structure map representation.

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MS54

Extending a Physics-Based Constitutive Model of Plastic Material Deformation Using Genetic Programming

Mathematical models are widely used in material science to describe material phenomena (e.g. phase transformation) and predict material properties (e.g. strength) under certain conditions (e.g. temperature, pressure, etc.). The major drawback of these models is the unknown parameters that cant be or are hard to measure and need to be calibrated to the experimental data. Thus, novel approaches need to be introduced to overcome this challenge. In the present work, we investigate the model that describes the material behavior at the microstructure level based on the physics laws. In particular, internal material variables such as dislocation density are used to describe the mechanical response under mechanical and thermal loading, which is expressed by the stress-strain curves. This constitutive model contains the three calibration parameters which should be varied depending on the input variables such as deformation temperature and rate. Using symbolic regression and genetic programming, the hidden correlation between the given parameters and input variables can be revealed in the form of short interpretable expressions. The derived expressions extend the physics-based constitutive model by replacing the calibration parameters with the mathematical expressions. This enables the interpolation between varying processing parameters during the deformation process. The approach is validated using the finite element simulation of a lab-scale hot compression test.

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MS54

Dynamic Boundary Conditions and Evolution of Grain Boundary Networks

I will present the dynamic boundary conditions in the general framework of energetic variational approaches. The focus is on the coupling between the bulk effects with the active boundary conditions. In particular, we will study applications in the evolution of grain boundary networks, in particular, the drag of trip junctions. This is a joint work with Yekaterina Epshteyn (University of Utah) and Masashi Mizuno (Nihon University).

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MS54

A Hybridizable Discontinuous Galerkin Method for the Phase Field Crystal Equation

The Phase Field Crystal (PFC) Equation is a sixth-order nonlinear time-dependent partial differential equation that was introduced by Elder and Grant (2004) as a continuum model to study the atomic-scale crystal growth over diffusive time scales. In this talk, we present a hybridizable discontinuous Galerkin method to solve the PFC equation with temporal discretization realized by the convex splitting scheme. We will discuss key properties of unique solvability and unconditional stability satisfied by the scheme and also present numerical experiments to illustrate the performance of our proposed method.

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MS55

Information Gamma Calculus: Convexity Analysis for Stochastic Differential Equations

We study the Lyapunov convergence analysis for degenerate and non-reversible stochastic differential equations (SDEs). We apply the Lyapunov method to the Fokker-Planck equation, in which the Lyapunov function is chosen as a weighted relative Fisher information functional. We derive a structure condition and formulate the Lyapunov constant explicitly. Given the positive Lyapunov constant, we prove the exponential convergence result for the probability density function towards its invariant distribution in the L1 norm. Several examples are presented: underdamped Langevin dynamics with variable diffusion matrices, quantum SDEs in Lie groups (Heisenberg group, displacement group, and Martinet sub-Riemannian structure), three oscillator chain models with nearest-neighbor couplings, and underdamped mean field Langevin dynamics (weakly self-consistent Vlasov-Fokker-Planck equations). This is based on a joint work with Qi Feng (FSU).

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MS55

Periodic and Stochastic Homogenisation of Transport Problems on Graphs

We discuss discrete-to-continuum limits of optimal transport problems, with particular attention to recent contributions in the periodic and the stochastic setting. We introduce a natural discretization of a broad class of dynamical transport problems and, in this talk, focus in particular on their convergence in the framework of stationary (and possibly ergodic) graphs with random transport problems. The content of the talk is based on a collaborations with Eva Kopfer, Peter Gladbach, and Jan Maas.

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MS55

On a Nonlinear, Nonlocal Parabolic Problem with Conservation of Mass, Mean and Variance

In this talk we show that the steepest descent of certain porous-medium type functionals with respect to the quadratic Wasserstein distance over a constrained (but not weakly closed) manifold gives rise to a nonlinear, nonlocal parabolic partial differential equation connected to the study of the asymptotic behavior of solutions for filtration problems. An interesting feature of the resulting Fokker-Planck equation is the nonlocality of its drift term occurring at the same time as its nonlinearity.

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MS56

Causal Inference and Statistical Reduced-Order Models for Extreme Damage Events

The mechanical behavior of high-purity polycrystalline metallic materials under stress is critical, impacting industries from aerospace to electronics. These materials comprise a network of grains, each with unique crystallographic orientations, creating a complex internal structure. In this talk, a causal inference framework is developed to discover the relationship between the microstructural factors and von Mises stress close to the grain boundaries. It uses information theory to facilitate the selection of crucial factors that contribute to the elevated stress state and build a nonlinear stochastic equation to the maximum von Mises stress. The method is applied to the data sets associated with a hierarchy of damage models with different complexities.

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MS56

Modeling Microstructure Descriptors Evolution with Stochastic Differential Equations

Modeling grain growth has been a subject of interest in computational material science, as it occurs in thermal-based processing methods such as annealing and sintering. Kinetic Monte Carlo with Potts model is a popular integrated computational materials engineering (ICME) grain growth model to simulate synthetic microstructures. In this talk, we discuss a data-driven stochastic calculus perspective on the kinetics of grain growth and model the microstructure evolution through the lens of stochastic differential equations, based on Langevin dynamics and Fokker-Planck equation to forecast the grain size distribution. We demonstrate that our proposed approach agrees reasonably well with the hybrid Potts-phase field kinetic Monte Carlo model using SPPARKS (spparks.sandia.gov) in forecasting the long-term evolution of grain size distribution.

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MS57

Wave Propagation in Periodic Half-Spaces

In this talk, we consider the 2D Helmholtz equation in presence of a periodic half-space. A numerical method has been proposed by Fliss, Cassan, Bernier (2010) to solve this equation under the critical assumption that the medium stays periodic in the direction of the interface. In fact, in this case, a Floquet-Bloch transform can be applied with respect to the variable along the interface, thus leading to a family of closed waveguide problems. The purpose of this work is to deal with the case where the medium is no longer periodic in the direction of the interface, that is, if the periodic half-space is not cut in a direction of periodicity. As it is done by Grard-Varet, Masmoudi (2015), we use the crucial (but non-obvious) observation that the medium has a quasiperiodic structure along the interface, namely, it is the restriction of a higher dimensional periodic structure. Accordingly, the idea is to interpret the studied PDE as the restriction of an augmented PDE in higher dimensions, where periodicity along the interface is recovered. This so-called lifting approach allows one to extend the ideas by Fliss, Cassan, Bernier (2010), but comes with the price that the augmented equation is non-elliptic (in the sense of the principal part of the differential operator), and thus more complicated to analyse and to solve numerically. Numerical results will be provided to illustrate the method.

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MS57

Waves in Fibonacci Quasicrystals: from Chaos to

Cantor Sets

Connections between distinct fields of mathematics are often valuable starting points for breakthroughs. This talk exploits links between elliptic periodic operators generated by Fibonacci tilings and a non-linear dynamical system. This non-linear second-order recursion relation describes the Lyapunov functions associated to the sequence of operators. This link allows us to make several breakthroughs. On the one hand, we can study how the spectral band gaps evolve under the Fibonacci tiling rule and prove the existence of "super band gaps" (band gaps that exist for all sufficiently large tilings). This characterises how periodic approximants (supercells) of Fibonacci quasicrystalline materials faithfully reproduce the main spectral gaps. Conversely, the density of states associated to the elliptic operators can be used to predict the statistics of the non-linear recursion relation, in spite of the apparent lack of an invariant measure. In both cases, these problems were solved by exploiting the connection between the two fields.

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MS57

Wave Propagation in One-Dimensional Quasiperiodic Media

This work is devoted to the solution of the Helmholtz equation in 1D unbounded quasiperiodic media. By this we mean that the coefficients appearing in the model are quasiperiodic functions of the 1D space variable, namely the trace along a line of a periodic function of n variables. When the coefficients are periodic (which is a special case), several methods have been proposed to characterize and compute the solution. However, when the coefficients are quasi-periodic without being periodic, the above methods cannot be applied directly. We use an original method, that we call the lifting method, which has been used in several papers on homogenization theory. The original problem can thus be lifted to an nD "augmented" problem with periodic coefficients, and the 1D solution is the trace along this line of the nD solution. The advantage is that the periodicity of the augmented problem enables to use the ideas proposed for solving periodic Helmholtz equations in periodic waveguides. However, since the augmented equation is a degenerate elliptic equation, the corresponding tools have to be adapted since new difficulties arise both in the analysis and in the design of the resulting numerical method. I will present our results for the Helmholtz equation with dissipation (where the solution decays at infinity) and then for the equation without dissipation (where the solution can propagate to infinity), analyzing the latter case using a limiting absorption principle.

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MS57

A Spectral Approach to Flat Lens Design

We consider the problem of finding a phase mask between an object and an imaging plane such that it maximizes the number of degrees of freedom that are transmitted between regions of interest in these planes. The optimization problem can be reformulated as an eigenvalue problem, which allows for an efficient solution and a characterization in terms of the classic thin lens phase.

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MS58

The Metamaterial That Trains Itself

Consider the generic goal of creating a physical system that performs a desired function, for example a circuit that classifies incoming signals. Typically, such an object is designed by hand, or with the help of digital optimization. Here Ill discuss an alternative approach, *learning metamaterials*: analog electronic networks made solely of copies of a single self-adjusting element. When shown examples of correct functionality (*e.g.* correctly classified signals), learning metamaterials respond by changing the conductance of each edge of the network. While the systems dynamics are entirely local and requires no external computation or memory its emergent behavior mimics error minimization of the training data, *training itself* to perform the task. Learning metamaterials are adaptive, and a single structure can be trained and retrained to perform a variety of nontrivial and nonlinear tasks, including classification. Similar to brains, learning metamaterials are ensemble systems that 'compute using nonlinear physical processes, making them potentially faster, more efficient, and more robust than digital computers at learning tasks. Ill discuss laboratory realizations of these systems, as well as what weve learned about how they accomplish global goals using only local rules, and modes of learning relevant to biological systems.

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MS58

Teaching Materials to Adapt Through Non-Equilibrium Training

The past two decades have seen dramatic advances in our ability to program material building blocks across lengthscales from the nano to the macro, generating metamaterials with impressive task-based functionalities. However, many desired material qualities are in fact better phrased as meta-functions, e.g. robustness, modularity, or adaptability. We show that adaptability naturally emerges when tunable synthetic materials are trained for different incompatible functions in sequence. By switching training goals, materials localize to special regions of their high-dimensional design spaces, where they have learned to be rapidly adaptive to a changing environment. Examining the resulting materials can reveal physical principles underlying material adaptability. This way of training works on top of existing design methods and can be applied across

a wide array of materials, real or simulated. We demonstrate our method in two different simulation contexts: disordered elastic structures and heteropolymers with tunable interactions.

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MS58

Nonequilibrium Design Strategies for Functional Self-Assembly

In this talk, I will discuss a nonequilibrium variational principle for optimizing the steady-state, dynamic properties of nanoclusters of DNA-coated colloids. Employing this principle within a stochastic optimization algorithm allows us to identify strategies to optimize the directed interconversion of colloidal cluster conformations and the hopping is particles between clusters within a microphase. This approach provides a general means of uncovering design principles for nanoscale, autonomous, functional materials driven far from equilibrium.

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MS58

Evolutionary Learning of Protocols for Molecular Self-Assembly

We show that neural networks trained by evolutionary methods can learn protocols that promote molecular self-assembly. Given a physical system, such as a collection of molecules or nanoparticles in water, we can encode the protocol to which it is subjected as a neural network. The neural networks inputs are the elapsed time of the experiment and any information we are able to measure from the system, while its outputs specify the values of the control parameters that comprise the protocol, such as temperature or pressure. We show, using simulations and experiments, that it is possible for a learning algorithm to produce neural networks of this nature whose protocols produce specified materials, choose between competing polymorphs, or perform open-ended synthesis to discover new materials.

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MS59

Propagation of Waves in 3D Periodic Media: Dispersion, Formation of Clusters, Analytical Determination of Gaps

We consider wave propagation through a periodic array of small inclusions of arbitrary shape described by the Helmholtz equation. The inclusion size a is much smaller than the array period. We derive the dispersion relation and show that there are exceptional frequencies for which the solution is a cluster of waves propagating in different directions with different frequencies. The approach is based on reducing the problem to the study of the condition for the existence of a zero eigenvalue of a specially constructed Dirichlet-to-Neumann operator. This allows us to use the regular perturbation techniques and obtain exact asymptotic results for the cutoff frequency in the case of homogeneous Dirichlet boundary conditions. We show that global gaps do not exist in any fixed interval $(\varepsilon, \varepsilon^{-1})$ of the time frequency ω if a is small enough. The notion of local gaps which depends on the choice of the wave vector $\mathbf{k}$, is introduced and studied. As one of the consequences, it will be shown that for $\mathbf{k}$ on the boundary of the first Brillouin zone, the local gaps exist if and only if $|\mathbf{k}| < \ell/\sqrt{2}$, where ℓ is the edge length of the Brillouin zone. The size of the gaps will be described.

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MS59

From Micro to Macro in Sea ice Modeling

Sea ice plays a key role in Earths climate and polar ecosystems, and it exhibits composite structure on length scales ranging over many orders of magnitude. A principal challenge in modeling sea ice is how to use information on smaller scale structure to find the effective behavior on larger scales relevant to climate and ecosystem models. The inverse problem of recovering smaller scale parameters from bulk measurements is also of interest. Well tour recent advances in the mathematics of modeling sea ice, from the fractal geometry of brine inclusions and surface melt ponds, to wave-ice interactions and the large-scale dynamics of the sea ice cover on the scale of the Arctic Ocean. Well focus on methods of homogenization, as well as unexpected topics that we encounter, including random matrix theory, Anderson localization, and topological data analysis. Finally, we'll give a brief report on an Arctic sea ice expedition with 7 math students, from high school to Ph.D., taking place in the 2 weeks prior to this conference.

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MS60

An Analysis of a Class of Variational Models for Heterogeneous Phase Separation

We present a variational model for the interaction between homogenization and phase separation in composite fluids based on the famous Modica-Mortola functional. We will survey physical motivations and recent works where the effective energies are characterized. They are shown to depend on the relative size of the homogenization scale and phase separation scale and are completely characterized using the tools of $\Gamma-$convergence.

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MS60

Energy Driven Pattern Formation in a Model for Two-Dimensional Frustrated Spin Systems

We are interested in pattern formation in two-dimensional magnetic compounds. We consider materials whose atoms are ordered in a regular crystalline structure and associate to each atom its so called spin, a unit vector in $\mathbb{S}^1$. Complex geometric structures in the spin field may be the result of the competition between anti- and ferromagnetic interactions. In ferromagnetic materials spins prefer to be aligned, whereas in antiferromagnetic compounds one cannot observe a global orientation of the spins. The competition between these two interactions leads to frustration mechanisms in the system. We consider the lattice energy of certain materials, in which antiferromagnetic (AF) and ferromagnetic (F) interactions coexist, and are modeled by the J_1 -J_3 F-AF model on a square lattice. In this talk we present our current research results. These include a Γ-convergence result which in a certain parameter regime relates the discrete model with a suitable continuous counterpart. Further, we present a scaling law for the optimal energy, which describes arising patterns in a minimal spin field. Next to the vortex free regimes, we also observe regimes which prefer using vortices to lower the interaction energy of a spin field. Finally, we briefly present some numerical experiments.

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MS60

Geometric Rigidity in Variable Domains, and Applications in Dimension Reduction for Materials with Voids

Quantitative rigidity results, besides their inherent geometric interest, have played a prominent role in the mathematical study of variational models related to elasticity/plasticity. For instance, the celebrated rigidity estimate of Friesecke, James, and Müller has been widely used in problems related to linearization, discrete-to-continuum or dimension-reduction within the framework of nonlinear elasticity. In this talk I will discuss an appropriate generalization to the setting of variable domains, where the geometry of the domain comes into play, in terms of a suitable surface energy of its boundary. As an application, we rigorously derive a Blake-Zisserman-Kirchoff theory for thin elastic rods with material voids, in a situation allowing for fracture.

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MS61

Numerical Solution of Diffuse Interface Models

Diffuse interface Cahn-Hilliard type models are presented. For their numerical solution energy dissipative Discontinuous Galerkin Finite Element (DG-FE) schemes are developed and numerically analyzed. Simulations that verify some of the numerical analysis results are shown.

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MS61

Boundary Effects in SmA-Type Phases of Liquid Crystals

We consider the de Gennes energy for Smectic A liquid crystals to study the effects of weak anchoring conditions on the onset of the undulation phenomenon due to an applied magnetic field. We present preliminary results on obtaining an estimate for the critical field for the onset of layer undulations. This is joint work with Laura Chavez-Gutierrez and Sookyung Joo.

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MS61

A Quasi-Incompressible Cahn-Hilliard-Darcy Model for Two-Phase Flows in Porous Media

The sharp interface model for two-phase flows in porous media, known as the Muskat's problem, can be ill-posed. In this talk we introduce a quasi-incompressible Cahn-Hilliard-Darcy model as a relaxation of the sharp interface model. We establish global existence of weak solutions. We then present a high-order bound-preserving and unconditionally stable numerical algorithm for solving the model.

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MS62

Diagrammatic Quantum Many-Body Linear Algebra

I will describe a new class of quantum approximation methods termed diagrammatic linear algebra. The basic idea is to describe primitives in linear algebra algorithms as applied to quantum-many body problems in terms of a new type of non-perturbative diagrammatic framework. This gives rise to a rich approximation structure and I will outline some of the promising directions and their applications to quantum-many body physics simulations.

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MS62

Learning Exchange-Correlation Functionals for the Time-Dependent Kohn-Sham Equation

We develop methods to learn the exchange-correlation potential (V_{xc}) for the time-dependent Kohn-Sham (TDKS) equation. We start by numerically solving the time-dependent Schrodinger equation for low-dimensional electronic Hamiltonians. From the resulting time-dependent wavefunctions, we compute the time-dependent electron densities that form our training data set. We treat V_{xc} as a feedback control, represented as a neural network, and then frame the learning problem as an optimal control problem. In this formulation, we seek neural network parameters that minimize the mismatch between reference electron densities and those computed via TDKS, with the discretized TDKS equation appearing as a time-dependent constraint. Applying adjoints and gradient-based optimization, we develop efficient methods to solve this optimal control problem and thereby learn V_{xc}. For 1D TDKS problems, we show how to learn V_{xc} functionals with memory, demonstrating one such model that yields excellent test set results. We compare the predictions of our learned V_{xc} models against widely used approximations of V_{xc}. We also report progress on our ongoing efforts to extend the above program to TDKS problems in 2D and 3D.

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MS62

A Collocation Method for Nonlinear Tensor Differential Equations on Low-Rank Manifolds

We present a new method for computing the solution to a nonlinear tensor differential equation with dynamical low-rank approximation. The idea of dynamical low-rank approximation is to project the differential equation onto the tangent space of a low-rank tensor manifold at each time. Traditionally, an orthogonal projection onto the tangent space is employed, which is challenging to compute for nonlinear differential equations. In this talk, we introduce a novel interpolatory projection onto the tangent space that satisfies the differential equation at a set of carefully selected indices and is easily computed for many nonlinear differential equations.

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MS63

Auxetic Composites with Checkerboard Structure: Asymptotic Rigidity and Variational Homogenization

Auxetic metamaterials are specifically designed to have a negative Poisson's ratio, meaning they expand perpendicular to applied forces under stretching. In this talk, we discuss homogenization via Γ-convergence for a model of auxetics made of elastic composites with stiff rotating squares that accounts for non-self-interpenetration. The challenging part of the proof is determining the admissible macroscopic deformation behavior, or in other words, characterizing the weak Sobolev limits of deformation maps whose gradients are locally close to rotations on the stiff components. To this end, we establish an asymptotic rigidity result, which confirms, under suitable scaling assumptions, that the attainable macroscopic deformations are affine conformal contractions. Our strategy is to tackle an idealized model with full rigidity on the stiff tiles first and then transfer the findings to the model with diverging elastic constants. The latter requires a new quantitative geometric rigidity estimate for non-connected touching squares and a tailored Poincar-type inequality for checkerboard structures.

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MS63

Asymptotically-inextensional Deformations of Periodic Shells

Surface isometries are typically classified into finite and infinitesimal. Recent investigations into the behavior of origami have shown that this classification leaves out an important class of deformations that are far too large to be infinitesimally isometric and far too rich to be strictly finitely isometric. Given that these deformations apply to origami, which is typically folded out of inextensible paper, they must be almost isometric in a sense. Here, the purpose is to theorize for a new class of asymptotically isometric deformations valid for periodic surfaces be them smooth or piecewise smooth (e.g., with straight/curved creases). The idea is to enforce length preservation to first order in the size of the unit cell of periodicity (rather than in the size of the deflection). This is quite reminiscent of two-scale asymptotics used in homogenization theory albeit here the purpose is not to minimize strain energy overall but, in a sense, to minimize membrane contributions. That being said, the presented theory is purely geometric. Its main result is a coarse-grained theorema egregium: a constraint that relates the effective metric of the periodic shell to its effective normal curvatures. Various corollaries regarding the (geometric) flexibility, and rigidity, of periodic shells are explored and exemplified using analytical and numerical methods.

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MS63

Mechanical Metamaterials: Exploring Geometric Frustration in Self Assembly Using a Generalized Elasticity Theory

Mechanical metamaterials have been studied extensively to explore their unusual properties owing to instabilities arising from their micro-structures. We explore a simple continuum framework for the mechanics of a mono-mode, metamaterial thin sheet in which a scalar field, coupled to the reference metric, captures the soft in-plane deformation of the material. In the Fpplvon Krmn limit, we show how the unusual elasticity of the sheet screens the curvature induced stress through soft deformation modes. In addition, we use this approach to explore the characteristic shapes of a metamaterial assembly system which is geometrically frustrated. In addition to the Fpplvon Krmn number, which dictates the competition between bending and stretching modes in a traditional elastic sheet, we show the existence of novel dimensionless numbers which dictate how the soft modes affect this competition and give rise to anomalous equilibrium shapes.

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MS63

Rigidity and Compactness Theorems for Origami and Kirigami-Based Metamaterials

Mechanical metamaterials such as kirigami and origami-inspired ones combine elasticity and geometry to create unusual bulk deformations at a low energy cost. Microscopically, the deformations involve coordinated rigid body motions known as "mechanisms"; macroscopically, a slowly varying field of mechanisms can lead to a non-trivial overall shape change. In the first part of this talk, we present a partial differential equation (PDE) for the bulk deformations of periodic kirigami designs, which we justify via an asymptotic argument based on a novel "mechanism-rigidity" inequality. In the second part of this talk, we discuss similar results for origami. In both cases, the key questions are (i) to determine the general class of non-affine maps that can be approximated by locally mechanistic motions of the underlying metamaterial design, and (ii) to prove a sharp lower bound on the energy required to do this approximation. This is joint work with Paul Plucinsky (USC); the part on origami is also with Zhimeng Wang (Rutgers).

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MS64

Across the Latent Space: Understanding the Organization of the Latent Space for Variational Autoencoders for Material Modeling Applications

Variational autoencoders (VAEs) are a deep neural network architecture that can be used to extract features from high-dimensional objects and to generate new, unique instances of the objects. In this talk, we investigate whether VAEs can be used to predict the mechanical properties of material microstructures. First, we train a VAE on 2D grain shapes in granular materials and probe the interpretability of the low-dimensional latent space created by the model. Next, we train a VAE on the initial configuration of small, representative volume elements (RVEs) of metals. We find that the resulting low-dimensional space discovered by the VAE organizes the microstructures by interpretable morphological features such as density. Finally, we add a regressor that takes as input a latent vector representation of an RVE initial condition and outputs the predicted mechanical response from finite element method (FEM) simulations. We study how the mechanical response of the regressor imposes additional organization on the latent space. The present organized, low-dimensional space provides opportunities for topology optimization, where microstructures with specific mechanical and morphological properties can be quickly designed by sampling the appropriate area of the latent space. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

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MS64

Improving Material Representations in Latent Space with Directional Autoencoders

Reducing high-dimensional materials data into low-dimensional representations is valuable for accelerating materials discovery, design, and understanding. Models such as autoencoders have proven to be exceptional at this dimensionality reduction task, reducing process-structure-property relationships into a small latent variable space. However, the learnt latent space often lacks the interpretability desired by subject matter experts, leading to limited understanding of the learnt representation. In this work, we enforce constraints on the latent space of autoencoders such that a subset of latent space directions correlate with variables deemed relevant by subject matter experts. We find these directional autoencoders to be as accurate as traditional autoencoders at reconstruction, while significantly improving latent space interpretability. We also discuss how constrained latent spaces can be applied to generative models, and downstream materials design tasks. These demonstrations are made on an exemplar problem of designing high hardness, low resistivity Pt-Au thin films. The directional autoencoders here aim to capture the structure of the films, represented as high-dimensional X-ray diffraction patterns or atomic force microscopy images, into low-dimensional latent spaces that correlate with variables identified by human intuition, such as peak width and surface roughness. Our approach can be applied to a wide variety of high-dimensional, multimodal materials datasets.

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MS65

Asymptotic Analysis of Composite Plate with Soft Pre-Strained Matrix

A theoretical study of simultaneous homogenization and dimension reduction of a composite plate in the framework of non-linear elasticity is presented. The examined composite plate comprises a periodic perforated plate made of stiff material with holes filled by soft matrix material. Two cases of asymptotic analysis are being considered: one without pre-strain and the other with matrix pre-strain. In both cases, the total elastic energy is in the von Krmn (vK) regime (ε^5). The asymptotic behavior of the Green-St Venant strain tensor in terms of displacements is derived by using the re-scaling unfolding operator. The vK plate model describes the limit homogenized model for the composite structure, which emerges as the Γ-convergence limit of the non-linear elasticity problem. Despite the nonlinear nature of the initial and homogenized problems, the cell problems associated with the vK plate are linear. The discussion of both cases with and without pre-strain aims to demonstrate that the soft matrix only plays a role in the homogenized plate if it has pre-strain. This behavior is attributed to the relative weakness of the matrix to the stiff part and the fact that the structure is stable (since the thickness and period are of the same order). The results find practical applications in 3D printing in the textile and aerospace industries.

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MS65

Homogenisation of High Contrast Spectral Problems. Part 2. Interpolation Operator

This is a natural continuation of the talk by Dr. Cooper. We discuss the implications of the general scheme for a concrete class of periodic problems and, in particular, we introduce a 'two-scale interpolation operator (an operator that lifts functions of one variable to functions dependent on slow and fast variables). This operator allows us to quantitively compare the solutions of degenerate highly oscillatory problems with the solutions of the corresponding two-scale operators. We shall discuss some properties of this operator as well as compare it to similar known objects. The talk is based on joint work with Dr. Cooper and Prof. Smyshlyaev.

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MS65

Negative Group Velocity and Negative Refraction in Laminates with (Relatively) High Contrast

I will demonstrate how the phenomenon of negative group velocity appears on a rigorous level in high-contrast periodic laminates described by scalar PDEs. The quantitative description of metamaterial properties observed in laminates crucially boils down to the complex-analytic properties of the associated generalised resolvent. Moreover, I will explain that inherently double-negative meta-properties of the effective medium by first principles cannot appear in the leading-order term of the asymptotics, thus bringing order-sharp norm-resolvent convergence estimates to the forefront of the analysis. Different versions of corrected estimates will be discussed in this context, and I will argue that the existing forms of the corrector, not taking into account the complex-analytic (in the frequency variable) behaviour of the model, have to be replaced by novel ones. The effective model of the laminate will be further discussed. The crucial bit of the puzzle here is that even in a scalar case, like the one describing acoustic laminates, the effective medium will be shown to be modelled by a matrix differential operator. Based on this, I will argue that the negative group velocity appears in laminates in what can be called an essentially non-Veselago way. Time permitting, I will also show the negative refraction on a half-space occupied by a high-contrast laminate both analytically and numerically.

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MS65

Homogenisation of High Contrast Spectral Problems. Part 1: Uniform Asymptotics with Error Esttimates

In this talk, we present a framework to study the asymptotic behaviour of (a large class of) periodic non-uniformly elliptic systems with respect to a (small period) parameter. We determine, under very few readily verifiable assumptions, the leading-order approximation of the solution and

derive error estimates, uniform in right-hand-side. Spectral asymptotics with error estimates directly follow. This is joint work with Prof. Ilia Kamotski and Prof. Valery Smyshlyaev.

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MS66

Computing Optimal Thermodynamic Protocols with Differentiable Simulation

Controlling the evolution of nonequilibrium systems to optimize thermodynamical quantities such as heat, work, and entropy is a key goal for designing nanotechnological devices like artificial molecular machines. Conversely, biological molecular machines have evolved to capitalize on the laws of nonequilibrium physics, in some cases achieving remarkable robustness and efficiency, but precisely how this is achieved remains elusive. Classical thermodynamics is ill-equipped to describe the physics of nonequilibrium systems, and new techniques are needed. Here, I introduce one such technique: repurposing the tools used in machine learning optimizations – in particular, automatic differentiation – to find optimal control protocols for nonequilibrium systems. Ill demonstrate the successful use of automatic differentiation to minimize the external energy required to unfold a protein or DNA molecule. I'll also illustrate how automatic differentiation can improve free energy landscape reconstructions for biologically relevant systems.

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MS66

Nonequilibrium Self-Assembly Time Forecasting

Many biological systems rely on the ability to self-assemble target structures from different molecular building blocks using nonequilibrium drives, stemming, for example, from chemical potential gradients. The complex interactions between the different components give rise to a rugged energy landscape with a plethora of local minima on the dynamic pathway to the target assembly. Inspired by many examples of nonequilibrium self-assembly in living systems, we set out to explore the added benefits achieved by nonequilibrium driving and identify distinctive collective phenomena that emerge in this regime. Exploring a toy physical model of multicomponent nonequilibrium self-assembly, we demonstrate that local driving can improve both the assembly time and kinetic stability of the target assembly, and show that a segmented description of the system dynamics can be used to provide predictions of the first assembly times. Based on data segmentation by a Bayesian estimator of abrupt changes (BEAST), we further present a general data-based algorithmic scheme, namely, the stochastic landscape method (SLM), for assembly time predictions. Our results can be used to establish a general quantitative framework for nonequilibrium systems and to improve control protocols of nonequilibrium self-assembly processes.

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MS66

Combining Markov State Models and Optimal Control Theory to Compute Optimal Nonequilibrium Self-Assembly protocols

The self-limited assembly of protein subunits into finite-sized structures underlies essential functions of cells and the pathogens that infect them. Recently, advances in DNA origami and protein design have enabled engineering synthetic subunits that are programmed for self-limited assembly, with precision rivaling that of natural proteins. Yet, achievable sizes of assembled structures fall far short of nature, because assembly is highly susceptible to kinetic traps that reduce target yields. In principle, such traps can be avoided by nonequilibrium assembly protocols, however, rationally computing a nonequilibrium assembly protocol has been computationally intractable for most systems. This talk describes a framework to combine Markov State Model (MSMs) with optimal control theory to construct an optimal time-dependent protocol that maximizes assembly yields at a finite time, and/or assembly rates. We show that MSMs enable simulating self-assembly reactions on timescales that are orders of magnitude longer than those accessible to straightforward simulations. Then, by constructing an MSM for a system as a function of its control parameters, an adjoint-based gradient descent method can be used to efficiently optimize the assembly protocol. The resulting protocols can increase yields and rates by orders of magnitude compared to equilibrium assembly protocols. The approach can be used to optimize a broad class of objective functions in diverse assembly systems.

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MS66

Discovery and Design of Emergent Behavior via Local Structure

Self-organization occurs in Nature at every length scale accessible to human inquiry, and results in a startlingly wide range of organic and inorganic materials with emergent and varied structural and dynamical properties. A primary goal of our lab is to understand and harness the subtle processes inherent in this self-organization, for the ultimate purpose of designing soft materials with tailor-made functionalities. I will focus in particular on our efforts to understand how local structure gives rise to global behavior in soft materials in two contexts. In the first, local structure emerges entirely due to entropic considerations in colloidal systems with very short-range interactions, and influences whether these materials crystallize or instead form glasses. In the second, local structure arises due to sample preparation in amorphous and jammed colloidal systems, and subsequently influences rearrangement dynamics and material memory under oscillatory shear. Given time, I will also discuss recent work characterizing local microstructure in the biological context of the human brain, and potential

applications related to better understanding brain development, aging, and disease. These examples illustrate the significant impact of local structure on complex global behavior in material and biological systems, and point toward exciting future directions related to the design of those behaviors.

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MS67

Homogenized Dynamics of Bistable Spring Arrangements

Bistable non-Hookean springs possess two stable equilibria in their stress-strain relation called a longer and a shorter phase. The state of minimal energy of the mass-spring chain of such springs (Maxwell law) is characterized by a transition from one phase to another at the critical elongation of the chain; the homogenized potential energy is the convex envelope of the nonconvex energy of the springs. Previous work has shown that the dynamic behavior of such chains produces waves and leads to sporadic phase transitions in proximity to the critical point; their intensity depends on the initial kinetic energy of the system. Here, we seek the homogenized dynamic behavior of chains and lattices of bistable springs; that is, we describe the long-time behavior of the entire system as a nonlinear homogenized stress-strain relation between its average deformation and externally applied forces."

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MS67

Homogenization of High-Contrast Dielectric Elastomer Composites

We will discuss the homogenization of high-contrast dielectric elastomer composites. The considered heterogeneous material consisting of an ambient material with inserted particles is described by a weakly coupled system of an electrostatic equation with an elastic equation enriched with electrostriction. It is assumed that particles gradually become rigid as the fine-scale parameter approaches zero. We will see that the effective response of this system entails a homogeneous dielectric elastomer, described by a weakly coupled system of PDEs. The coefficients of the homogenized equations are dependent on various factors, including the composite's geometry, the original microstructure's periodicity, and the coefficients characterizing the initial heterogeneous material. Particularly, these coefficients are significantly influenced by the high-contrast nature of the fine-scale problem's coefficients. Consequently, as anticipated, the high-contrast coefficients of the original yield non-local effects in the homogenized response.

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MS67

Two Dimensional Problem of An Elastic Matrix Containing Multiple Gurtin-Murdoch Material Surfaces Along Straight Segments

In this talk, we present the study of the plane strain problem of an infinite isotropic elastic medium subjected to far-field load and containing multiple Gurtin-Murdoch material surfaces arbitrarily located along straight segments. Each material segment represents a membrane of vanishing thickness characterized by its own elastic stiffness and residual surface tension. We provide a brief overview of the governing equations and boundary conditions for the problem, and present analytical integral representations for elastic fields everywhere in the material system in terms of unknown density functions. The problem is reduced to the system of coupled hypersingular boundary integral equations for the unknown density functions. Further, we provide the closed-form expressions for the stress intensity factors at the tips of the membranes. The numerical algorithm and several results of the numerical simulations will be presented to demonstrate the effectiveness of the proposed approach and study the influence of dimensionless parameters involved in the problem. The possible applications of our work are in modeling the local and overall properties of composite materials that utilize ultra-thin, stiff, and prestressed membranes as reinforcements.

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MS68

Dynamical Stability of the Surface Diffusion Flow in the Flat Torus

We show that, in the N-dimensional flat torus, the surface diffusion flow, with initial datum sufficiently close in $C^{1,1}$ to a strictly stable critical set of the perimeter, exists for all times and converges, as the time goes to infinity, to a suitable translate of such critical set exponentially fast.

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MS68

A Gibbs-Thomson Relation for Inhomogeneous Phase Separation

We consider a variational model for inhomogeneous phase separation. In particular, we investigate the asymptotic behavior of the first variation λ_ε of a heterogeneous variant of the Modica-Mortola energy as the width of the diffuse interface ε goes to 0. Our convergence result corresponds to a Gibbs-Thomson relation for inhomogeneous surface tension. Starting from this information, one can show that (weak) solutions of the AllenCahn equation with spatially dependent double well potential W converge to BV solutions to an inhomogeneous mean curvature flow (under an energy convergence hypothesis). As a next step in our analysis, we aim to establish a weak-strong uniqueness principle for BV solutions to inhomogeneous mean curvature flow.

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MS68

On the Sharp Interface Limit for Models of Tumor Growth

Phase-field models are nowadays often adopted in the description of biological systems involving complex geometric structures. Indeed, they provide a simpler framework, from both the analytical and the numerical viewpoint, while still remaining close to the original problem. Within this approach interfaces are replaced by steep transitions, say of thickness $\varepsilon > 0$, of a phase variable, in the spirit of the Modica-Mortola (or Allen-Cahn) approximation of the perimeter. Hence, geometric flows are rewritten as easier partial differential equations. Understanding the behaviour of the limit $\varepsilon \to 0$, named sharp interface limit, of such smoothed models thus becomes a crucial issue in order to validate the phase-field approach. In this talk we present phase-field models of tumor growth affected by the presence of a nutrient evolving via a reaction-diffusion equation. The resulting system consists in the Cahn-Hilliard equation for the phase-field variable nonlinearly coupled through suitable transmission functions with the Allen-Cahn equation for the nutrient. We then discuss their sharp interface limits, showing that the resulting evolutions follow in a very weak sense (varifold solutions) a Mullins-Sekerka type flow still coupled with the Allen-Cahn equation for the nutrient in the tumor region. The talk is based on a joint work with E. Rocca.

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MS68

The Effect of the Geometry of the Domain in Martensitic Phase Transformations

We study scaling laws for singular perturbation problems associated with a class of two-dimensional martensitic phase transformations for which we deduce a domain dependence of the scaling law in the singular perturbation parameter. Firstly, we prove a general lower bound estimate illustrating that in settings in which the domain and well geometry are incompatible (in the sense of the Hadamard-jump condition) then necessarily at least logarithmic losses occur in the associated scaling laws. Secondly, for specific phase transformation in two-dimensional settings we prove that this gives rise to a dichotomy involving logarithmic losses in the scaling law for generic domains and optimal linear scaling laws for very specific, highly compatible polygonal domains. We discuss both the geometrically linearized and nonlinear settings. This is a joint work with Janusz Ginster, Angkana Rland and Barbara Zwicknagl.

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MS69

Adaptive Randomized Sketching for Dynamic Nonsmooth Optimization

Dynamic optimization problems arise in many applications including optimal flow control, phase field modeling, full waveform inversion, and medical imaging, where they are plagued by significant computational challenges. For example, memory is often a limiting factor on the size of problems one can solve since the evaluation of derivatives requires the entire state trajectory. Additionally, many applications employ nonsmooth regularizers such as the L^1-norm or the total variation as well as auxiliary constraints on the optimization variables. In this talk, we introduce a novel trust-region algorithm for minimizing the sum of a smooth, nonconvex function and a nonsmooth, convex function that addresses these two challenges. Our algorithm employs randomized sketching to store a compressed version of the state trajectory for use in derivative computations. By allowing the trust-region algorithm to adaptively learn the rank of the state sketch, we arrive at a provably convergent method with near optimal memory requirements. We demonstrate the efficacy of our method on various realistic numerical examples.

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MS69
Dna Clusters and Viral Structures

Problems of packaging, organization and condensation of DNA, either in confined domains, capsids, or in free solution, present many mathematical challenges. A key ingredient to our recent studies of organized DNA is the earlier discovery that, under confinement, DNA arranges itself as an hexagonal chromonic liquid crystal. Such an arrangement plays an important role on how efficiently a certain class of virus, bacteriophages, infect bacteria. Viruses, with highly organized DNA in their encapsidated, quiescent (non-infective) state, present evolutionary advantages with respect to the disordered ones in terms of their infection function. This motivates us to study problems on chromonic liquid crystal clustering and bacteriophage infection, withing the framework of the order tensor theory of Landau and de Gennes. Our mechanically based models lead to energy minimization problems and their associated free boundary problems. There is a growing interest in the medical community to study these viruses, in connection with the development of new therapies, such as against antibiotic resistant bacteria. I will present an overview of our results as well as recent studies of the dynamics of the infection process.

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MS69
On a Regularized Model for Brittle Fracture in Strain-Limiting Elastic Solids

Over the last several years, the study of cracks and damages in elastic bodies has been a challenging topic for applied mathematicians and engineers. In the last few decades, a lot of progress has been made in formulating mathematically well-posed models for the crack evolution problem. However, many of these approaches suffer glaring inconsistency due to enduring linear constitutive relations. In this talk, first I will emphasize the need for a new class of constitutive relations to characterize the response of elastic solids. The class of models considered allows a nonlinear relationship between the primitive mechanical variables that have hitherto defined competent explanations about the evolution of cracks. The novel theory leads to a nonlinear system of partial differential equations that presents several challenges. Then, I will explain the analysis and implementation of a staggered iterative scheme for a two-field variational inequality system obtained from a regularized model for the quasi-static crack evolution problem. The proposed method involves a continuous Galerkin-type finite element discretization of two subproblems with each containing stabilization terms to improve the efficiency and robustness of the overall algorithm. Finally, I will present some interesting results from the direct numerical simulations of quasi-static crack evolution in elastic solids.

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MS69
Modeling Fracture in Porous Elastic Solids Whose Material Moduli Depend Upon the Density

In this talk, I will discuss about mathematical and mechanical aspects of porous elastic solids using a novel class of nonlinear implicit constitutive theories. Such a description is necessary to characterize the response of many materials such as rocks, concrete, bones, and high-strength titanium alloys. Starting from the implicit theory, I will derive a sub-class of nonlinear relations wherein the stress and the linearized strain appear linearly, and one cant obtain such constitutive relations starting from the classical theory of linear elasticity. Then, a mixed variational formulation for the three field variables such as displacement, deviatoric stress, and spherical stress will be presented for a static and quasi-static crack problem. The existence theorem for the well-posedness of the regularized problem will be discussed. Finally, I will present some interesting finite element simulation results that can be directly correlated with the response of real-world engineering materials.

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MS70
Biophysics-Inspired Topology

While most DNA has either linear or circular topology, a variety of exotic DNA topologies exist including branched, knotted, and linked molecular architectures. Knotted DNA is investigated as a model system to study polymer entanglement, and trypanosome parasites store their mitochondrial DNA in a topologically linked chainmail network called a kinetoplast. Here, I will discuss a few recent mathematical results inspired by the biophysics of topologically complex DNA. These include investigations into the ropelength of complex knots (the relationship between the crossing number and minimum contour length of a physical knot), as well as the percolation threshold of Borromean networks (inseparable linked-ring systems in which no two rings share a common topological link).

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MS70
Statistical Mechanics of Compressed Filaments

Filaments are everywhere, and across a wide range of scales, from supercoiled DNA and folded tissues to the waves of leaves and the petals of flowers. While much progress has been made over the last two centuries in understanding and predicting the equilibrium shapes of stressed single filament, the emergence of order in a collection of filaments continues to pose interesting theoretical and computational challenges. In this talk, I will discuss our recent joint theoretical and experimental efforts to understand how order emerge in a canonical example of a

collection of beams that are compressed.

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MS70

Understanding Topological Effects in Polymers Using a Gauge-Invariant Field Theory and Molecular Dynamics Simulations

In this talk, I will present our on-going work related to understanding topological effects in melts of linear chains, rings and trefoil knotted polymers. The talk will introduce a gauge-invariant field theory applicable to polymer melts and concentrated solutions. Use of the gauge invariance in the field theory of polymers to model orientational order in confinements and knots will be discussed. Near the end, use of computational tools for quantifying topological effects in molecular dynamics will be presented.

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MS70

Topological Dynamics of Knotted and Tangled Matter

Knots and tangles play a fundamental role in the dynamics of biological and physical systems, from DNA and root networks to surgical sutures and shoelaces. Despite having been studied for centuries, the subtle interplay between topology and mechanics in tangled elastic filaments remains poorly understood. Here we investigate the dynamical rules governing the behavior of knotted and tangled matter. We first study the human-designed knots used to tie ropes together. By developing an analogy with long-range ferromagnetic spin systems, we identify simple topological counting rules to predict the relative mechanical stability of commonly used climbing and sailing knots. Secondly, we examine the complex tangling dynamics exhibited by California blackworms, which form living tangled structures in minutes but can rapidly untangle in milliseconds. Using ultrasound imaging datasets, we construct a minimal model that explains how the kinematics of individual active filaments determines their emergent collective topological dynamics. By identifying generic dynamical principles of topological transformations, our results can provide guidance for designing classes of self-adaptive topological metamaterials.

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MS71

Consensus-Based Construction of High-Dimensional Free Energy Surface

We propose a consensus sampling-based approach to construct free energy surfaces (FESs) by reformulating the construction as a minimax problem which simultaneously optimizes the function representation and the training set. In particular, the maximization step establishes a stochastic interacting particle system to achieve the adaptive sampling of the max-residue regime by modulating the exploitation of the Laplace approximation of the current loss function and the exploration of the uncharted phase space; the minimization step updates the FES approximation with the new training set. By iteratively solving the minimax problem, the present method essentially achieves an adversarial learning of the FESs with unified tasks for both phase space exploration and posterior error-enhanced sampling. We demonstrate the method by constructing the FESs of several molecular systems.

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MS71

Learnable Equivariant Representations of Stochastic Heat Bath Models via the Atomic Cluster Expansion (ACE)

Rigorously derived dynamics of coarse-grained particle systems via the Mori-Zwanzig projection formalism take the form of a (generalized) Langevin equation with, in general, configuration-dependent friction and diffusion tensors. In this talk, I will introduce a class of equivariant representations of tensor-valued functions based on the Atomic Cluster Expansion (ACE) framework that allows for efficient learning of such configuration-dependent friction and diffusion tensors from data. Besides satisfying the correct equivariance properties with respect to the Euclidean group E(3), the resulting heat bath models satisfy a fluctuation-dissipation relation. Moreover, such models can be extended to include additional symmetries, such as momentum conservation, to preserve the hydrodynamic properties of the particle system.

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MS71

Data-Driven Learning for Mori-Zwanzig Formalism: Theory and Potential Applications

More than half a century ago, Mori and Zwanzig (MZ) developed a mathematically rigorous formalism for constructing reduced-order models for dynamical systems using functional projection operators. Several recent studies have established that with Mori's linear projection operator, it is possible to adopt a data-driven approach to learn the MZ operators using the time series of the resolved dynamics. In this talk, I will present our latest proposition of using regression analysis to define the projection operators, and a data-driven method for learning the associated MZ operators using time-series data. The newly proposed method can be considered as a generalization of our recently proposed method (Lin et al. 2021, SIADS) because it is not restricted to linear regressions. As we gradationally increased the complexity of the regression models, we observed a consistent improvement of the learned reduced-order models on a few test examples. We still observed considerable improvements by including the MZ memory effect in these nonlinear projections, justifying the necessity of accounting for the past histories of under-resolved systems. We believe that the proposed method for learning MZ operators is promising because it is applicable to most data-driven methods (e.g., approximate Koopman and SINDy) for learning dynamical systems.

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MS72

Cross-Scale Covariance for Material Property Predictions

A simulation can stand its ground against experiment if and when its accuracy and uncertainty are known and quantified. Uncertainty of an atomistic simulation based on an interatomic potential (IP) can be large and, worse still, unknown. To improve accuracy and to quantify uncertainty of large-scale atomistic simulations (1B atoms) here we propose to regress their predictions on predictions obtained with the same IPs on much smaller scales where quantum-accurate calculations are feasible. To establish and quantify covariance of a large-scale quantity of interest (metal strength) to small-scale properties of the same model material, we perform 178 large-scale Molecular Dynamics simulations of crystal plasticity using a set of 178 interatomic potentials available in the OpenKIM repository for face-centered-cubic (FCC) metals. Simultaneously, we extract a set of small-scale (indicator) properties precomputed for the same 178 potentials in OpenKIM. In a manner similar to statistical studies in public health, we analyze correlations of strength with small-scale indicators, build a regression function and quantify uncertainty of cross-scale strength on indicators regression over the same statistical pool of interatomic potentials. Indicators found to be most covariant with strength are then recomputed using expensive quantum-accurate calculations and used to predict strength for seven FCC metals within uncertainty bounds established in our statistical study.

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MS72

Indicator Configurations: An Information-Matching Method of Data Reduction for Training Interatomic Potential

Interatomic potentials (IPs) are often trained by fitting IP parameters to energies, atomic forces, or similar quantities for many atomic configurations. These training quantities are typically obtained from DFT calculations, and collecting data from enough unique configurations to constrain all IP parameters is computationally expensive. A critical problem is identifying when the training data is sufficient to constrain the predictions of the IP for material properties of interest. We present an information-matching method for selecting a minimal set of configurations, i.e., indicator configurations, that constrain the predictions of an IP for target material properties. Central to our analysis is the Fisher Information Matrix (FIM), which quantifies the information that the data carries about the IP parameters. We calculate the FIM for the target quantities of interest and for, e.g., the energy and forces of each candidate configuration. Then, we down-select from these candidate configurations so that their combined FIM matches that of the quantities of interest, i.e., the indicator configurations are those whose information content is the same as the target predictions. We demonstrate this method on the Stillinger-Weber potential for several systems and target materials properties. In addition to improving the efficiency of the data-generation process, the indicator configurations reveal the physics and mechanisms relevant to the materials properties of interest.

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MS72

Reliable Molecular Simulations with Uncertainty-Quantified Machine Learning Potentials

Machine learning (ML) interatomic potentials offer new opportunities to accurately simulate larger material systems for longer periods of time. In the past decade, a large number of ML potential models have been proposed, but the assessment of their reliability and the quality of the simulation results largely lag behind. It is imperative to quantify the uncertainty in such ML potentials since their functional forms are overly flexible and do not explicitly have the bonding information between atoms baked in. In this talk, I will discuss a class of dropout uncertainty neural network potentials that provide rigorous uncertainty estimates that can be understood from both Bayesian and frequentist statistics perspectives. I will demonstrate the strengths and potential limitations of this approach using examples involving the fitting of carbon allotropes, as well as how to propagate the model uncertainty in molecular simulations. Additionally, I will discuss recent new de-

velopments in the field, including model uncertainty and calibration.

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MS73

Robust Asymmetric Interface Transport in Topological Insulators

The surprising robustness to perturbation of the asymmetric transport observed along interfaces separating distinct insulating bulks has a topological origin. This talk reviews recent classifications of partial differential operators modeling such systems. A classification by means of domain walls provides a topological invariant whose calculation as an explicit integral is straightforward. A general bulk-interface correspondence then proves that the invariant also describes the quantized aforementioned asymmetric transport. The theory is illustrated on several examples of applications and in particular gated twisted bilayer graphene models.

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MS73

Modeling of electronic dynamics in twisted bilayer graphene

We consider the problem of numerically computing the quantum dynamics of an electron in twisted bilayer graphene. The challenge is that atomic-scale models of the dynamics are aperiodic for generic twist angles because of the incommensurability of the layers. The Bistritzer-MacDonald PDE model, which is periodic with respect to the bilayer's moiré pattern, has recently been shown to rigorously describe these dynamics in a parameter regime. In this work, we first prove that the dynamics of the tight-binding model of incommensurate twisted bilayer graphene can be approximated by computations on finite domains. The main ingredient of this proof is a speed of propagation estimate proved using Combes-Thomas estimates. We then provide extensive numerical computations which clarify the range of validity of the Bistritzer-MacDonald model.

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MS73

Continuum Limits of Stacked 2d Materials

Twisted bilayer graphene and other stacked 2d materials are naturally analyzed at the moiré scale: the scale of oscillation of the interlayer disregistry. This scale is generally much longer than the constituent materials' lattice constants, making this a considerable modeling simplification. I will discuss mathematical results justifying this simplification when modeling the stackings' electronic and mechanical properties.

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MS74

Band Theory and Boundary Modes of High-dimensional Representations of Infinite Hyperbolic Lattices

Periodic lattices in hyperbolic space are characterized by symmetries beyond Euclidean crystallographic groups, offering a new platform for classical and quantum waves, demonstrating great potentials for a new class of topological metamaterials. One important feature of hyperbolic lattices is that their translation group is nonabelian, permitting high-dimensional irreducible representations (irreps), in contrast to abelian translation groups in Euclidean lattices. Here we introduce a general framework to construct wave eigenstates of high-dimensional irreps of infinite hyperbolic lattices, thereby generalizing Bloch's theorem, and discuss its implications on unusual mode-counting and degeneracy, as well as bulk-edge correspondence in hyperbolic lattices. We apply this method to a mechanical hyperbolic lattice, and characterize its band structure and zero modes of high-dimensional irreps.

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MS74

Robust Geometry Processing for Physical Simulation in Metamaterial Design

The numerical solution of partial differential equations (PDE) is ubiquitously used for physical simulation in scientific computing and engineering. Ideally, a PDE solver should be opaque: the user provides as input the domain boundary, boundary conditions, and the governing equations, and the code returns an evaluator that can compute the value of the solution at any point of the input domain. This is surprisingly far from being the case for all existing open-source or commercial software, despite the research efforts in this direction and the large academic and industrial interest. To a large extent, this is due to lack of robustness and generality in the geometry processing algorithms used to convert raw geometrical data into a format suitable for a PDE solver. I will discuss the limitations of the current state of the art, and present a proposal for an integrated pipeline, considering data acquisition, meshing, basis design, and numerical optimization as a single challenge, where tradeoffs can be made between different phases to increase automation and efficiency. Finally, I will present a differentiable elastodynamic simulator based on this robust approach and discuss its use for designing metamaterial families using shape optimization with non-linear material models and accounting for the contact forces appearing in large deformation regimes.

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MS74

Tessellated Granular Metamaterials

Jammed packings of granular materials display complex mechanical response that is qualitatively different from continuum solids. The elastic behavior of jammed packings depend on, among other factors, the interparticle interactions present in the packing. By modifying how particles interact with each other, we can tune the properties of a packing. For example, the ensemble-averaged shear modulus ¡G¿ increases as a power law in pressure for static packings of soft spherical particles that can rearrange during compression. In this talk, I will present 'tessellated granular metamaterials where both G as well as the ratio of shear to bulk modulus (G/B) decrease with increasing pressure, even in the large system limit. Tessellated granular metamaterials are made from flexible tessellations that are connected to each other, each containing a small number of solid particles. For under-constrained tessellations, the dominant contributions to G and B are the particleparticle and particlecell interactions. Tessellating a system prevents particles in once cell of the tessellation from interacting with particles in other cells, resulting in unexpected behavior, such as G/B¡¡1 at large pressures. Our work demonstrates that tessellated granular metamaterials provide a platform for the design of soft materials with specified mechanical properties.

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MS75

Localized Curvature and Generalized Volterra Defects in Thin Sheets

Defects in elastic solids are singular sources of elastic fields. Within a geometric description of elasticity, defects are described as local deviations of the reference metric, describing rest lengths in the solid, from being euclidean. For example, disclinations and dislocations are metric defects that induce non trivial residual stresses in elastic bodies. Mathematically, metric defects are quantified as geometric incompatibility that violates Gauss equation. Thin elastic sheets are characterized not only by a reference metric, but also by a reference curvature. As such, metric defects do not constitute a complete description of localized sources of elastic fields in thin sheets. In this talk I will show that another class of defects, complementing metric defects and termed curvature defects, corresponds to a reference curvature that violates Gauss-Peterson-Mainardi-Codazzi equations at a discrete point. We show that curvature defects appear naturally as neutral layered metric defects in a bilayer structure, and are constructed via generalized Volterra constructions. We present a geometric theory of such singularities discussing the incompatibility field whose localization characterizes the defect. We present a complete classification of curvature defects based on the associated charge and their classification into topological and non topological defects. We also discuss some results about the mechanics and interaction of such defects in thin sheets.

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MS75

Variational Models for Pattern Formation in Biomembranes

Biological membranes are thin structures that are composed of various components. The different components often form microdomains, called lipid rafts, that are arranged in complex patterns. To explain this pattern formation, variational models based on Cahn-Hilliard type energies have been introduced that couple the local composition of the membrane to its local curvature, which renders the resulting functionals nonlocal. The main focus of this talk lies on the derivation of the Γ-limit in a certain parameter regime where the limiting functional turns out to be of perimeter-type. As a main novelty, we will present a technique to include Neumann-boundary conditions in the construction of a recovery sequence. Additionally, in the remaining parameter regimes scaling behavior of the infimal energy will be discussed.

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MS75

Fracture and Curvature in Thin Structures

We report on some recent results on effective theories for thin and ultrathin structures which are subject to both elastic deformations and fracture. In particular, we will consider the formation of folds and cracks in two scenarios: 1. atomistically thin rods and 2. membranes and and plates with soft inclusions.

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MS76

Finite Element Approximation of Thin Liquid Crystal Polymer Networks

Liquid crystal polymeric networks (LCNs) are materials where a nematic 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 discretize a stretching energy of LCNs with conforming piecewise linear finite elements and add a higher order bending energy regularization to address the lack of convexity. We prove that minimizers of the discrete energy converge to zero energy states of the membrane energy in the spirit of Gamma convergence. We solve the discrete minimization problem via an energy stable gradient flow scheme, and this talk emphasizes the algorithmic aspects of the scheme, including an analysis of an inner Newton solver for each gradient flow step. We finally present computations showing the geometric effects that arise from liquid crystal defects as well as computations of nonisometric origami. The nonisometric origami simulations also go beyond theory by including examples with incompatible stretching. This work is joint with R.H. Nochetto and S. Yang.

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MS76

Relaxation and Numerics for Single Crystal Strain Gradient Plasticity

We will consider non-convex models for single-crystal elasto-plasticity, where the non-convexity arises through so-called cross-hardening, i.e., deformation in one slip system is prohibiting deformation in a different slip system at the same position. Such models are typically ill-posed and require relaxation. A different avenue to pursue is the addition of a strain-gradient term which regularizes the model by introducing a length scale on which the plastic strain may oscillate. We will see that physically reasonable strain gradient penalizations, which only assign an energy to geometrically necessary dislocations - penalizing only the curl of the plastic strain - still require some relaxation. Further issues arise regarding numerical implementation of the strict conditions of infinite cross-hardening. We will thus regularize the side-condition by introducing a large cross-hardening penalty into the plastic energy. The regularized model is then amenable to implementation with finite-element methods, and, with the aid of div-curl arguments, one can show that it Gamma-converges to the single-plane model for large penalization. Finally we show some microstructures arising in the numerical implementation of this model.

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MS76

Simulation of the Stretching and Bending Deformation of Thin Structures with Folding

We study the elastic behavior of prestrained thin plates which can undergo large deformations and achieve nontrivial equilibrium shapes even without external forces. The deformation is driven by stretching/shearing and bending, and the plate is allowed to fold across a prescribed crease. The mathematical problem consists in minimizing an energy of the form $E(\mathbf{y}) = E_S(\mathbf{y}) + \theta^2 E_B(\mathbf{y})$, where $\mathbf{y}$ is the deformation of the midplane, θ is the thickness of the plate, E_S is the (nonconvex) stretching energy, and E_B is the bending energy. We introduce a discrete energy based on a continuous finite element space and a discrete Hessian operator involving the jump of the gradient of the deformation across the interelement sides. We establish the Γ-convergence of the discrete energy, present an energy-decreasing gradient flow for finding critical points of the discrete energy, and provide numerical simulations illustrating the capabilities of the model.

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MS77

Homogenization for Problems Concerning Composites with Evolving Microstructures

Phase transition processes (e.g, between different phases in steel) are examples of problems where the geometry is allowed to evolve and where microscopic effects (growing nucleation cells) influence the macroscopic properties of the system. As a consequence of the changes in geometry, the resulting mathematical problems are generally highly nonlinear and complex in and of itself; but the scale separation adds further difficulties in particular for proving necessary regularity estimates. With the Hanzawa transformation, we present a popular technique for moving boundary problems and discuss how it can be applied in a multiscale setting. In the simplified case of uniform cell evolutions, we use this transformation to show well-posedness of the moving boundary problem and to conduct a limit analysis with respect to the scale parameter. Finally, we mention some of the difficulties in extending these results to the case of more general cell evolutions.

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MS77

Scattering by a Random Thin Coating of Nanoparticles

We study the time-harmonic scattering by a heterogeneous object covered with a thin layer of randomly distributed nanoparticles. The size of the particles, their distance between each other and the layer thickness are all of the same order but small compared to the wavelength of the incident wave. Solving numerically Maxwells equations in this context is very costly. To circumvent this, we propose via a multi-scale asymptotic expansion of the solution, an effective model where the layer of particles and the object are replaced by an equivalent boundary condition. The coefficients in this equivalent boundary condition depend on the solutions to corrector problems of Laplace-type defined on unbounded random domains. Under the assumption that the particles are distributed given a stationary and ergodic random point process, we study the behavior at infinity of those solutions and the well-posedness of the associated problems with both homogeneous Dirichlet and Neumann boundary conditions on the particles. We then establish quantitative error estimates for the effective model and present numerical simulations that illustrate our theoretical results.

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MS77

Variational Homogenization Estimates for Viscoplastic Fluid Flow through Porous Media

Modeling the flow of complex fluids through porous media is of crucial importance in many industrial and naturally occurring processes. For this reason, there have been numerous attempts to generalize Darcy's law, relating the flow velocity to the pressure drop by the permeability of the porous medium, for various types of non-Newtonian fluids. This work is concerned with the flow of yield-stress (viscoplastic) fluids through rigid porous media under Stokes flow conditions. The porosity distribution may be periodic, or random and statistically uniform, but not necessarily isotropic. Variational estimates are obtained for the nonlinear permeability or mobility of the viscoplastic fluid under macroscopically uniform flow conditions through a generally anisotropic porous medium, with given microstructure, in terms of the porosity and the permeability tensor for the flow of a comparison Newtonian fluid through a porous medium with the same microstructure.

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MS77

Quantitative Analysis of Passive Intermodulation and Surface Roughness

I will discuss a quantitative analysis of the phenomenon of passive intermodulation (PIM) when the underlying surface conductor is rough. PIM occurs when multiple signals are active in a passive device that exhibits a nonlinear response. It is known that certain nonlinearities (e.g. the electro-thermal effect) which are fundamental to electromagnetic wave interaction with matter cannot be ignored. In this talk, I will discuss existence and uniqueness of solutions to a simple model for PIM when the domain is Lipschitz. By introducing a characteristic angle of the surface, we track the dependence of the fields on this parameter through various estimates. I will also discuss the regularity of the fields, which is lower than one might expect due to the presence of the rough surface. This is joint work with E. Cherkaev and N. Wellander.

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MS78

Hyperoptimization Insight for Computational Morphogenesis

The nonlinear relationship between the form and function of physical structures in our built environment raises challenges for design. Modern design methods, such as topology optimization, provide structural solutions but obscure the relationship between the form of the solution and the formulation of the underlying design problem. Here, we show how to extend classical molecular dynamics methods to provide novel forms of insight into the origin and organization of design features in morphogenesis problems. Our computational approach to morphogenesis implements a version of the digital alchemy methods that were introduced to solve inverse-design problems for self-assembled materials. The framework we present here for problems in morphogenesis surmounts known design problems including grayscale ambiguity, manufacturing inaccuracy, and artificially over-specified criteria. Our results give examples where molecular methodologies can be used to derive results for macroscopic systems.

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MS78

The Nanocaterpillar's Random Walk: or How to Move Precisely with Random Sticky Feet?

Particles with sticky feet - or nanoscale caterpillars - in biological or artificial systems, beat the paradigm of standard diffusion to achieve complex functions. Some cells (like leucocytes) use ligand-receptor contacts (sticky feet) to crawl and roll along vessels. Sticky DNA (another type of sticky feet) is coated on colloids to design programmable interactions and self-assembly. Predicting the dynamics of such sticky motion is challenging since sticky events (attaching/detaching) often occur on very short time scales compared to the overall motion of the particle. Even understanding the equilibrium statistics of these systems (how many feet are attached in average) is largely uncharted. Yet, controlling the dynamics of such particles is critical

to achieve these advanced functions – for example facilitating motility is critical for long-range alignment of DNA coated-colloids crystals. Here we present advanced theory and experimental results on a model system. We rationalize what parameters control average feet attachment and how they can be compared to other existing systems. We investigate furthermore how various motion modes (rolling, sliding or skipping) may be favored over one another.

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MS78

Electric Transport Through Networks with Tunable Disorder

Open lattice materials can be designed to feature tunable electrical and heat transport properties, as well as superior mechanical stiffness, with minimal material and weight. Yet mathematical theory is lacking especially for disordered network structure. I will discuss some recent results from both experiments and simulations of electric transport, measured as resistivity, through 2D networks. The disorder of the network is slowly removed through iterations of Lloyds algorithm that moves nodes to the center of mass of their Voronoi cells. Connections are drawn to the graph Laplacian, other network statistics, and measures of hyperuniformity (long-range correlations in node location).

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MS78

Jointly Optimizing Design and Control of Soft Robots through Reinforcement Learning and Modular Model Order Reduction

This work provides a complete framework for the simulation, co-optimization, and sim-to-real transfer of the design and control of soft legged robots. Our approach leverages a reinforcement learning-based co-optimization framework, showcasing its capability to identify soft crawling robots that surpass expert baselines through zero-shot sim-to-real transfer. Further, we explore the framework's generalization to novel terrains, evaluating the effectiveness of domain randomization as a strategy to enhance sim-to-real transfer. In this work, we show that adding design optimization into the soft legged robot control problem improves performance and investigate sim-to-real transfer of the optimized robots for trained in simulation environments of varying accuracy. The results show novel designs and controllers that outperform expert-developed baselines and zero-shot sim-to-real transfer of many of these legged robots to new terrains. The presented framework has the potential to accelerate current robot development processes by creating virtual development tools that are fast and accessible to non-experts.

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MS79

Radiation Conditions for Null-Solutions of the Helmholtz Operator

In this talk I aim to identify a very broad spectrum of radiation conditions for null-solutions of the vector Helmholtz operator. This contains, as particular cases, the Sommerfeld, Silver-Mller, and McIntosh-Mitrea radiation conditions corresponding to scattering by acoustic waves, electromagnetic waves, and null-solutions of perturbed Dirac operators, respectively. This is joint work with Dorina Mitrea and Marius Mitrea from Baylor University.

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MS79

Heterogeneous Effects in Nonlocal Models

The wide applicability of nonlocal models in different areas of science (continuum mechanics, biology, image processing, neural networks) has catapulted them to the center of many analytical investigations. In this talk I will present some recent results on nonlocal systems that exhibit heterogeneous behavior via domain operators or boundary conditions. Of particular interest is the study of the limiting behavior of the nonlocal system as the horizon of interaction shrinks to zero. For the emergent system we identify the classical (differential) counterparts and their physical interpretation.

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MS79

A Problem for a Material Surface Attached to the Boundary of An Elastic Semi-Plane

A problem for a nano-sized material surface attached to the boundary of an elastic isotropic semi-plane is considered. A normal external traction is applied to a boundary of the material surface. The material surface is modeled using the Steigmann-Ogden form of surface energy. The problem is solved by using integral representations of stresses and displacements through certain unknown functions. With the help of these functions, the problem can be reduced to either a system of two singular integral equations or a single singular integral equation. Two types of material surface tip boundary conditions are considered: free tip conditions and conditions with compensated surface prestress term. The numerical solution of the system of singular integral equations is obtained by expanding each unknown function into a series based on Chebyshev polynomials. Then the approximations of the unknown functions can be obtained from a system of linear algebraic equations. Accuracy of the numerical procedure is studied. Various numerical examples for different values of the surface energy parameters are considered. It is shown that both the surface parameters and the type of tip conditions have significant influence on the behavior of the material system.

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MS80

A Scaling Law for a Model of Epitaxial Growth with Dislocations

Epitaxy is a special form of crystal growth and of great importance in modern technology. We consider a crystalline film that is deposited on a (rigid) substrate. The misfit between the crystal structure of the film and the substrate can lead to dislocations and can have an influence on the morphology of the film. Dislocations are topological defects of the crystallographic lattice. In this talk we will study a variational model from the literature which is based on linearized elasticity and takes into account the surface energy of the film's free surface as well as the dislocation nucleation energy. In particular we will discuss a new scaling law for the infimum of the energy. The results indicate that in certain parameter regimes, the formation of dislocations is expected.

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MS80

Variational Models with Eulerian-Lagrangian Formulations Allowing for Material Failure

Variational models featuring mixed Eulerian-Lagrangian formulations arise naturally in many multiphysics problems. The underlying energy functional depends on the deformation of the body, classically set on the reference configuration, and an Eulerian map defined on the deformed configuration in the actual space. The latter has often to comply with nonlinear constraints determined by the context. Concrete examples concern the modeling of liquid crystals and magnetic elastomers, where the Eulerian map represents the nematic director and the magnetization field, respectively. In this talk, we present an existence theory for minimizers of abstract mixed Eulerian-Lagrangian energies. Building upon previous works by D. Henao and C. Mora-Corral, our results move beyond the purely elastic case and investigate models that allow for material failure. First, we focus on soft materials possibly exhibiting cavitation, that is, the abrupt formation of voids inside the material in response to mechanical stresses. Subsequently, we investigate brittle materials that might experience fracture. Deformations will thus be modeled as Sobolev maps and special maps with bounded variation, respectively. The regularity of Eulerian maps will be specified in each of these settings according to the geometric and topological properties of the deformed configuration. Effectiveness and limitations of the theory will be illustrated by means of explicit examples covering relevant applications.

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MS80

Discrete model for partial dislocations

I will present a discrete two dimensional toy model for crystal defects based on nearest neighbours and next to nearest neighbours interaction, via a period potentials. In the asymptotic limit as the lattice spacing tends to zero, in terms of Gamma convergence, the model accounts for the formation and interaction of partial dislocations and stacking faults.

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MS80

Derivation of Line Tension Models for Dislocations from 3d Nonlinear Energies

In this talk we will introduce a 3D variational model for dislocations which is obtained through a regularisation procedure. Afterwards we show that the asymptotics, via Gamma convergence, is independent of the specific choice of the energy and of the regularisation. Moreover we show that the limit is characterised by the sum of an elastic energy and a line tension term. This is based on joint works with Sergio Conti, Adriana Garroni Riccardo Scala.

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MS81

MINIMIZERS FOR THE DE GENNES-CAHN-HILLIARD ENERGY UNDER STRONG AN-

CHORING CONDITIONS

In this talk, I will discuss the study that employs the Nehari manifold and the eigenvalue problem for the negative Laplacian with Dirichlet boundary condition to analyze minimizers for the de Gennes Cahn-Hillard energy with a quartic double-well potential and Dirichlet boundary condition on a bounded domain. The analysis uncovers a bifurcation phenomenon dependent on the boundary value and a bifurcation parameter that characterizes the thickness of the transition layer segregating the binary mixtures two phases.Specifically, when the boundary value aligns precisely with the average of the pure phases and the bifurcation parameter surpasses or equals a critical threshold, a unique minimizer emerges, representing the homogeneous state. Conversely, if the bifurcation parameter falls below this critical value, two symmetric minimizers arise. Symmetry breaking occurs when the boundary value deviates from the average of the pure phases, resulting in a unique minimizer.Furthermore, the study derives bounds for these minimizers, incorporating boundary conditions and features of the de Gennes-Cahn-Hilliard energy. This research is conducted jointly with Shibin Dai.

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MS81

C0 IP Methods for Phase Field Crystal Equations

A relatively new class of mathematical models known as phase field crystal models has emerged as a way to simulate physical processes where atomic- and microscales are tightly coupled. In this talk, we present numerical schemes for two such models which rely on a C0 interior penalty finite element method spatial discretization. We show that the numerical methods are unconditionally energy stable and unconditionally convergent and support our conclusions with a few numerical experiments.

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MS81

Numerical phase-field models on manifolds and applications in bioengineering

We present a scalar auxiliary variable (SAV) method to solve the Cahn–Hilliard equation with degenerate mobility posed on a smooth closed surface Γ. The SAV formulation is combined with adaptive time stepping and a geometrically unfitted trace finite element method (TraceFEM), which embeds Γ in $\mathbb{R}^3$. The model was applied to study the fusogenicity of positively charged phased-separated lipid vesicles. Experimental findings are supported by numerical simulations using a mathematical model for phase-separated charged liposomes. Findings of this study may be used for design and development of highly fusogenic liposomes with minimal level of toxicity.

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MS81

A Non-Isothermal Phase Field Crystal Model with Lattice Expansion

The phase field crystal modeling framework describes materials at atomic space scales on diffusive time scales. It has been used to study grain growth, fracture, crystallization, and other phenomena. In this talk I will describe some recent work with collaborators developing a thermodynamically consistent phase field crystal model that includes heat transport and lattice expansion and contraction. We use the theory of non-equilibrium thermodynamics, a formalism developed by Alt and Pawlow, and Onsagers principle to give consistent laws of entropy production, and mass and energy conservation. I will show some preliminary numerical simulation results involving heat transport during solidification, and I will discuss some ideas on developing entropy and energy stable numerical methods.

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MS82

Interacting Models for Twisted Bilayer Graphene: Towards a Quantum Chemistry Approach

We present a numerical study of an interacting Bistritzer-MacDonald (IBM) model of Twisted Bilayer Graphene (TBG) using a suite of methods in quantum chemistry, including Hartree-Fock, coupled cluster singles, doubles (CCSD), and perturbative triples (CCSD(T)), as well as a quantum chemistry formulation of the density matrix renormalization group method (DMRG). At integer filling, all numerical methods agree in terms of energy and $C_{2z}T$ symmetry breaking. Additionally, as part of our benchmarking, we explore the impact of different schemes for removing double-counting in the IBM model. Our results at integer filling suggest that cross-validation of different IBM models may be needed for future studies of the TBG system. After benchmarking our approach at integer filling, we perform a systematic study of the IBM model near integer filling. In this regime, we find that the ground state can be in a metallic and $C_{2z}T$ symmetry breaking phase. The ground state appears to have low entropy, and therefore can be relatively well approximated by a single Slater determinant. Furthermore, we observe many low entropy states with energies very close to the ground state energy in the near integer filling regime.

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MS82

Data Driven Approach for Local Density of State on the Moir Scale

Classical machine learning emerges as a potent ally in the realm of quantum material science and electronic structure exploration. The formidable challenge posed by the exponential resource demands for larger system sizes prompts

the question: what role can classical machine learning truly play in the physical sciences? While it might seem implausible, numerous captivating electronic properties do not necessitate computations at the scale of quantum many-body systems. Moreover, these observables often exhibit super-low dimensions, liberating them from the burdensome shackles of exponential scaling. In this context, we aim to illuminate how classical computers can unravel the intricacies of intriguing electronic properties, exemplified by the Local Density of States, and show how to search for flat band with the help of operator learning.

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MS82

Algebraic Aspects of Spectra for Periodic and Quasi-Periodic Media

Certain aspects of the spectrum of multi-layer electronic media are informed by the algebraic structure of the Fermi surface. In Bernal-stacked bi-layer graphene, these include creation of non-symmetry-induced bound defect states, localization of defects, and effects of magnetic potentials. I will discuss progress and interesting questions related to the role of commutative algebra in electronic media.

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MS82

The Role of Electron-Phonon Coupling in the Superconductivity of Twisted Bilayer Graphene

The origin of superconductivity in twisted bilayer graphene (tBLG) has been a topic of heated debate since its discovery. In magic-angle tBLG, the electronic bands significantly flatten, leading to enhanced electronic correlation, a potential precursor to superconductivity. However, the role of electron-phonon coupling has often been overlooked. To accurately describe electron-phonon coupling in moir systems, there are nearly insurmountable challenges related to the incommensurability at general twist angles and the large number of degrees of freedom, including both electron and phonon momenta. In this work, we overcome these computational challenges by employing a first-principles-based multi-scale continuum model to accurately and efficiently describe electron-phonon coupling due to moir phonons in twisted bilayer graphene. We estimate the twist-angle dependence of the superconducting critical temperature without relying on an adiabatic approximation.

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MS83

Ribbon Gridshells Soft Elasticity and Inverse Design

In this talk, we discuss the properties of a two-dimensional metamaterial composed of thin inextensible ribbons connected together to form a gridshell. We study both in-plane and out-of-plane deformations of such ribbon gridshells and point out their exotic geometric and mechanical properties. In particular, ribbon gridshells demonstrate anomalous softness with respect to some modes of deformation. At the same time, they are highly rigid with respect to other modes and conserve global geometric invariants. Shaping these objects constitutes a hyperbolic PDE system, and therefore properly imposing initial conditions on a one-dimensional subset rigidifies them and fully determines their shape. We further show that exploiting structural degrees of freedom in ribbon gridshells allows tuning their soft modes in various ways. In particular, we can encode shapes into them – for example to make a flat object that can be accurately deformed into an arbitrary target surface shape. We demonstrate our results with experiments and suggest useful design and technology applications to our findings.

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MS83

Existence Theorems and Regularity Properties for Highly Deformable Elastic Surfaces

We consider a class of single-director Cosserat shell models accounting for both curvature and finite mid-plane strains. We assume a convexity condition for the stored-energy function that reduces to a physically correct membrane model in the absence of bending. Among other things, we argue that this model is suitable for predicting wrinkling observed in thin sheets. With appropriate growth conditions, we establish the existence of orientation-preserving energy minimizers for this model. We then focus on the pure membrane version of this model which is not even rank-one convex for deformations into $\mathbb{R}^3$. Nevertheless, we prove that it admits energy-minimizing configurations when constrained to lie on some prescribed oriented surface. With a few additional assumptions, we show that these minimizers are globally invertible and satisfy the weak Eulerian form of the equilibrium equations. This is joint work with Tim Healey.

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MS83

Sharp Ridges in a Variational Problem for Convex

Functions

We consider energy minimization for a thin elastic sheet with two disclinations in the von Kármán approximation. Under the simplifying assumption that the out-of-plane deformation is a convex function, we show that any map with sufficiently low energy will display a sharp ridge stretching from one disclination to the other. On the level of the energy, we prove upper and lower bounds that match up to a logarithmic factor in the thickness of the sheet.

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MS84

Simulation As a Crucial Tool in the Understanding of Grain Growth in Polycrystals

Most technologically useful materials are polycrystalline composed of small monocrystalline grains that are separated by grain boundaries of crystallites with different lattice orientations. One of the central problems in materials science is to design technologies capable of producing an arrangement of grains that delivers a desired set of material properties. A method by which the grain structure can be engineered in polycrystalline materials is through grain growth (coarsening) of a starting structure. Grain growth in polycrystals is a very complex multiscale process. It can be modeled as the anisotropic evolution of a large cellular network via a set of deterministic local evolution laws for the growth of an individual grain combined with stochastic models for the interaction between them. In this talk, we will discuss new perspectives on computational modeling and simulation in the analysis and experiments of the evolution of the grain boundary network in polycrystalline materials.

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MS84

A Discontinuous Galerkin Method for Optimal Control of the Obstacle Problem

In this talk, we discuss the a priori error estimates for an optimal control problem constrained by an elliptic obstacle problem where the finite element discretization is carried out using the symmetric interior penalty discontinuous Galerkin (SIPG) method. The main proofs are based on the improved L^2-error estimates for the obstacle problem, the discrete maximum principle, and a well-known quadratic growth property. All the existing results require restrictive assumptions on mesh, which is not assumed here. A quasi-optimal rate of convergence is derived for both state and control variables in a realistic, locally distributed optimal control setting.

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MS84

Structural Properties of Multiphase Multicomponent Porous Flow Models

Many problems of contemporary interest involve thermal effects and phase changes. Three dimensional printing of metallic components, and the release of green houses gasses beneath thawing permafrost are prototypical examples. This talk will review how classical thermodynamics enters into the structural properties of of the partial differential equations modeling some thermo–mechanical problems, and the challenges that arise in the numerical simulation of their solutions.

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MS85

Optimal Multimaterial Composites

The paper discusses the exact bounds for the effective properties of multimaterial composites. The problem is to find sets of supporting fields of the quasiconvex envelope of a multiwell Lagrangian; these are fields in optimal structures. Because all structures are compared, the components of the optimal gradient fields in the wells are either constant or do not affect the bound; they depend on several parameters: properties and fractions of mixed materials and applied excitation. We show that the optimal supporting fields vary in restricted domains. The optimal bounds are solutions to nonlinear programming problems. The found inequalities modify the Translation method and lead to exact bounds in several examples. A unified approach to deriving a set of constraints in the supporting fields is yet to be developed.

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MS85

Homogenization of a Space-time Quasiperiodic Parabolic Problem

We investigate the homogenization of a linear parabolic problem exhibiting coefficients which we could consider as describing properties of a both spatially and temporally quasiperiodic material. An effective homogenization method for periodic materials is the two-scale convergence technique and it would be desirable to be able to use it also in this case. Quasiperiodic materials can often be described by periodic structures in higher spatial dimensions that are cut by particular two- or three-dimensional sections and projected onto $\mathbb{R}^2$ or $\mathbb{R}^3$, respectively, rendering a quasiperiodic pattern. This cut-and-projection technique enables the use of an extension of two-scale convergence to homogenize quasi-periodic materials. The problem we study also involves quasiperiodic variations in time. Again, there are methods for the periodic case, namely very weak convergence, introduced exactly for the purpose of homogenizing periodic problems exhibiting also rapid scales in time. Combining the cut-and-projection technique and very weak multiscale convergence makes it pos-

sible to study the homogenization of materials with properties varying quasi-periodically in both space and time.

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MS85

Band Structure and Dirac Points of Real-space Quantum Optics in Periodic Media

The field of photonic crystals is almost exclusively based on a Maxwell model of light. To capture light-matter interactions, it natural to study such systems under a quantum-mechanical photon model instead. In the real-space parametrization, interacting photon-atom systems are governed by a system of nonlocal partial differential equations. In this talk, we study resonant phenomena of such systems. Using integral equations, we phrase the resonant problem as a nonlinear eigenvalue problem. In a setting of high-contrast atom inclusions, we obtain fully explicit characterizations of resonances, band structure, and Dirac cones. Additionally, we present a strikingly simple relation between the Green's function of the nonlocal equation and that of the local (Helmholtz) equation. In particular, we generalize existing lattice-summation methods to the nonlocal case. Based on this, we are able to achieve efficient numerical calculations of band structures of interacting photon-atom systems.

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MS85

Very Weak Multiscale Convergence with an Extension from the Periodic to the Quasiperiodic Setting

We present very weak multiscale convergence, a concept applicable to homogenization of periodic problems with rapid temporal oscillations. An extension to the quasiperiodic setting enabling homogenization of problems exhibiting rapid quasiperiodic temporal oscillations is also presented. The incentive of introducing very weak multiscale convergence is to handle sequences that may not be bounded in any Lebesgue space appearing in the homogenization of problems with rapid temporal oscillations. It was first employed to homogenize parabolic problems with rapid periodic oscillations in both space and time. The cut-and-projection technique has been utilized to enable the homogenization of quasiperiodic materials. As a way to manage also quasiperiodicity in time we introduce a cut-and-projection version of very weak multiscale convergence.

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MS86

Harnessing Floppy Modes to Engineer Mechanics and Thermodynamics of Geometrically Frustrated Self-Assemblies

This talk focuses on advancing theoretical frameworks for exploiting geometrically-frustrated assemblies (GFAs) to realize size-controlled, self-limiting assembly. Because soft and self-assembling materials tolerate some measure of misfit at least over some size range, such systems can exhibit scale-dependent thermodynamics, in particular a finite self-assembly size that is controllable through local building block properties. Motivated by efforts to put this concept into practice for intentionally engineered, misfit building blocks (e.g. via DNA origami), we investigate limits of the inter-assembly propagation of stress gradients that lead to finite size selection via a combination of discrete-particle and continuum theory descriptions. Since elasticity of multi-particle assemblies itself, places tight limits on the extent to which cumulative frustration can be extended beyond the particle dimensions, we explore a new paradigm for introducing "floppy modes' into self-assembled structures as means to engineer their response to shape frustration. In particular, we show introducing floppy (auxetic) modes to membrane assemblies frustrated by hyperbolic curvature leads to stress accumulation that is akin to 2D liquid crystalline materials, and extends over substantially larger size scales. We test this prediction via a simple, discrete model of "tapered, square-twist' particles, and further explore the size-dependent stiffness of the assemblies themselves.

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MS87

Line Defects in Hard and Soft Materials: What Is Common?

Line defects in hard (metal) and soft (liquid crystal) materials have been studied with widely different approaches. We focus on an approach that capitalizes on a common thread for such studies, and one which puts equal emphasis on topological properties as well as energetic aspects. A unified kinematical basis for the description of topological defects in soft or hard materials, based on a characterization of integrability of specified distortion fields will be discussed. This kinematics is embedded into a continuum mechanical framework consistent with non-negative dissipation. The resulting model will be illustrated through select examples of dislocation and disclination statics and dynamics in nematic liquid crystals and, separately, in single and polycrystalline metals.

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MS87

Ab-Initio Study of Energetics of Pyramidal Dislocations in Mg Alloys: Implications to Ductility

In this talk, we apply the massively parallel finite-element based DFT framework (DFT-FE) (https://github.com/dftfeDevelopers/dftfe) to study the dislocation core energetics of Pyramidal ¡c+a¿ screw dislocations in magnesium, and the influence of dilute solute alloying on these energetics. We perform systematic cell-size convergence studies of these energetics that indicate requirement of large cell sizes reaching 6,000 atoms (60,000 electrons). Subsequently, we use the obtained ab-initio energetics data to inform a mesoscopic model of ductility in dilute magnesium alloys. We demonstrate that the use of cell-size converged ab-initio inputs significantly influence the mesoscopic model predictions in Mg-Y alloy, and finally we provide quantitative predictions of Y concentration range with improved ductility.

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MS87

The Topological Origin of the Peierls-Nabarro Barrier

Crystals and other condensed matter systems described by density waves often exhibit dislocations. Here we show, by considering the topology of the ground state manifolds (GSMs) of such systems, that dislocations in the density phase field always split into disclinations, and that the disclinations themselves are constrained to sit at particular points in the GSM. Consequently, the topology of the GSM forbids zero-energy dislocation glide, giving rise to a Peierls-Nabarro barrier.

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MS88

Novel topological metrics of entanglement of polymeric material

Filamentous material may exhibit structure dependent material properties and function that depends on their entanglement. Even though intuitively entanglement is often understood in terms of knotting or linking, many of the filamentous systems in the natural world are not mathematical knots or links. In this talk we will introduce a novel framework in knot theory that can characterize the complexity of (collections of) open curves in 3-space in general. This leads to novel metrics of entanglement of open curves in 3-space that generalize classical topological invariants, like, for example, the Jones polynomial and Vassiliev invariants. For open curves, these are continuous functions of the curve coordinates and tend to topological invariants of classical knots and links when the endpoints of the curves tend to coincide. We will apply our methods to polymeric systems and show that the topological entanglement captured by these mathematical methods indeed captures polymer entanglement effects in polymer melts and solutions.

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MS88

Topological constraint release in blends of ring and linear polymers

Blends of linear and ring polymers can have slower dynamics and higher viscosities than the pure individual components. This is due to the threading of ring polymers by linear polymers, which introduces topological constraints that hinder chain diffusion. We simulate blends of linear and ring polymers for long time scales and evaluate the

relaxation of the topological constraints using the periodic linking number. By using the software TEPPP, which employs MPI parallelization, we can evaluate threading between hundreds of millions of pairs of ring and linear polymers over a simulation trajectory. We find that the diffusion time of a ring polymer scales like $N_L^{3.4} * N_R^2$ in ring linear blends, where N_L and N_R represent the length of the linear polymer and ring polymer, respectively. The scaling of ring diffusion time in a blend is partially explained by the relaxation of ring-linear threads, which have a relaxation time that scales like $N_L^{3.4}$.

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MS89

Dynamics of Dislocations with Time-Space Nonlocal Effects

Dislocation dynamics and its relaxation to the metastable transition profile are crucial for understanding the plastic deformation caused by line defects in materials. The global stability of a stationary dislocation profile is proved for bulk-interface coupled dynamic system, where the bulk diffusion equation is coupled with a dynamic boundary condition on the Interface. Due to the presence of dislocation, a nonconvex misfit potential yields an interfacial reaction term on the interface. The nonlocal nature of dislocation appears in both space and time due to the interaction between bulk and interface. We proved that the dynamic solution to this bulk-interface coupled system will uniformly converge to the metastable transition profile, which has a bistates with fat-tail decay rate at the far fields.

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MS89

A New Proof of the Steady State Solution to a 2D Smoluchowski Equation

In this talk we revisit a 2D Smoluchowski equation that is used to model nematic liquid crystalline polymers. In particular, we give a new proof to the study of steady state solutions to the 2D Smoluchowski equation: if the intensity constant is less or equal than 4, then there exists a unique (trivial) solution; if the intensity constant is greater than 4, then there are exactly two solutions that correspond to the isotropic and nematic phases, respectively. The proof depends purely on calculus and is rather transparent.

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MS90

Analysing the Temporal Accuracy of a Hierarchy of Coarse-Grained SDE Models

For complex models such as those used in molecular dynamics, the process of coarse-graining enables longer and larger simulations to be conducted with given computational resources. However, there is no free lunch: fewer degrees of freedom necessarily means lower accuracy of the resulting model. Here, I will discuss work with Helen Li in which we derived a hierarchy of models to coarse-grain simple systems and analysed the resulting coarse-grained models. Our results focus particularly on the temporal accuracy of coarse-grained models, which is where memory effects in the dynamics can play an important role.

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MS90

Arbitrarily Accurate, Nonparametric Coarse Graining with Markov Renewal Processes and the Mori-Zwanzig Formulation

Stochastic dynamics, such as molecular dynamics, are important in many scientific applications. However, summarizing and analyzing the results of such simulations is often challenging due to the high dimension in which simulations are carried out and, consequently, due to the very large amount of data that are typically generated. Coarse-graining is a popular technique for addressing this problem by providing compact and expressive representations. Coarse graining, however, potentially comes at the cost of accuracy, as dynamical information is, in general, lost when projecting the problem in a lower-dimensional space. We show how to eliminate coarse-graining error using two key ideas. First, we represent coarse-grained dynamics as a Markov renewal process. Second, we outline a data-driven, non-parametric MoriZwanzig approach for computing jump times of the renewal process.

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MS90

Data-Driven Scale-Bridging Approaches for Complex Alloys

The extremely large compositional space of complex alloys such as High Entropy Alloys (HEA) promises the development of highly tailored materials solutions with unique combinations of properties. However, the correspondingly astronomically large configurational space of local atomic environments makes the predictions of mesoscale materials properties, such as radiation resistance or elasto-plastic response, from atomistic simulations extremely challenging. We present a comprehensive computational framework to accelerate the development of atomistic-to-mesoscale scale-bridging models through i) physics-informed machine learning to learn how the properties of local atomic environments affect the response of the material, and ii) uncertainty-quantification (UQ) to guide the generation of additional atomistic data to optimally inform the mesoscale models. We present two examples,

the prediction of defect transport coefficients and the development of flow rules for crystal plasticity, that were autonomously developed using a large-scale computational framework guided by UQ. This approach offers a promising avenue to exploit massive scale computing to assist the exploration of the chemical space of HEA for specific applications.

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MS90

Nonlinear Model Reduction for SlowFast Stochastic Systems Near Unknown Invariant Manifolds

We introduce a nonlinear stochastic model reduction technique for high-dimensional stochastic dynamical systems that have a low-dimensional invariant effective manifold with slow dynamics and high-dimensional, large fast modes. Given only access to a black-box simulator from which short bursts of simulation can be obtained, we design an algorithm that outputs an estimate of the invariant manifold, a process of the effective stochastic dynamics on it, which has averaged out the fast modes, and a simulator thereof. This simulator is efficient in that it exploits of the low dimension of the invariant manifold, and takes time-steps of size dependent on the regularity of the effective process, and therefore typically much larger than that of the original simulator, which had to resolve the fast modes. The algorithm and the estimation can be performed on the fly, leading to efficient exploration of the effective state space, without losing consistency with the underlying dynamics. This construction enables fast and efficient simulation of paths of the effective dynamics, together with estimation of crucial features and observables of such dynamics, including the stationary distribution, identification of metastable states, and residence times and transition rates between them.

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MS91

Accelerating Phase Field Simulations Through Time Extrapolation Using Fourier Neural Operators and Unets

Computational simulation of phase field dynamics can be prohibitively expensive when using standard numerical solvers. For example, high-fidelity simulations often use very small time steps due to stability considerations, which can become a bottleneck when the target quantities of interest require predictions far out in time. To address this challenge, we employ machine learning-based surrogate models to help extrapolate forward in time, enabling predictions at time horizons beyond what is achievable through traditional methods alone. Specifically, we investigate two deep learning architectures, Fourier Neural Operators (FNOs) and UNets, and train them to predict future states with much coarser time steps thus encapsulating multiple high-fidelity steps within a single surrogate evaluation. While this approach enables more rapid predictions through autoregressive evaluation of the surrogate, the incurred error is essentially uncontrolled. To alleviate this, we adopt a hybrid prediction strategy which alternates between surrogate evaluations which leap forward in time and high fidelity simulation steps which reduce errors and bring the system state back to the solution manifold. Moreover, we show that including periodic retraining or online fine-tuning can provide further control on the error growth. We illustrate these methods on two examples, a canonical Cahn-Hilliard system and a liquid metal dealloying model.

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MS91

Accelerating Phase Field Simulation of Microstructure Evolution in Additive Manufacturing with Surrogate Machine Learning

Phase-field (PF) modeling is a versatile physics-based computational method that has been used to simulate the evolution of microstructures. The PF method can produce accurate microstructures but suffers from a high computational cost, limiting its use in length scales relevant to additive manufacturing (AM). Using small-scale PF simulations as training data, we trained a surrogate machine learning (ML) model as a computationally cheaper alternative. We use a three-dimensional (3D) U-Net convolutional neural network and predict microstructure evolution with initial microstructure and thermal history as inputs. The ML model can predict the resulting grain orientations at a high accuracy compared to the PF model. Computationally, the ML model is orders of magnitudes faster than the direct PF simulation in a GPU implementation, and scales favorably with increasing number of cells. By spatiotemporally composing multiple ML model predictions at the small-scale, we demonstrate a large-scale 64-layer simulation of a 2 mm 2 mm 2 mm cube for a powder bed fusion additive manufacturing process. The ML results revealed a mixture of equiaxed, columnar, and curved grains, comparable to experimental observations. Microstructures resulting from different toolpath strategies, and lack of fusion defects are also demonstrated. This approach paves the way for microstructure-driven process design in AM.

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MS91

Rethinking Phase-Field Simulations: Blending Di-

rect Numerical Simulations with Neural Operator

Direct numerical simulations are accurate but computationally expensive for predicting materials evolution across timescales, due to the complexity of the underlying governing equations and the nature of spatiotemporal interplays across scales. In this talk I will present a method that blends numerical solvers with neural operators to accelerate such simulations. This methodology is based on the integration of a common numerical solver, in this case a finite-difference phase-field solver, with a U-Net neural operator enhanced by a temporal conditioning mechanism that enables accurate and efficient time-to-solution predictions of the dynamics. This framework will be demonstrated on simulations of microstructure evolution during physical vapor deposition (PVD). PVD simulations exhibit high spatial gradients due to the co-evolution of different material phases with simultaneous slow and fast materials dynamics. I will discuss the accuracy and speedup gained by such hybrid solver and offer thoughts on improvements moving forward. This methodology is generalizable to a broad range of evolutionary models, from solid mechanics, fluid mechanics, to climate. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy National Nuclear Security Administration under contract DE-NA0003525.

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MS91

Phase Field Modeling with Neural Operators

Phase-field modeling serves as a powerful yet computationally demanding approach for capturing the intricate morphological and microstructural changes at the mesoscale, simulating material failures, as well as climate modeling. Consequently, there is a pressing need for fast and generalizable surrogate models to mitigate the computational burden associated with these intricate processes. The inherent discontinuity in microstructures poses a challenge when training surrogate models. In this research endeavor, we introduce an algorithm that combines an autoencoder with a deep neural operator, known as DeepONet, to capture the dynamic evolution of systems within a lower-dimensional latent space. Our study not only highlights the efficacy of this hybrid framework but also provides concrete demonstrations across diverse applications in material science, fracture mechanics, and climate modeling. Furthermore, we establish the superiority of our framework by comparing its accuracy and efficiency against the conventional DeepONet framework.

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MS92

The Materials Genome and the Search for Universal and Continuous Structure Representations

The development of crystallography over the previous century has revolutionized our ability to understand the material universe. However, crystallography has limitations: It results in classifications that are not unique and are discontinuous under small distortions of the structure and it is not well suited to comparing the similarity of different structures. Here we explore alternative representations for rigid periodic structures that overcome these limitations. We seek descriptors (invariants) that are straightforwardly and rapidly computed for any given structure which lead to mathematically valid distance metrics between crystal structures that allow us to easily and rapidly compare their similarity. I will describe measures based on partial atomic pair distribution functions, that can be shown to be unique and complete continuous invariants for crystal structures. Materials can then be mapped into a continuous space to gain insights into how they cluster, where there are gaps (*terra incognita*) that can guide searches for novel materials. As well as being mathematically rigorous, these invariants are very rapid to compute. As a first exploration of what can be learned from this approach we have computed these structure invariants for more than a quarter of a million structures from the Cambridge structural database (CSD) and the Inorganic Crystal Structure Database (ICSD).

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MS92

Crystal-GFN: Sampling Crystals with Desirable Properties and Constraints

Accelerating material discovery holds the potential to greatly help mitigate the climate crisis. Discovering new solid-state crystals such as electrocatalysts, ionic conductors or photovoltaics can have a crucial impact, for instance, in improving the efficiency of renewable energy production and storage. In this paper, we introduce Crystal-GFN, a generative model of crystal structures that sequentially samples a crystal's composition, space group and lattice parameters. This domain-inspired approach enables the flexible incorporation of physical and geometrical constraints, as well as the use of any available predictive model of a desired property as an objective function. We evaluate the capabilities of Crystal-GFN by using as objective the formation energy of a crystal structure, as predicted by a new proxy model trained on MatBench. The results demonstrate that Crystal-GFN is able to sample diverse crystals with low formation energy.

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MS92

Realizations of the Abstract Regular Platonic Polyhedra

An abstract regular polyhedron $\mathcal{P}$ is the combinatorial analog of a classical regular geometric polyhedron. It is a partially ordered set of elements called faces that are completely characterized by a string C-group (G, T), which consists of a group G generated by a set T of involutions. A realization R is a mapping from $\mathcal{P}$ to a Euclidean G space

that is compatible with the associated real orthogonal representation of G. This work discusses an approach to the theory of realizations of abstract regular polyhedra with an emphasis on the construction of a realization of an abstract Platonic polyhedron and its decomposition as a blend of subrealizations. In the fields of chemistry and materials research, regular polyhedra and related structures such as complexes and nets play a prominent role in the study of materials such as crystals, nanotubes, and viruses

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MS92

The Geometry of Highly Symmetric Realizations of (Periodic) Graphs

A graph Γ is an abstract object, but the molecule or material it represents is geometric, and that geometry may be represented by a 'realization' $\rho(\Gamma)$ in Euclidean space. If it is highly symmetric, it may be treated as one component of a 'derived graph' from a 'voltage graph' Δ, in which the 'voltages' are isometries of the appropriate Euclidean space. Fixing Δ, the isometries that may be asigned as voltages form a 'parametrization space', and all possible realizations of Γ that have Δ as a quotient may be realized by an assignment of voltages from this parametrization space. If the graph is to represent a crystal (and thus the symmetry group of its realization should be crystallographic) or a periodic layer or rod (and thus the symmetry group of its realization should be subperiodic), and is to satisfy certain a priori symmetry and geometric restrictions, we can construct the space of all voltage assignments that produce realizations with these restrictions. This space is an ensemble of Euclidean spaces, with realizations of crystallographic or subperiodic structures of higher symmetry being represented by vector subspaces in the Euclidean spaces making up the parametrization space. All possible crystal and subperiodic structures may be represented in this way, facilitating searches for structures of desired symmetry and geometric properties.

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MS93

Bending Measures for Plates and Shells

We present new kinematic bending measures and quadratic energies for isotropic elastic plates and shells, with certain desirable features not present in commonly employed models in soft matter elasticity. These are (informally) justified in a direct approach by a physical definition of pure stretching in terms of the through-thickness strain profile, and complementarily through a reduction from a three-dimensional energy quadratic in stretch. The measure of plate bending is dilation-invariant, coupling stretch and curvature in a generalization of primitive bending strains for straight rods. The extension to naturally-curved rods and shells differs from other forms previously suggested in the literature. The corresponding field equations and boundary conditions feature moments linear in the bending measures, and respond to application of a pure moment by isometric deformation of a unique neutral surface, a primitive behavior in agreement with classical linear response, but not displayed by many analytical models. We briefly comment on relations between our energies, those derived from a neo-Hookean bulk energy, and a commonly used discrete model for flat membranes.

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MS93

Wrinkling Instability Induced by Geometrical Frustration

Thin elastic sheets are characterized by their deformability and exhibit various mechanical instabilities. One common instability is wrinkling. Wrinkling is familiar in sheets that adhere to a soft substrate or fluid interface under compression (e.g., skin), and the interplay between the substrate deformation and the bending of the sheet determines their wavelength. Surprisingly, wrinkles also appear in isolated thin sheets that undergo non-uniform growth, yet their properties are still poorly understood. In this work, we investigate wrinkles of the second type, from a geometrical point of view. We use latex sheets that swell non-uniformly one half of the sheet is exposed to a solvent that swells it, while the other is not, meeting at a sharp transition. This geometry corresponds to two cylinders of different radii joined by a smooth transition region, like a wine bottle. However, we show that when the radius of one of the cylinders is fixed to a non-equilibrium value, a smooth isometric embedding of the system is no longer possible, and longitudinal wrinkles appear to prevent the stretching of the material. We study the origin of this phenomenon and identify the scaling of the wavelength and size of the wrinkled domain. We find that when the radius grows to infinity, the system behaves like hanging drapes. The study results are relevant to other cases where differential swelling induces wrinkling instability, such as in plants and synthetic responsive materials.

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MS93

Linking Energy to Irregularity in Prestrained Elastic Sheets

This talk will delve into the link between prestrain regularity and energy in non-Euclidean thin elastic sheets. We show that in 2d stretching+bending models, prestrain irregularity implies a lower bound on the energy of the system. We also analyze the example of incompatible inclusions, a problem with applications in thin nematic elastomer sheets. In this example, we show a lower bound for general 3d elastic energy functionals and a matching upper bound, constructed by a combination of origami maps and Brehm isometries.

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MS93

Discretization Methods for Large-Strain Director Shells

Various models of continuum mechanics involve degrees of freedom that do not form linear spaces. A prime example are large-strain director shell models that describe shear and drilling motions by fields of unit vectors or orthogonal matrices. Such models cannot be discretized by standard finite elements, because these methods cannot represent the nonlinear structure of the configuration space. We show how to generalize polynomial interpolation to obtain finite elements that approximate direction and orientation fields without violating the nonlinear nature of the configuration space. Such geometric finite elements preserve frame indifference, and they satisfy optimal approximation error bounds. We apply them to a geometrically nonlinear Cosserat shell model, and we prove existence of finite element solutions. We then show various wrinkling and buckling simulations, both for free-standing shells and for shells coupled to an elastic substrate.

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MS94

Discretization of the Monge-Ampre Equation and Application to Optical Lens Design

The Monge-Ampre equation is a nonlinear degenerate elliptic equation that arises from the field of optimal transport and that has various applications. I will discuss in particular an application to refractor design in nonimaging optics, which is motivated by recent engineering progress in the manufacturing process of arbitrarily-shaped optical lens. A common approach for solving the Monge-Ampre equation numerically is to discretize a reformulation of the equation in Hamilton-Jacobi-Bellman form. I will describe such a discretization, using monotone finite differences on a Cartesian grid and tools originating from the theory of low-dimensional lattice geometry. The resulting numerical scheme features good consistency properties and can be solved efficiently using a simple Newton method, even in the case of degenerate data. It is compatible with the optimal transport boundary condition that typically arises in applications. The existence and the convergence of numerical solutions are proved at least in the case of Monge-Ampre equations associated with the quadratic optimal transport cost, and numerical experiments validate the method in a more general setting.

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MS94

Modelling Abscission of Plant Organs As Inspiration for the Separation of Artificial Materials Systems

We develop a finite element model to understand the abscission process of different species of cacti. In particular, the cactus species *Opuntia ficus-indica* and *Cylindropuntia bigelovii* exhibit a vastly different effective fracture toughness, while relying as all plants do on a very limited set of basic materials as building blocks. We thus include the available morphometric and biomechanical data of our cactus species in the variational framework of brittle fracture presented by Bourdin et. al in 2008 and study their behavior compared to fictional cacti to isolate the effect of different geometric, microstructural, and materials features on the effective fracture toughness. The results are compared to experimental testing. The main motivation of this research is to gain inspiration for novel methods aiding the separation of artificial materials systems to sort raw materials for sustainable reuse and recycling.

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MS95

Bicrystallography-Informed FrenkelKontorova Model for Interlayer Dislocations in Strained 2D Heterostructures

The weak van der Waals interactions between the two-dimensional (2D) lattices of a bilayer graphene (BG) offer high fidelity in tuning the local atomic environments, allowing control over quantum properties. Small-twist BG is the most prominent example, wherein flat bands emerge at a specific magic twist angle. However, the electronic structure of a twisted BG is sensitive to the structural relaxation that accompanies the twist. The exciting possibility of discovering magic heterostrains in 2D heterostructures motivates us to develop a mesoscale model to predict structural relaxation. Building on the observation that partial dislocations are responsible for structural relaxation in a small-twist BG, we hypothesize that interface dislocations also play a critical role in large-twist/strained 2D heterostructures. In this talk, we will demonstrate the validity of this hypothesis using atomistics and formulate a mesoscale model for heterostructure relaxation. We note that unlike in a small-twist BG, the Burgers vector in a relaxed large-twist BG is much smaller than the lattice vector of graphene. Smith normal form (SNF) bicrystallography implies that the Burgers vector in such systems belongs to the displacement shift complete lattice (DSCL). Recognizing that the stacking fault energy of the two lattices should reflect the symmetry of the DSCL, we formulate a bicrystallography-informed Frenkel–Kontorova model to predict structural relaxation in 2D heterostructures.

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MS95

Solutions of Design Problems in the Actuation of Liquid Crystal Glass Sheets Via Duality

A novel dual variational principle [Arora, A. PhD Thesis, Carnegie Mellon University (2023).] is developed for inverse and forward design problems in the actuation of liquid crystal glass sheets based on the PDEs arising from continuum mechanics ideas [Acharya, A. J Elast 136, 237–

249 (2019).]. A Newton-Raphson algorithm is developed to obtain the approximations of critical point solutions of the dual functional, with a consistent nonlinear mapping between the primal and dual fields, with the guarantee that the primal PDE is solved in a well-defined sense. For complicated design shapes, an elliptic regularization of the dual PDE is introduced, and the solutions obtained for the regularized problem are used as an initial guess for the unregularized problem. Examples of both forward and inverse design problems are computationally demonstrated using the developed framework. The quality factor (error) of the obtained solution is measured based on the L^2 norm of the difference between the prescribed stretches and the computed principal stretches of the Right-Cauchy Green tensor of the deformation, mapping the actuated and the unactuated shape. The solutions obtained for the inverse design problems of shapes with non-zero Gauss curvature such as a hemisphere and a hat shape have less than 2.5% error, which is a decent result, given the complexity of the governing equations in the prescribed principal stretches formulation.

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MS95

Emergent Defect Mechanics in Soft, Supramolecular Networks

Amphiphilic molecules can self-assemble into ordered phases, from the classical lamellar, columnar, and sphere phases, to complex bicontinuous networks. Given that these phases can have either 1D, 2D, or 3D crystalline symmetries, they host a rich variety of defects. However, the essential interplay between interfacial geometry and molecular packing complicates the study of defects in these materials; in fact, little is known about the response of amphiphilic assemblies to symmetry-breaking deformations and disruptions of crystalline order. With the ultimate goal of arriving at a detailed picture of defect mechanics and thermodynamics in amphiphilic assemblies, we investigate their collective responses to various disruptions in crystalline symmetry. In particular, we focus on mesoscale mass transport as a key feature of near-equilibrium response of these assemblies. In the context of network phases, we explore material response through the lens of mechanical networks via "liquid network theory," a coarse-grained model governed by the mathematics of length-minimizing Steiner networks, which gives rise to new modes of stress relaxation seen in previous experiments on block copolymers.

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MS96

New Measures of Entanglment of Collections of Open Curves in 3-Space

The entanglement of open curves in 3-space appears in many physical systems and affects their material properties and function. A new framework in knot theory was introduced recently, that enables to characterize the complexity of collections of open curves in 3-space using the theory of knotoids and linkoids, which are equivalence classes of diagrams with open arcs. In this talk, we discuss new invariants of linkoids via a surjective map between linkoids and virtual knots. This leads to a new collection of strong invariants of linkoids that are independent of any given virtual closure. This gives rise to a collection of novel measures of entanglement of open curves in 3-space, which are continuous functions of the curve coordinates and tend to their corresponding classical invariants when the endpoints of the curves tend to coincide.

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MS97

Rigidity of the Eikonal equation with L^p Entropies

The Aviles-Giga functional is a classical problem in the calculus of variations. The energy functional in 2D has been used to model smectic liquid crystals and thin film blisters. The Gamma-convergence of the Aviles-Giga functional remains a challenging open problem, which requires better understanding of the fine structure of the underlying function space, namely the space of finite entropy solutions of the Eikonal equation. In this talk, I will give an introduction to the above mentioned problem, and present our recent progress towards understanding finite entropy solutions of the Eikonal equation in 2D. Our result supports the conjecture that entropy measures of finite entropy solutions concentrate on 1D sets, and completes the picture on the rigidity/flexibility threshold of the 2D Eikonal equation in the Besov space scaling. This is joint work with Xavier Lamy and Andrew Lorent

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MS97

Equlibrium Shape of an Elastic Beam in a Rigid Cylinder

In this talk, we will present the findings regarding the equilibrium shape of an elastic beam contained in a rigid right

circular cylinder. This is a constrained minimization problem, where the energy to be minimized is the elastic energy of the beam, subject to the hard constraint that the beam has to be inside the cylinder, oriented transversely to its axis. Based on observations from desktop experiments, we derived and numerically solved the Euler-Lagrange equations together with suitable boundary conditions and other constraints that depend on the length of the beam. We hope that our findings from studying the elastic beam in the rigid cylinder can offer valuable insights for dealing with more general obstacles.

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MS98

Sharp Error Estimates for the Target Measure Diffusion Maps

We obtain asymptotically sharp error estimates for the consistency error of the Target Measure Diffusion map (TMDmap) (Banisch et al. 2020), a variant of diffusion maps featuring importance sampling and hence allowing input data drawn from an arbitrary density. The derived error estimates include the bias error and the variance error. The resulting convergence rates are consistent with the approximation theory of graph Laplacians. The key novelty of our results lies in the explicit quantification of all the prefactors on leading-order terms. We also prove an error estimate for solutions of Dirichlet BVPs obtained using TMDmap. The solution error is controlled by consistency error. We use these results to study an important application of TMDmap in the analysis of rare events in systems governed by overdamped Langevin dynamics using the framework of transition path theory (TPT). The cornerstone ingredient of TPT is the solution of the committor problem, a boundary value problem for the backward Kolmogorov PDE. Remarkably, the TMDmap algorithm is particularly suited as a meshless solver to the committor problem due to the cancellation of several error terms in the prefactor formula. Furthermore, significant improvements in bias and variance errors occur when using a quasi-uniform sampling density. Our numerical experiments show that these improvements in accuracy are realizable in practice when using $\bar{\delta}$-nets as spatially uniform inputs to the TMDmap algorithm.

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MS98

Deforming Domain Methods for Nonequilibrium Molecular Dynamics

In the molecular scale simulation of fluid flow, a wide range of numerical techniques are employed for the efficient computation of quantities of interest. One class of techniques simulates molecular fluids with a steady background flow and involves the use of deforming simulation geometry. The time-periodic and quasiperiodic deforming domains as well as the nonreversible nature of the flow provides analytical and computational challenges for showing the existence and convergence to nonequilibrium steady states. We will discuss the existence of steady-states for general nonequilibrium flows in three-dimensions as well as techniques for accelerating sampling.

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MS98

Enhanced Sampling Methods for the Calculation of Nonequlibrium Steady States

The calculation of steady-states of systems which are both non-reversible and metastable presents a major computational challenge. Here we present work on a class of methods that seek to overcome this challenge by stratifying the underlying space, that it, breaking it up into parts and sampling on each part. Iterative Aggregation Disaggregation (IAD) is a model of such methods, and we present a result showing why it can accelerate convergence to the steady state for many systems.

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MS98

Global Space Time Formulation of the Schrdinger Equation for Low Rank Methods

In this project, we mathematically and numerically study new methods for solving time-dependent electronic structure calculation problems in order to provide accurate numerical approximations over long time scales. More specifically, we numerically simulate the time evolution of the state of an electron system in a molecule or a periodic solid over long time scales. Most electronic structure calculations carried out in practice involve solving the stationary problem, i,e, determining the lowest energy state of the electrons in the molecule or material of interest. However, these stationary calculations are not sufficient to predict the electronic properties of a system interacting with the external environment. This is the case, for example, when one wishes to study the interactions of the molecule or material in question with photons, a phenomenon that plays a crucial role in the properties of photovoltaic materials. It is important in this context to be able to perform accurate simulations of the evolution of the electron system of interest over long time scales. To do this, we reformulate the evolution problem as a minimization problem, for which verifying the well-posed nature of the obtained variational problems requires the use of results from spectral theory. We then combine the obtained variational principles with nonlinear numerical approximation methods such as tensor methods to compute an approximation of the solution.

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MS99

Multi-Phase Field Model Development for Electrochemical Dealloying Corrosion

Dealloying corrosion is the selective dissolution of a metal into a corrosive agent, resulting in the formation of a

topologically-complex structure composed of the more-noble metal element(s). The topology of dealloyed structures depends on the metals microstructure and the corrosive agents chemistry, which inform the nature of the corrosion reactions occurring at their solid-liquid interface. The phase field method is an excellent candidate for modeling microstructure evolution during dealloying corrosion. However, the fine-scale structures that dynamically emerge during dealloying impose numerical constraints that usually require very small time-steps to guarantee numerical stability and accuracy. This work proposes using an advanced semi-implicit time integration scheme, using spectral methods, to accelerate phase field modeling of electrochemical dealloying corrosion. This numerical approach makes large 2D and 3D simulations tractable by enabling the use of very large time steps. We exercise this numerical scheme to simulate a Ni-based alloy undergoing dealloying corrosion in a molten salt. We consider the roles of relative electrochemical overpotentials for metallic species, the concentration of oxidants in the molten salt, and assumptions regarding charge conservation in the system. We find that the corrosion rate and morphology of alloy depend strongly on solute transport rates within the metal and molten salt, and along their solid-liquid interface.

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MS99

Investigating Grain Growth Using a Physics-Regularized Interpretable Machine Learning Model

Physics-based mesoscale models of grain growth have been unable to accurately represent the grain growth behavior of real materials. We are developing the Physics Regularized Interpretable Machine Learning Microstructure Evolution (PRIMME) model learns to predict grain growth directly from grain growth data. The PRIMME algorithm uses a multi-level neural network to predict grain growth in a voxelated domain. It uses a regularization function that encourages evolution that never increases the number of nearest neighbor voxels assigned to different grains. PRIMME helps to interpret and understand its learned grain growth behavior by determining the likelihood of a voxel changing to the grain of neighboring voxels. It was originally trained using data from 2D isotropic simulation results. It is now being extended to 3D isotropic and 2D anisotropic behavior. It will begin to be trained using experimental data rather than just simulation results soon.

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MS100

Micromechanics of Light-Induced Phase Transformation in Molecular Crystals

Molecular crystals that respond to a light stimulus are emerging as a new class of photo-mechanical materials that find numerous engineering applications, ranging from remote actuation to flexible electronics. These materials consist of discrete molecules that are held together by intermolecular interactions and have a crystalline order that is intermediate to inorganic crystals and polymers. On exposure to light, these molecular crystals undergo a chemical reaction (e.g., cis-trans isomerization or dimerization) that is accompanied by an abrupt mechanical response, such as bending, coiling, twisting, and at their most extreme, jumping to distances several orders of magnitude their size. In this talk, I will present a continuum model to understand how underlying structural transformations of lattices and microstructural evolution pathways play an important role in the photomechanical behavior of a representative molecular crystal (Salicylideneimine). We show that a model rooted in the Finite Deformation Theory and the Cauchy-Born Rule describes the bending and twisting deformation in these materials.

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MS100

Structure determination and constructive interference by group invariance

The effectiveness of X-ray methods in determining atomic structure stems from the group invariance of Maxwells equations. Specifically, certain forms of radiation interact with atoms in the structure, whose positions correspond to the orbit of a transformation group. This interaction leads to constructive interference in specific directions in the far field, while strong destructive interference occurs in other directions. Essentially, the group generating the radiation aligns with the group generating the atomic structure. Instead of atoms, emitters (such as dipole sources) can be positioned based on the orbit of a group, offering greater flexibility since each emitter can be independently controlled, unlike the oscillations of atoms in a crystal structure. Emitters also provide a wider range of group options, including conformal or Lorentz groups. In this context, we develop a theory of constructive interference. Additionally, we redefine a general solution of Maxwells equations from a differ-

ent perspective. This solution holds practical significance, as it can be effectively approximated by superposing finite plane waves. The convergence is remarkably fast due to the rapid convergence of the trapezoidal rule for the integration of a periodic analytical function.

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MS100

Dipole amplification: bounds and optimal designs

What is the optimal geometrical/material pattern for extracting radiation from a dipole, or reciprocally concentrating radiation to a point? This question has ramifications for imaging, quantum communication, Purcell-factor enhancement, and mode volume minimization. I will discuss: ideal scaling laws (as a function of minimum feature size), why conventional bowtie structures fall far short, bounds showing that two-material designs must always fall short, and three-material design patterns that can approach the optimal scaling laws.

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MS101

Phase Separation in Heterogeneous Media

Modern technologies and biological systems, such as temperature-responsive polymers and lipid rafts, take advantage of engineered inclusions, or natural heterogeneities of the medium, to obtain novel composite materials with specific physical properties. To model such situations using a variational approach based on the gradient theory of phase transitions, the potential and the wells may have to depend on the spatial position, even in a discontinuous way, and different regimes should be considered. In the critical case case where the scale of the small heterogeneities is of the same order of the scale governing the phase transition and the wells are fixed, the interaction between homogenization and the phase transitions process leads to an anisotropic interfacial energy. The supercritical case for fixed wells is also addressed, now leading to an isotropic interfacial energy. In the subcritical case with moving wells, where the heterogeneities of the material are of a larger scale than that of the diffuse interface between different phases, it is observed that there is no macroscopic phase separation and that thermal fluctuations play a role in the formation of nanodomains. This is joint work with Riccardo Cristoferi (Radboud University, The Netherlands) and Likhit Ganedi (Aachen University, Germany), USA), based on previous results also obtained with Adrian Hagerty (USA) and Cristina Popovici (USA).

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MS101

Function Space Identification for Peridynamics

In the model of linearized peridynamics the associated function space is a subspace of $L^p(\Omega)$ that contains the fractional Sobolev space $W^{s,p}(\Omega)$. The question is whether for Lipschitz domains $\Omega \subset \mathbb{R}^n$ the function space is in fact $W^{s,p}(\Omega)$. The question has been answered positively by Mengesha and Scott in the case when Ω is either the entire space $\mathbb{R}^n$ or the half space. We answer the question affirmatively for bounded Lipschitz domains Ω with small Lipschitz constant (in partiicular C^1 domains). This is joint work with H. Mikayelyan, T. Mengesha, and J. Scott.

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MS101

Dynamic Energy Balance and Continuum Damage

A nonlocal model for dynamic damage evolution is introduced that consists of two branches one elastic and the other inelastic. Evolution from the elastic to the inelastic branch depends on material strength and is mediated through the constitutive law relating force to strain. For two dimensional problems with a straight crack, power balance delivers the crack tip velocity in terms of the rate of work done by the load and the change in both the kinetic energy and elastic potential energy of the specimen. Passage to the limit of vanishing nonlocality in a pre-cracked plate subjected to mode I loading delivers a sharp fracture evolution that agrees with classic dynamic fracture mechanics.

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MS101

On the Landau-de Gennes model with planar anchoring and a weak magnetic field

In this talk I will discuss the 3D Landau-de Gennes model for nematic liquid crystal with an external magnetic field around an immersed particle. I will show that if we impose strong planar anchoring on the surface, then in the large particle limit, and assuming a weak magnetic field, we can

characterize the defects that occur. We will see that only point defects can occur for minimizers in this regime.

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MS102

An Anisotropic Poincare Inequality in $GSBV^p$ and an Application to an Anisotropic Mumford-Shah Energy

In this talk we discuss a Poincare inequality for functions in $GSBV^p$ that have a small variation in 2 of 3 spatial directions. It will be shown that such a function is close to a function of one variable outside an exceptional set. For the exceptional set bounds on the volume and the perimeter in two directions are provided. As a key tool we prove an approximation result for such functions. For this we present a two-dimensional countable ball construction that allows to carefully remove the jumps of the function. As a simple application, we present the G-convergence of an anisotropic three-dimensional Mumford-Shah model to a one-dimensional model.

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MS102

Discrete Differential Geometry for $C^{1,1}$ Hyperbolic Surfaces of Non-Constant Curvature

We develop a discrete differential geometry for surfaces of non-constant negative curvature, which can be used to model various phenomena from the growth of flower petals to marine invertebrate swimming. Specifically, we derive and numerically integrate a version of the classical Lelieuvre formulas that apply to immersions of $C^{1,1}$ hyperbolic surfaces of non-constant curvature. In contrast to the constant curvature case, these formulas do not provide an explicit method for constructing an immersion but rather describe an immersion via an implicit set of equations. We propose an iterative method for resolving these equations. Because we are interested in scenarios where the curvature is a function of the intrinsic material coordinates, in particular, on the geodesic distance from an origin, we suggest a fast marching method for computing geodesic distance on manifolds. We apply our methods to generate surfaces of non-constant curvature and demonstrate how one can introduce branch points to account for the sort of multi-generational buckling and subwrinkling observed in many applications.

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MS102

Origami As a Limit of Confined Thin Elastic Sheets

Origami-inspired design is a familiar approach to engineering shape change: folds can be viewed as building blocks whose arrangement can be optimized. At the same time, folds arise naturally from confining thin elastic sheets, in a poorly understood process known as stress concentration. Does nature suggest optimal fold patterns for achieving macroscopic shape change? To make progress on this question, we consider a thin elastic sheet that is confined along its midplane and constrained to lie within a small vertical gap. We prove that stress must concentrate in this setup onto a lower dimensional fold set, which we define. Similarly, we prove a compactness theorem that establishes strong convergence of minimizers towards an origami limit map, in an asymptotic limit where the gap size for the confinement and the sheet thickness go to zero. Time permitting, we discuss limit formulas for the asymptotic line energy of the folds. This is joint work with Ian Tobasco (Rutgers) and Sergio Conti (Bonn).

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MS103

Modeling of Experimentally Observed Topological Defects Inside Bulk Polycrystals

A scheme is developed for computing elastic fields, on the microscale, generated by experimentally observed defect structures within grains in a polycrystal that has undergone some deformation. An existing data set, collected using near-field high energy diffraction microscopy (nf-HEDM) measurement, is analyzed. A topologically interesting feature was identified in the orientation field. This feature is present in the interior of a grain of zirconium after tensile deformation. At the scale of the observations, we use g.disclination theory, to compute the stress fields for the identified intra-granular orientation discontinuities.

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MS103

Higher-Order Defects in Soft Materials

Hyperbolic thin elastic sheets support a novel type of defects, that we call *branch points*, corresponding to discontinuities in the second derivatives of the displacement. These defects confer novel mechanical properties to such thin sheets. I will present a brief discussion of discrete differential geometric (DDG) methods for studying the kinematics of thin hyperbolic sheets. I will also discuss some recent results on the distribution of and interactions between branch point defects. This is joint work with Ari Bormanis and Christian Parkinson.

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MS103

A Tensor Density Measure of Topological Charge and Disclination Kinematics in Three Dimensional Nematics

An exact kinematic law for the motion of disclination lines in nematic liquid crystals as a function of the tensor order parameter Q is derived. Unlike other order parameter fields that become singular at their respective defect cores, the tensor order parameter remains regular. Following earlier experimental and theoretical work, the disclination core is defined to be the line where the uniaxial and biaxial order parameters are equal, or equivalently, where the two largest eigenvalues of Q cross. This allows an exact expression relating the velocity of the line to spatial and temporal derivatives of Q on the line, to be specified by a dynamical model for the evolution of the nematic. By introducing a linear core approximation for Q, analytical results are given for several prototypical configurations, including line interactions and motion, loop annihilation, and the response to external fields and shear flows. Behavior that follows from topological constraints or defect geometry is highlighted. The analytic results are shown to be in agreement with three-dimensional numerical calculations based on a singular Maier-Saupe free energy that allows for anisotropic elasticity. We also show that the kinematic law can be related to a three-dimensional invariant measure via a tensor density, function of the line tangent, and nematic rotation vector.

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MS104

On Energy Minimizers with Planar Anchoring in Nematic Liquid Crystals

Motivated by experiments with nematic liquid crystal droplets, we study harmonic maps that arise as minimizers of the the one-constant approximation of the Oseen-Frank energy subject to strong anchoring tangential boundary condition. In this talk, I will present a reflection method allowing us to analyze the regularity of minimizers up to the boundary. We also obtain results on the type and location of defects that can occur, such as boundary "boojums' and interior vortices. The talk is based on joint work with L. Bronsard and A. Colinet.

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MS104

Core Shells and Double Bubbles in a Weighted Nonlocal Isoperimetric Problem

We consider a sharp-interface model of ABC triblock copolymers, for which the surface tension σ_{ij} across the interface separating phase i from phase j may depend on the components. We study global minimizers of the associated ternary local isoperimetric problem in $\mathbb{R}^2$, and show how the geometry of minimizers changes with the surface tensions σ_{ij}, varying from symmetric double-bubbles for equal surface tensions, through asymmetric double bubbles, to core shells as the values of σ_{ij} become more disparate. Then we consider the effect of nonlocal interactions in a droplet scaling regime, in which vanishingly small particles of two phases are distributed in a sea of the third phase. We are particularly interested in a degenerate case of σ_{ij} in which minimizers exhibit core shell geometry, as this phase configuration is expected on physical grounds in nonlocal ternary systems.

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MS104

A Nonlinear Smectic A Liquid Crystal Model

We will review some recent progress on a nonlinear model for Smectic A liquid crystal. We present some compactness results as well as some asymptotic upper and lower bounds on the energy functional. This talk is based on joint work with Michael Novack.

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MS105

Mathematical Model of Materials with Nonlocal Behavior in Space and Time

In this talk, we consider a model of materials with nonlocality in both space and time. The nonlocality in space corresponds to a bond-based peridynamic material model, where progressive bond failure leads to the emergence of crack-like defects. The nonlocality in time corresponds to viscoelasticity with a non-constant complex-valued stiffness tensor, allowing the material to have different responses for different frequencies. This approach results in a causal viscoelastic peridynamic model. We present numerical simulations with applications to fracture, in particular, crack propagation in a block of sea ice with interconnected brine channels.

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MS105

Topological Anderson Insulators by homogenization theory

A central property of (Chern) topological insulators is the presence of robust asymmetric transport along interfaces separating two-dimensional insulating materials in different topological phases. A Topological Anderson Insulator is an insulator whose topological phase is induced by fluctuations. We propose a mathematical model of perturbed Dirac equations and show that for sufficiently large and highly oscillatory perturbations, the system is in a different topological phase than the unperturbed model. In particular, a robust asymmetric transport indeed appears at an interface separating perturbed and unperturbed phases. The theoretical results are based on careful estimates of resolvent operators in the homogenization theory of Dirac equations and on the characterization of topological phases by the index of an appropriate Fredholm operator.

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MS105

Asymmetric Transport for Magnetic Dirac Equations

This talk concerns the asymmetric transport associated with a low-energy interface Dirac model of graphene-type materials subject to external magnetic and electric fields. We show that the relevant physical observable, an interface conductivity, is quantized and robust to a large class of perturbations. These include defects that decay along or away from the interface, and sufficiently small or localized changes in the external fields. An explicit formula for the interface conductivity is given by a spectral flow.

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MS105

Classification of Strongly-Disordered Topological Insulators

In this talk I will describe some of the mathematical aspects of strongly-disordered topological insulators. These are novel materials which insulate in their bulk but (may) conduct along their edge; the quintessential example is that of the integer quantum Hall effect. What characterizes these materials is the existence of a topological index, experimentally measurable and macroscopically quantized. Mathematically this is explained by applying algebraic topology to the space of appropriate quantum mechanical Hamiltonians. I will survey some recent results mainly concentrating on the classification problem for spectrally gapped 1D systems.

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MS106

Variational Model for Nematic Soap Films

In this talk I discuss the existence and the derivation of some geometrical properties of minimizers for the energy functional penalizing both the area contribution, as in the classical Plateau problem, and the Frank free-energy, typically arising from soft materials like nematic liquid crystal.

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MS106

On the Sparsity of h-Wasserstein Barycenters

The Multi-Marginal Optimal Transport problem will be presented, showing the relation, in case of Coulomb cost, with the Wigner crystallization conjecture, for which a gas of electrons at low density will crystallize and form a lattice. This can be seen as an OT problem, and the difficulties will be emphasized, also in connection with the MMOT problem of the h-Wasserstein barycenter, where h is a nonnegative strictly convex function. This is a generalization of the better known 2-Wasserstein barycenter, which has been widely studied lately as it provides a way for averaging probability distributions, by respecting their geometry. It appeared first in [Agueh and Carlier,Barycenters in the Wasserstein space, 2011] and was further studied, among the others, in [Pass, Multi-marginal optimal transport and multi-agent matching problems: Uniqueness and structure of solutions, 2014]. It is a highly nonlinear problem, but it can be reduced to a MMOT problem, which is a linear programming problem, but - a priori- of higher dimension. The goal is to prove the sparsity of the optimal plan for the MMOT formulation, which for the 2-case has been proved in [Gangbo and Swiech, Optimal Maps for the Multidimensional Monge- Kantorovich Problem, 1998]. Here we provide a proof of the absolute continuity of the h-Wasserstein barycenter, which implies that the optimal plan is a map and thus its dimension coincides with the dimension of the support of only one marginal.

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MS106

An Approach to Topological Singularities Through Mumford-Shah Type Functionals

The talk concerns an ongoing work with L. De Luca and R. Scala about the asymptotic variational equivalence, at any logarithmic scaling regime, between Ginzburg-Landau energies (then Core Radius energies, as well) and suitable Mumford-Shah type energies. This extends a recent work by De Luca-Scala-Van Goethem which first employs such Mumford-Shah type functionals to approximate the energy of finitely many dislocations in a simplified topological setting.

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MS107

Applications of Isometry Invariants on Material Property Prediction

Periodic material or crystal property prediction using machine learning has grown popular in recent years as it provides a computationally efficient replacement for classical simulation methods. A crucial first step for any of these algorithms is the representation used for a periodic crystal. While similar objects like molecules and proteins have a finite number of atoms and their representation can be built based upon a finite point cloud interpretation, periodic crystals are unbounded in size, making their representation more challenging. Isometry invariants offer a consistent way to represent and compare crystal structures. In the present work, we adapt two isometry invariants, the Pointwise Distance Distribution (PDD) and Average Minimum Distance (AMD) as a representation for our learning algorithm. The PDD and AMD distinguished all (more than 660 thousand) periodic crystals in the Cambridge Structural Database as purely periodic sets of points without atomic types. For machine learning models, the composition of a crystal contains crucial information needed for making accurate predictions. We introduce a method for combining the geometric information contained in the isometry invariants with compositional information and show its effectiveness on the commonly used Jarvis-DFT and Materials Project datasets.

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MS107

Graph Theory Establishes Nonlinear Dependence of Complexity on Chirality

Nano-, micro- and macrostructures obtained by the self-assembly of chiral nanoparticles demonstrated emergence of complexity, that is spontaneous increase of structural hierarchy and non-randomness seemingly prohibited by thermodynamics. These observations mirror the structural evolution of biological materials that combine nano-, meso- and microscale chirality. We applied graph theoretical (GT) measures of complexity to nanoparticle assemblies and found that (a) formation of complex structures does not require monodispersity; (b) competing thermodynamic restrictions in self-limited systems increase their complexity; (c) complexity depends on chirality non-linearly; (d) synthetic particles can have higher complexity than their biological prototypes. The GT description can be expanded to include other nanoscale structures, such as complex porous particles and superlattices,creating analogs of chemical formulas for complex particle systems (chiral, racemic and achiral) for the use in ML predictions. References - Science, 2020, 368, 642; Nature 2023, 615, 418.

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MS107

New Mathematical Principles in Materials Science

This talk will describe two new principles developed in a new area of Geometric Data Science. The most fundamental models of molecules and periodic crystals are finite and periodic sets of atomic centers. The strongest equivalence of such atomic sets in practice is rigid motion because there is little sense to distinguish between

molecules and crystals that are related by translations and rotations. This relation motivates the problem to design complete (DNA-style) invariants that uniquely identify any molecule or crystal up to rigid motion. Since all real data are noisy, practically useful invariants should continuously change under perturbations: if any atom is displaced by epsilon, the invariant should change up to C*epsilon in a suitable metric d, where C is a constant. We developed generically complete and continuous invariants for finite and periodic sets of unordered points. In the periodic case, the new invariants uniquely identified all periodic crystals in the Cambridge Structural Database through 200+ billion pairwise comparisons within two days on a modest desktop computer. The resulting Crystal Isometry Principle (CRISP) justifies a geographic-style map covering all known and not yet discovered periodic crystals, see http://kurlin.org/projects/Crystal-Isometry-Principle-maps.pdf. For finite clouds of unordered atoms, the new invariants continuously quantified structure-property relations in the QM9 database of 130K+ molecules for a molecular analog of CRISP.

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MS108

Deformation and Motion of Structures by Light

Photo-mechanically active materials are able to couple light and mechanical deformation. These materials enable mechanical deformation of structures with light. However, the action is non-local in both space and time: as the structure absorbs light and deforms, the conditions of illumination change across the structure, and this, in turn, changes the nature of subsequent deformation. We develop a simple model of slender structures beams, rods and shells – of photomechanically active materials, and show through examples that this non-locality leads to very unusual phenomena. Examples includes the emergence of cyclic or periodic motion under steady illumination and the emergence of orientational tracking/avoidance of light sources.

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MS108

Patterned Illumination for Complex Spatio-temporal Morphing of LCE Sheets

Liquid crystal elastomers are rubbery solids containing molecular LC rods that align along a common director. On heating, the alignment is disrupted, leading to a substantial ($\sim 50\%$) contraction along the director. In recent years, there has been a great deal of interest in fabrication LCE sheets with a bespoke alignment pattern. On heating, these patterns generate corresponding patterns of contraction that can morph a sheet into a bespoke curved surface such as a cone or face. Moreover, LCEs can also be activated by light, either photothermally or photochemically, leading to similarly large contractions. Stimulation by light also introduces an important new possibility: using spatio-temporal patterns of illumination to morph a single LCE sample into a range of different surfaces. Such stimulation can enable non-reciprocal actuation for viscous swimming or pumping, and control over the whole path taken by the sheet through shape-space rather than just the final destination. In this talk, I will start by with an experimental example of a spatio-temporal pattern of illumination being used to actuate an LCE peristaltic pump. I will then introduce a second set of experiments, in which a monodomain sheet morphs first into a cone, an anti-cone and then an array of cones upon exposure to different patterns of illumination. Finally, I will then discuss the general problem of how to choose a pattern of illumination to morph a director-patterned sheet into an arbitrary surface, first analytically for axisymmetric cases, then numerically for low symmetry cases. This last study exceeds our current experimental capacity, but highlights how, with full spatio-temporal control over the stimulation magnitude, one can choreograph an LCE sheet to undergo almost any pattern of morphing.

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MT1

Multi-Modal Data Driven and Physics-Informed Machine Learning with Uncertainty for Materials Applications

This tutorial explores state-of-the-art data fusion and machine learning under uncertainty for materials applications, divided into three components forming a unified framework through shared applications that can be applied for wide-ranging problems in materials science. The code/activities will be shared with participants in the mini tutorial for additional study after the conference. The first part focuses on merging materials data from diverse sources, using variational inference to create multimodal embeddings and integrate physical models for unsupervised feature identification. The example uses molecular dynamics simulations of metal lattices for multimodal data fusion. The second part delves into advanced techniques for operator learning, employing deep neural networks to model physical processes and address material science problems, enhancing accuracy with labeled datasets or domain-specific knowledge. The tutorial also addresses pervasive uncertainties in data-driven materials modeling, including imprecision, noise, bias, and data scarcity. It explores methods like physics-informed Gaussian processes, polynomial chaos expansions, and Bayesian neural networks for quantifying uncertainties, with a focus on Bayesian neural networks' strengths and limitations in materials modeling, data fusion, and operator learning.

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MT1

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MT1

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MT2

Numerical and Mathematical Aspects of Nonlocal Models for Fracture

See description

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MT2

Numerical and Mathematical Aspects of Nonlocal Models for Fracture

See description

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PP1

Advances Toward Parameter-Free Reconstruction of Grain Orientation Data

Polycrystalline materials consist of clusters of various crystal grains. Electron-backscatter diffraction (EBSD), a technique utilized in scanning electron microscopy (SEM), is employed to gather data on the orientation of these grains. This information is crucial for the quantitative analysis and comprehension of the materials' properties. However, EBSD images frequently contain numerous misorientation pixels that resemble noise, and these images may also exhibit areas where data is absent. Many algorithms that are used to reconstruct the grain orientation data need tuning of algorithm-specific parameters. This tuning of parameters is problematic since it requires a sophisticated understanding of the algorithms being used. In this talk, we present our ongoing work in making the reconstruction of the grain orientation parameter-free. We will present our work on using weighted total variation (TV) flow that uses estimation of the noise as a way to automate the stopping criteria of the weighted TV flow. We also present our latest efforts on grain reconstruction using U-nets, a convolutional neural network. We will present a statistical comparative analysis of these methods in our talk.

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PP1

Instability in Porous Elastomers and Relaxation via Domain Formation

Porous elastomers actuated pneumatically are an interesting candidate for soft active materials. Here we explore the behavior of porous elastomers under plane strain, building on previous estimates [Lopez-Pamies & Ponte Castañeda, 2004, J. Elasticity 76, 247] derived from nonlinear homogenization theory for an incompressible neo-Hookean elastomer containing aligned cylindrical voids distributed randomly and isotropically. The incremental homogenized response was found to lose strong ellipticity for certain loading conditions, corresponding to the development of an instability in its mechanical response. We investigate the relaxed response by computation of the rank-one convexification of the energy via a sequential lamination procedure [Kohn & Strang, 1986, Pure Appl. Math 39, 139], corresponding physically to the formation of lamellar domains following onset of the instability. We find the relaxed solution to give rise to soft modes of deformation, which are

of interest in active materials.

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PP1

2D Piezoelectric Metamaterial Model for Large Deflection Amplification

Metamaterials are materials engineered at the nano or micro scale with repeating unit structures designed to exhibit properties that are not available with other materials. The unit structure is carefully arranged to create unique electromagnetic, acoustic, thermal, or mechanical behaviors. Smart metamaterials or adaptive metamaterials are a special category of metamaterials that can dynamically alter their properties in real-time due to external stimuli or changes in the environment. Adaptability is achieved through incorporating active elements in the metamaterial microstructure. Smart metamaterials, while promising, have been limited in their response properties primarily due to low strain values. To overcome this restriction, a unique metamaterial has been developed that is capable of large strain outputs. The concept is numerically analyzed using a multi-physics approach that incorporates the piezoelectric expansion/contraction effect, non-linear stress/strain, and large-scale deflection modeling.

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PP1

The Saturn Ring Defect for Two Colloidal Particles

The study of nematic liquid crystals and the defects that arise due to various energy configurations has been of great interest to both mathematicians and physicists alike. In particular, it has been shown in the physics literature that there are several varieties of line defects which can be studied using a plethora of mathematical and physical models. In their 2016 paper, Alama, Bronsard & Lamy showed, using the Landau-de Gennes model for liquid crystals in a particular regime, that for a single spherical colloid immersed within such a nematic material, a ring defect is formed when the particle is sufficiently small, called the 'Saturn ring defect'. They also showed that the defect is formed at the positions where there is an exchange of the dominant eigenvalues from the Q-tensor. This tensor is the solution to the Laplace equation with Dirichlet boundary conditions on the particle. In this poster presentation, we will summarize the mathematics behind the Saturn ring defect, and we will present our extended problem analyzing the ring defect(s) that may arise for two colloidal particles. We will describe how, in this case, changing the domain to bispherical coordinates allowed us to obtain an analytic solution for the Q-tensor, and how we were able to numerically map the structure of the defects in the planar region situated exactly halfway between the colloids.

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PP1

Optimization of a Lattice Spring Model with Elastoplastic Conducting Springs: A Case Study

We consider a simple lattice spring model in which every spring is elastoplastic and is capable to conduct current. The elasticity bounds of spring i are taken as $[-c_i, c_i]$ and the resistance of spring i is taken as $1/c_i$, which allows us to compute the resistance of the system. The model is further subjected to a gradual stretching and, due to plasticity, the response force increases until a certain terminal value. We demonstrate that the recently developed sweeping process theory can be used to optimize the interplay between the terminal response force and the resistance on a physical domain of parameters c_i. The proposed methodology can be used by practitioners for the design of multi-functional materials as an alternative to topological optimization. In this way we introduce a simple conceptual model for the design of optimal multi-functional materials. We stick to a particular feasible domain of parameters c_i for which a formula for the terminal response force has been recently obtained in the literature over a sweeping process approach.

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PP1

Dft-Fe: Massively Parallel Hybrid CPU-GPU Code for Large-Scale Density Functional Theory Calculations Using Finite-Element Basis

Kohn-Sham density functional theory (DFT) calculations have been instrumental in providing many crucial insights into materials behaviour and occupy a sizable fraction of the world's computational resources today. However, the stringent accuracy requirements necessary to compute meaningful material properties, in conjunction with the asymptotic cubic-scaling computational complexity of the underlying eigenvalue problem, demand enormous computational resources for these calculations. Thus, these methods are routinely limited to high-throughput calculations with a maximum of a few thousand electrons. This poster explores recent advancements in real-space DFT calculations through DFT-FE, an open-source finite-element (FE) based DFT code designed for hybrid CPU-GPU architectures. DFT-FE employs adaptive FE discretisation that handles pseudopotential and all-electron calculations while accommodating fully periodic, semi-periodic and non-periodic boundary conditions. It integrates scalable and efficient solvers for the solution of the Kohn-Sham equations, significantly delaying the onset of cubic scaling computational complexity to large system sizes reaching up to 30,000 electrons. The poster showcases these recent HPC-centric methodological developments and capabilities in the DFT-FE code, with wide-ranging implications for tackling diverse scientific challenges involving large-scale material systems in energy storage, device materials, catalysis, and alloy design.

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PP1

Goal-Oriented Optimal Experimental Design in Linear Bayesian Inverse Problems

We consider goal-oriented optimal experimental design (gOED) in the context of Bayesian inversion. In this setting, the goal is considered as an operator on the inversion parameter. While the classical optimal experimental design (OED) problem seeks a sensor distribution, or design, that satisfies a Bayesian optimality condition on the inversion parameter, gOED produces a design that satisfies a Bayesian optimality condition on the goal. We consider the case when inverse problem is linear with a Gaussian prior, and the goal operator is a quadratic functional on the inversion parameter. With these assumptions, we derive a novel goal-oriented optimality criterion–an analytic expression for the expected variance of the goal. Minimizing this criterion over the design space results in a goal-oreinted optimal design problem. In addition to developing the theoretical framework to solve gOED problems under the stated assumptions, we outline a scalable numerical approach. We illustrate the features of the proposed approach in a model inverse problem governed by an advection-diffusion equation in a two-dimensional domain.

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PP1

An Experimentally Informed Continuum Grain Boundary Model

We present a continuum grain boundary model that incorporates experimentally determined grain boundary energy data as a function of misorientation. Unlike traditional curvature-driven models, this approach takes into account the non-convex nature of grain boundary energy, supported by experimental evidence and incorporating rotational invariance. Simple gradient descent dynamics of the energy are used for idealized microstructure evolution, which requires higher-order regularization of the energy density for the model to be well-set. Mathematically, the constructed energy functional formally is of the Aviles–Giga/Cross–Newell type but with unequal well–depths, resulting in a difference in the structural feature of solutions that can be identified with grain boundaries. The model explores 1-D and 2-D scenarios, simulating grain boundary evolution and microstructure changes. It also delves into grain boundary metastability, affirming their persistence before transitioning to more energetically favorable configurations. In 2-D simulations, the model illustrates grain rotation and the transformation of curved boundaries into straight ones, as expected in experiments. Additionally, it demonstrates grain growth from diverse initial conditions. Overall, this approach provides valuable insights into grain boundary behavior and microstructure evolution, diverging from the simplifications observed in conventional models.

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PP1

Global Sensitivity Analysis with Sparse Polynomial Chaos Classifiers for Thermal-Barrier Coating Applications

We present a novel approach for training soft-max classifiers with built-in Polynomial chaos expansions (PCE) that enhance sparsity in the PCE representation and makes them suitable for classification problems in the small-data regime. Next, we use the proposed classifier to perform variance-based global sensitivity analysis by using Monte Carlo to evaluate the first order Sobol indices. We demonstrate the performance of our proposed method on a few numerical examples, including the challenging problem of designing thermal-barrier coating experiments for Industrial Gas Turbine blade coating with desired pattern characteristics.

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