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1 Plenary Talks

1.1 Automatic Discovery of Algorithms and Neural Architectures in Scientific Machine Learning

Plenary Speaker: George Karniadakis (Brown University)

Abstract. We will first review deep neural operators, which we will use as foundation models for scientific machine learning tasks. Then, we will design two classes of ultra-fast meta-solvers for linear systems arising after discretizing PDEs by combining neural operators with either simple iterative solvers, e.g., Jacobi and Gauss-Seidel, or with Krylov methods, e.g., GMRES and BiCGStab, using the trunk basis of DeepONet as a coarse preconditioner. The idea is to leverage the spectral bias of neural networks to account for the lower part of the spectrum in the error distribution while the upper part is handled easily and inexpensively using relaxation methods or fine-scale preconditioners. We create a pareto front of optimal meta-solvers using a plurality of metrics, and we introduce a preference function to select the best solver most suitable for a specific scenario. This automation for finding optimal solvers can be extended to neural architectures for predicting time series as well as to nonlinear systems and other setups, e.g. finding the best meta-solver for space-time in time-dependent PDEs.

1.2 Mathematics of Vector-borne Diseases

Plenary Speaker: Abba Gumel (University of Maryland)

Abstract. Vector-borne diseases (VBDs), such as malaria, dengue, Lyme disease, leishmaniasis, and West Nile virus, constitute over 17% of all infectious diseases of humans, causing in excess of 1 million deaths annually (with malaria alone accounting for about 600,000 of these deaths, mostly in children under the age of five in malaria-endemic areas). These vectors are typically controlled using insecticide-based control methods, and their lifecycle (and those of the pathogens they vector) are greatly affected by changes in local climatic conditions, such as temperature, precipitation, and humidity. Although much progress has been recorded in the battle against several VBDs, particularly malaria, over the last few decades (prompting a renewed quest for malaria eradication, for instance), these efforts are unfortunately threatened by several factors, such as widespread resistance to the currently-available insecticides used in vector control, evolution of drug resistance, changes in local climatic conditions (which affect all aspects of the lifecycle stages of the vectors), land-use changes, emergence of invasive species, human mobility (rural-urban migration), and quality of public health infrastructure and care. I will discuss some of these advances and challenges associated with the mathematical modeling and analysis of the transmission dynamics of VBDs, using malaria and possibly Lyme disease as case studies. One of the key questions to address is whether or not anthropogenic climate change will lead to a range expansion or a shift of the vectors to new areas. Furthermore, the potential effectiveness of alternative biocontrol/genetic approaches (such as sterile insect technique) on controlling the population abundance of the disease vectors will be discussed.

1.3 Asymptotic Robustness of DG Schemes for the Convection Diffusion Equation

Plenary Speaker: Noel Walkington (Carnegie Mellon University)

Abstract. Numerical schemes for problems involving both transport and diffusion often frequently fail when the diffusion coefficient is small and the convective velocity is non-smooth. In this talk, we show that schemes using discontinuous Galerkin (DG) approximations of the elliptic (diffusion) term and classical upwinding for the convective term exhibit asymptotic robustness; that is, solutions converge strongly in $L^2(\Omega)$ independently of how the diffusion constant and mesh parameters tend to zero. The major technical difficulty involves identifying the trace (boundary values) of weakly convergent approximations. This is done using Boyer's (2005) extension of the DiPerna Lions theory for transport equations.

1.4 Finite Element versus Finite Neuron Methods

Plenary Speaker: Jinchao Xu (King Abdullah University of Science and Technology, Pennsylvania State University)

Abstract. An interesting consequence is that a piecewise linear finite element space, when defined in terms of ReLU neural networks, avoids the curse of dimensionality for sufficiently smooth functions, whereas the classical linear finite element space still suffers from it. We further introduces a bit-centric perspective, showing that parameter count alone is not a reliable measure of model complexity or approximability. Collectively, these results bridge finite element analysis and deep learning theory, offering new mathematical insights into scientific machine learning.

2 Minisymposium

2.1 Theory, Computation, and Applications for Nonlocal Models

MS Abstract. This minisymposium brings together researchers that work on advancing the state of the art of nonlocal modeling and simulation. Nonlocal models provide a new framework to overcome limitations and challenges present in classical PDE-based models. For instance, peridynamics, a nonlocal extension of classical continuum mechanics, admits discontinuous solutions and naturally describes material failure and damage. Similarly, nonlocal and fractional diffusion models can represent anomalous diffusion and heat transfer. Furthermore, nonlocal models introduce length scales, which can be used for multiscale modeling. Recent years have witnessed a tremendous advance in modeling, mathematical analysis, and computational practice for nonlocal problems. This minisymposium will highlight recent developments in peridynamics, nonlocal and fractional diffusion, and related areas, with a focus on new mathematical insights, numerical methods, and emerging applications.

- **Interacting particle dynamics for sampling in high dimensions**

Speaker: Dejan Slepcev (Carnegie Mellon University)

Co-authors: Elias Hess-Childs (Carnegie Mellon University), Lantian Xu (Carnegie Mellon University)

Abstract. Motivated by the task of sampling measures in high dimensions we introduce a new geometry on the space of measures called Radon-Wasserstein geometry and show that gradient flows of Kullback-Leibler divergence with respect to the Radon-Wasserstein geometry can be approximated well by interacting particles in high dimensions. We will discuss the properties of the mean-field flow and its convergence towards the desired measure. We will also show that the flow of the interacting particle system can be computed accurately and efficiently in high dimensions using a slicing technique.

- **Compactness Results for a Nonlocal Dirichlet Energy and some applications**

Speaker: Tadele Mengesha (University of Tennessee)

Abstract. In this talk I will present a compactness result for function spaces with finite Dirichlet energy of half-space nonlocal gradients. 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. We use the compactness result to study the nonlocal heterogeneous anisotropic diffusion problems as well as a nonlocal optimal control problem. This is based on a joint work with Z. Han and X. Tian.

- **Recent advances on asymptotically compatible schemes for nonlocal models**

Speaker: Xiaochuan Tian (University of California, San Diego)

Abstract. Asymptotically compatible schemes are a cornerstone of numerical methods for nonlocal models with finite-range nonlocal interactions. These schemes provide robust discretizations that are insensitive to the modeling parameters in nonlocal models, thereby avoiding inaccurate numerical solutions caused by inappropriate choices of model or discretization parameters. This talk highlights recent advances in asymptotically compatible schemes, including their application to nonlinear nonlocal problems and nonlocal models with heterogeneous localization.

- **Nonlocal models with local boundary conditions in semi-supervised learning**

Speaker: James M. Scott (Auburn University)

Abstract. We state and analyze nonlocal problems with classically-defined, local boundary conditions. The model takes its horizon parameter to be spatially dependent, vanishing near the boundary of the domain. We establish a Green's identity for the nonlocal operator that recovers the classical boundary integral, which permits the use of variational techniques. Using this, we show the existence of weak solutions, as well as their variational convergence to weighted classical counterparts as the bulk horizon parameter uniformly converges to zero. In certain circumstances, global regularity of solutions can be established, resulting in improved modes and rates of variational convergence. We conclude by discussing applications of these results to convergence in Laplacian learning and graphon-based variational problems.

- **Data-Driven Particle Dynamics: A Structure-Preserving Method for Emergent Behavior in Nonequilibrium Systems**

Speaker: Max Win (University of Pennsylvania)

Co-authors: Quercus Hernandez (University of Pennsylvania, Emmi AI), Thomas O'Connor (Carnegie Mellon University), Paulo Arratia (University of Pennsylvania), Nathaniel Trask (University of Pennsylvania)

Abstract. When coarse-graining a dynamical system, nonlocality, dissipation, and stochastic fluctuations naturally emerge. These emergent properties possess strict geometric and thermodynamic constraints: coarse-grained dynamics must satisfy a first/second law of thermodynamics, and work done by fluctuations must balance dissipation in a discrete fluctuation-dissipation theorem. We present a data-driven framework in which metriplectic brackets may be inferred from observations of particle positions and velocities, providing a meshfree nonlocal models guaranteed to preserve these structural properties by construction. We demonstrate the model by learning coarse-grained dynamics of polymer melts and from experimental observations of colloidal systems. The framework is open-source and we provide code to evaluate extracted models at exascale using LAMMPS.

- **Emergent Nonlocal Effects in Metamaterials**

Speaker: Kaushik Dayal (Carnegie Mellon University)

Abstract. (empty)

- **Nonlocal Models for Traffic Flow**

Speaker: Wen Shen (Pennsylvania State University)

Abstract. Classic traffic flow models in PDE is typically a nonlinear scalar conservation law. Adding certain details on the drivers behavior, the flux function becomes a nonlocal term which includes an integral term over space and possibly time. We present several models of this type, and present some main results and challenges.

- **Seamless multiphysics coupling with peridynamics enabled by nodal finite element approximation**

Speaker: Prashant K. Jha (South Dakota School of Mines and Technology)

Abstract. This presentation discusses ongoing research in the seamless coupling of physics, such as diffusion of chemical components (corrosion) and temperature, with the peridynamics theory of fracture. This is achieved by a recently proposed and published nodal finite element approximation (NFEM) of peridynamics (Jha, Diehl, Lipton (2025) CMAME). NFEM provides a finite element representation of the deformation of structures at a computational cost comparable to mesh-free methods. Corrosion and heat distribution based on partial differential equations usually employ finite element approximation. Thus, the coupling is easily introduced by combining NFEM for peridynamics and FEM for other physics. After discussing formulation and numerical methods, some preliminary results will be presented, including cracking of two-dimensional structures in corrosive fields and under inhomogeneous temperature distribution.

- **Nonlinear Fractional Modeling of Viscoelasticity in Biotissues**

Speaker: Ziwei Yang (Lehigh University)

Co-authors: Jihong Wang (Lehigh University), Maedeh Makki (University of California, Riverside), Chung-Hao Lee (University of California, Riverside), Yanzhi Zhang (Missouri University of Science and Technology), Yue Yu (Lehigh University)

Abstract. Biotissue is a heterogeneous material which presents complex biomechanical properties. Typically, its memory effect is captured by viscoelastic models using integer-order differential equations, such as the generalized Kelvin model. Herein, we propose a novel viscoelastic model for biotissues by incorporating fractional-order derivatives into a nonlinear generalized kelvin (NGK) model, so as to capture their nonlinear and viscoelastic responses. Based on this model, a learning framework is developed to obtain optimal parameters from uniaxial mechanical testing experimental data under force-controlled and displacement-controlled conditions. The proposed model was tested on two representative biotissues, and its performances were compared against the integer-order differential equation models. We found that the fractional model not only achieves a more effective prediction of the nonlinear viscoelastic behavior, but also generalizes better in downstream predictions. To further investigate the influence of the fractional order and other internal parameters on the model-predicted response, we perform additional sensitivity analysis and parameter studies with respect to different loading conditions and tissue statues. Our results suggest that the fractional model offers a powerful alternative to capture the transient dynamics of viscoelastic materials, possibly because of their inherent long-tail memory.

- **Monotone Nonlocal Neural Operator for Material Modeling with Conditionally Unique Solutions**

Speaker: Yue Yu (Lehigh University)

Co-authors: Jihong Wang (Lehigh University), Xiaochuan Tian (University of California, San Diego), Zhongqiang Zhang (Worcester Polytechnic Institute), Stewart Silling (Sandia National Laboratories), Siavash Jafarzadeh (Lehigh University)

Abstract. Data-driven methods have emerged as powerful tools for modeling the responses of complex nonlinear materials directly from experimental measurements. Among these methods, the data-driven constitutive models present advantages in physical interpretability and generalizability across different boundary conditions/domain settings. However, the well-posedness of these learned models is generally not guaranteed a priori, which makes the models prone to non-physical solutions in downstream simulation tasks.

In this study, we introduce monotone peridynamic neural operator (MPNO), a novel data-driven non-local constitutive model learning approach based on neural operators. Our approach learns a nonlocal kernel together with a nonlinear constitutive relation, while ensuring solution uniqueness through a monotone gradient network. This architectural constraint on gradient induces convexity of the learnt energy density function, thereby guaranteeing solution uniqueness of MPNO in small deformation

regimes. To validate our approach, we evaluate MPNO’s performance on both synthetic and real-world datasets. On synthetic datasets with manufactured kernel and constitutive relation, we show that the learnt model converges to the ground-truth as the measurement grid size decreases both theoretically and numerically. Additionally, our MPNO exhibits superior generalization capabilities than the conventional neural networks: it yields smaller displacement solution errors in down-stream tasks with new and unseen loadings. Finally, we showcase the practical utility of our approach through applications in learning a homogenized model from molecular dynamics data, highlighting its expressivity and robustness in real-world scenarios.

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2.2 Advances in the Mathematics of Infectious Diseases

MS Abstract. Mathematical models play a vital role in providing insight and understanding of the transmission dynamics and control of emerging and re-emerging infectious diseases of major public health significance. These models, which are typically calibrated and validated using real-data, are often used to inform effective public health strategies and policies for combating the spread of diseases in populations. This minisymposium brings together interdisciplinary researchers, employing diverse modeling frameworks, to highlight recent advances and challenges in the mathematical modeling of infectious diseases and assessment of the effectiveness of public health interventions, with particular emphasis on the complex interplay between associated biological, behavioral, and environmental factors. Some of the specific topics to be discussed include the modeling and dynamics of vector-borne diseases subject to fluctuations in ecological and environmental conditions, the role of human behavior in shaping epidemic outcomes, the combined effects of vaccination and screening strategies on the spread of human papillomavirus and related cancers, novel biological and ecological methods to control vectors of major vector-borne diseases, and the role of age-stratified vaccination on the spread and control of malaria.

- **Exploring the Feedback Loop Between Behavior and Public Health**

Speaker: Alice Oveson (University System of Maryland)

Co-authors: Abba Gumel (University of Maryland)

Abstract. The interplay between individual behavior and infectious disease dynamics creates feedback loops that shape epidemic trajectories in ways classical models cannot capture. In this talk, I present two modeling frameworks that highlight these dynamics: a measles vaccination model with explicit child-adult structure, and a COVID-19 transmission model stratified by race and age with empirically grounded contact matrices. The measles model examines how vaccination uptake, exemptions, and heterogeneous mixing sustain pockets of susceptibility despite high statewide coverage. The COVID-19 model investigates how behavioral heterogeneity—driven by differential risk acceptance and demographic contact patterns—modulates reproduction numbers and disease burden across groups. Together, these models demonstrate how feedback between population behavior and public health interventions can produce counterintuitive outcomes, including persistence of outbreaks in highly vaccinated populations and disproportionate impacts across demographic groups. I conclude by discussing implications for designing more effective and equitable public health strategies.

- **Leveraging inter-species competition to improve the effectiveness of the sterile insect technique**

Speaker: Alex Safsten (University of Maryland)

Co-authors: Abba Gumel (University of Maryland)

Abstract. Mosquitos top the list of the deadliest animals in the world due to the diseases they carry and transmit to humans, including malaria, West Nile virus, and dengue, with malaria being the most important vector-borne disease of mankind. Existing methods of mosquito control heavily rely on using

chemical insecticides to kill them. Unfortunately, however, in the context of malaria for instance, the heavy and widespread use of these insecticides in endemic areas has resulted in widespread resistance to all the chemical compounds currently used in vector control. This necessitates the use of alternative methods for vector control. The sterile insect technique (SIT), which entails the periodic mass release of sterilized male mosquitoes into an environment where adult female mosquitoes are abundant, is one of the main promising approaches being proposed. The eggs laid by females that mated with sterile male mosquitoes will not hatch, thereby potentially reducing the population of the wild mosquitoes in the environment. I will present an ODE model of SIT and several strategies eliminating disease-carrying mosquitoes including using optimal and feedback control for adjusting the rate of release of sterile males as the wild population is reduced and leveraging interspecies competition from less-harmful species. I will also present a PDE model of SIT which demonstrates the spatio-temporal dynamics of SIT and allows for the development of strategies for, e.g., inducing counter invasions of non-disease-carrying mosquitoes that have recently been pushed out of their historical ranges by their disease-carrying cousins.

- **Mathematical assessment of the role of temperature variability on Lyme disease dynamics in Maryland**

Speaker: Salihu Musa (University of Maryland)

Co-authors: Abba Gumel (University of Maryland)

Abstract. Lyme disease, transmitted by ticks, is the most important vector-borne disease in the United States and in Europe. It is endemic in many regions of the United States, particularly the Northeast (costing an estimated average of up to \$1.4 billion annually in direct medical costs in the United States). This talk is based on using a mathematical model for gaining insight into the impact of climate change, which strongly affects the life cycle of ticks and the reservoir host (rodents and other small mammals), on the geospatial dynamics of Lyme disease in the reservoir and incidental (human) host populations within the state of Maryland. The model is simulated using relevant climate and Lyme disease data to determine the optimal temperature range within which ticks activity and Lyme disease intensity are maximized in Maryland, informing when control efforts (against ticks and the reservoir host) should be intensified. Furthermore, the key question on whether or not climate change will lead to a range expansion of ticks and Lyme disease, or shift to new areas, in Maryland will be addressed, under current and projected mean monthly temperature. The effectiveness of various control strategies will be discussed.

- **Mathematical assessment of the roles of vaccination and Pap screening on the incidence of HPV and related cancers in the Republic of Korea**

Speaker: Soyoung Park (University of Maryland)

Co-authors: Hyunah Lim (University of Maryland), Abba Gumel (University of Maryland)

Abstract. Human Papillomavirus (HPV) is a major sexually-transmitted infection that causes various cancers and genital warts in humans. In addition to accounting for about 99% of cervical cancer cases, it significantly contributes to anal, penile, vaginal, and head and neck cancers. Although HPV is vaccine-preventable (and highly efficacious vaccines exist for preventing infection with some of the most oncogenic HPV subtypes in the targeted population), the disease continues to cause major public health burden globally (largely due to inequity in access to the main control resources (i.e., access to Pap smear and vaccination) and low vaccination coverage in most communities that implement routine HPV vaccination).

This lecture is based on the use of a new mathematical model (for the natural history of HPV, together with the associated neoplasia) for assessing the combined population-level impacts of Pap cytology screening and vaccination against the spread of HPV. The model, which takes the form of a deterministic system of nonlinear differential equations, will be calibrated and validated using HPV-related cancer data from South Korea. Theoretical and numerical simulation results will be presented. Conditions for achieving vaccine-derived herd-immunity threshold (for achieving HPV elimination in Korea) will be derived.

- **Mathematical modeling of the impact of age-targeted and dose-structured vaccination on malaria dynamics**

Speaker: Arnaja Mitra (University of Maryland)

Co-authors: Abba Gumel (University of Maryland)

Abstract. Malaria, a parasitic disease spread to humans via an effective bite by an infectious adult female *Anopheles* mosquito, continues to exude a major burden in endemic areas (causing in excess of 600,000 deaths annually, mostly in children under the age of five). Much progress was made over the last two or three decades in the fight against malaria, largely due to the heavy and large-scale use of chemical insecticides (particularly in the form of long-lasting insecticidal nets and indoor residual spraying) to kill the malaria mosquito, promoting a renewed quest for malaria eradication. Unfortunately, such heavy use has also resulted in widespread *Anopheles* resistance to all the main chemical insecticides used in vector control, posing challenges to the eradication objective. New anti-malaria vaccines have been approved recently, and are being deployed in a number of countries in sub-Saharan Africa. In this talk, I will present a new mathematical model, in the form of a system of delayed-differential equations, for assessing the population-level impact of one of the approved vaccines in curtailing the disease burden in the targeted (vaccinated) population.

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2.3 Recent Mathematical and Computational Modeling Advances in Life Sciences

MS Abstract. Mathematical and computational modeling have become indispensable tools for exploring the complexity of biological systems, offering quantitative insights that complement experimental and clinical studies. Recent years have witnessed significant advances in modeling frameworks, analytical techniques, and data-driven approaches tailored to address emerging challenges in the life sciences. This minisymposium will showcase recent developments in mathematical analysis, numerical simulation, and scientific computing, with applications ranging from neuroscience and infectious diseases to cancer dynamics, cardiovascular modeling, and systems biology. Featured topics will include multiscale modeling and the integration of data-driven techniques with mechanistic models. By bringing together researchers from mathematics, computational science, and biology, the sessions aim to foster interdisciplinary collaboration and highlight new directions at the intersection of theory, computation, and biomedical applications.

- **Modeling and nonlinear simulation of solid tumor growth**

Speaker: Shuwang Li (Illinois Institute of Technology)

Abstract. In this talk, we develop a computational model for simulating the nonlinear dynamics of a tumor-host interface within the sharp interface framework. We are interested in solid tumor growth with chemotaxis and cell-to-cell adhesion, together with the effect of the tumor microenvironment by the variability in spatial diffusion gradients, the uptake rate of nutrients inside/outside the tumor. We model the heterogeneous distribution of vasculature using complex far-field geometries. We solve the nutrient field and the Stokes/Darcy flow field using a spectrally accurate boundary integral method. Numerical results highlight the complexity of the problem, e.g. development of spreading branching-patterns and encapsulated morphologies in a long period of time.

- **Synchronized Optimal Transport**

Speaker: Yanxiang Zhao (George Washington University)

Abstract. Optimal transport has been an essential tool for reconstructing dynamics from complex data. With the increasingly available multifaceted data, a system can often be characterized across multiple spaces. Therefore, it is crucial to maintain coherence in the dynamics across these diverse

spaces. To address this challenge, we introduce Synchronized Optimal Transport (SyncOT), a novel approach to jointly model dynamics that represent the same system through multiple spaces. With given correspondence between the spaces, SyncOT minimizes the aggregated cost of the dynamics induced across all considered spaces. The problem is discretized into a finite-dimensional convex problem using a staggered grid. Primal-dual algorithm-based approaches are then developed to solve the discretized problem. Various numerical experiments demonstrate the capabilities and properties of SyncOT and validate the effectiveness of the proposed algorithms.

- **Evaluate the role of impulsive intervention on some network models**

Speaker: Yanyu Xiao (University of Cincinnati)

Abstract. We examined the transmission dynamics of certain preventable infectious diseases using a network-based model with impulsive control strategies. We derived a threshold value, established the global stability of the disease-free periodic solution, and demonstrated the persistence of the disease.

- **Convergence of the Regularised Immersed Boundary Method**

Speaker: Alexandre Milewski (Courant Institute of Mathematical Sciences)

Co-authors: Charles Peskin (Courant Institute of Mathematical Sciences)

Abstract. Developed in 1972, the immersed boundary method has since been used as a means to simulate fluid-membrane interactions. However, whilst the numerical convergence of such a method has been empirically verified, it is theoretically unproven due to the singular forcing terms present in the governing equations. In this talk, I introduce a variant of the immersed boundary method that deals with co-dimension 2 surfaces in a Navier-Stokes fluid (the co-dimension being defined as the dimension of the fluid minus the dimension of the boundary) and demonstrate that it is numerically convergent in theory as well as in practice.

- **Data-Driven Modeling of Amyloid-beta Targeted Antibodies for Alzheimer’s Disease**

Speaker: Kobra Rabiei (Pennsylvania State University)

Abstract. Alzheimer’s disease (AD) is characterized by the accumulation of amyloid beta, which is strongly associated with disease progression and cognitive decline. Despite the approval of monoclonal antibodies targeting A-beta, optimizing treatment strategies while minimizing side effects remains a challenge. This study develops a mathematical framework to model A-beta aggregation dynamics, capturing the transition from monomers to higher-order aggregates, including protofibrils, toxic oligomers, and fibrils, using mass-action kinetics and coarse-grained modeling. Parameter estimation, sensitivity analysis, and data-driven calibration ensure model robustness. An optimal control framework is introduced to identify the optimal dose of the drug as a control function that reduces toxic oligomers and fibrils while minimizing adverse effects, such as amyloid-related imaging abnormalities (ARIA). The results indicate that Donanemab achieves the most significant reduction in fibrils. These findings provide a quantitative basis for optimizing AD treatments, providing valuable insight into the balance between therapeutic efficacy and safety

- **Virtual Cohorts for Within-Host Cholera and Immune Dynamics**

Speaker: Harsh Jain (University of Minnesota, Duluth)

Abstract. Cholera remains a critical global health concern, particularly in regions with compromised water and sanitation infrastructure. Existing population-level models capture epidemic trends but fail to account for how malnutrition and other stressors impair immune function, potentially exacerbating disease severity. In this talk, we present an ordinary differential equation (ODE) system model of Cholera’s within-host pathogen – immune system dynamics, incorporating key variables such as bacterial load in the gut and epithelium – factors not easily measured in clinical settings, as well as bacterial loads in stool – factors that can be measured with fecal samples. By leveraging available

clinical and laboratory data, we construct “virtual patients” to explore the interplay between immune health and infection risk at an individual level. This approach lays the groundwork for coupling detailed within-host simulations with person-to-person transmission models, ultimately enabling more accurate forecasts of epidemic trajectories under varying immune conditions.

- **Modeling treatment of osteoarthritis with standard therapy and senolytic drugs**

Speaker: Nourridine Sieue (Rochester Institute of Technology)

Co-authors: Avner Friedman (The Ohio State University)

Abstract. Osteoarthritis (OA), the most common form of joint disease, involves the progressive degradation of articular cartilage and is a major cause of chronic disability in aging populations. Since OA is associated with severe deficiency of collagen type II, clinical trials considered treatment of OA by injection with undenatured collagen type II (UC-II). Recent studies consider also injection of senolytic drugs, like fisetin, that eliminates senescent chondrocytes in aging patients, to reduce the negative effect of these senescent cells on cartilage structure. In this paper we develop a mathematical model of OA for men and, separately, for women, and use the model to assess the efficacy of treatment by UC-II and by fisetin, alone or in combination. Our computations show the benefits of starting treatment early. They also show that although the effect of treatment by fisetin on slowing the progression of OA is much smaller compared to UC-II treatment, its effect in combination with UC-II is significantly increased.

- **Toward Governing Equations for Agent-Based SIR Models: Calibrating Time-Varying Transmission**

Speaker: Erick Anderson (University of Minnesota, Duluth)

Abstract. Agent-based epidemic models (ABMs) capture heterogeneity and test targeted interventions, but they are difficult to calibrate from incidence data alone, especially when transmission varies over time. We propose a governing-equation pathway that links aggregate dynamics and individual-level simulations. Starting from a well-mixed SIR system, we introduce an evolution law for the transmission rate (β)—such as logistic dependence on prevalence or a fitted ODE $\dot{\beta} = f(\beta, p)$ —and calibrate parameters to the classic British boys’ boarding-school influenza dataset. Fitting minimizes error in daily incidence while enforcing a terminal susceptible constraint, producing a dynamic $\beta(t)$ that reflects changes in effective transmission.

This calibrated $\beta(t)$ is then mapped into a discrete time-step ABM by replacing β with explicit contacts and transmission probabilities. The result is an ABM that reproduces epidemic size and peak timing without hand-tuned rules, while also revealing the micro-mechanisms that realize aggregate dynamics. Beyond matching incidence curves, the ABM framework enables exploration of interventions (e.g., co-horting, isolation, schedule changes) and generates heterogeneity and distributional outcomes invisible in the ODE model. I will compare against constant- β baselines, discuss identifiability and uncertainty, and demonstrate how the learned β function generalizes to out-of-sample simulations.

- **A Systematic Computational Framework for Practical Identifiability Analysis**

Speaker: Shun Wang (Pennsylvania State University)

Abstract. Practical identifiability is a fundamental challenge in the data-driven modeling of biological systems, as many model parameters cannot be directly measured and must be estimated from experimental data. I introduce a novel mathematical framework for practical identifiability analysis in dynamic models. Starting from a rigorous mathematical definition, it is proved that practical identifiability is equivalent to the invertibility of the Fisher Information Matrix (FIM). The relationship between practical identifiability and coordinate identifiability is further established, introducing an efficient metric that simplifies and accelerates identifiability assessment compared to traditional profile likelihood methods. To address non-identifiable parameters, new regularization terms are incorporated, enabling uncertainty quantification and improving model reliability. To support experimental design,

an optimal data collection algorithm that ensures all model parameters are practically identifiable is proposed. Applications to Hill functions, neural networks, and biological models demonstrate the effectiveness and computational efficiency of the proposed framework in uncovering critical biological processes and identifying key observable variables.

- **Who’s In and Who’s Out: Leveraging Homogeneous Preclinical Data to Extrapolate Tumor Growth Outcomes Across Heterogeneous Populations**

Speaker: Chloe George (University of Minnesota, Duluth)

Co-authors: Harsh Jain (University of Minnesota, Duluth), Brygida Boryczka (Marquette University), Nam Phung (University of Minnesota, Duluth), Ava Peterson (University of Minnesota, Duluth)

Abstract. High failure rates in preclinical and clinical studies remain a major obstacle in anti-cancer drug development. A key factor is the lack of heterogeneity in preclinical models, which typically use genetically identical mice or monoclonal cell lines that fail to reflect real-world variability. Additionally, preclinical data are often aggregated, obscuring important individual-level insights. Here, we introduce a computational framework specifically designed to address these challenges. Using a lung cancer xenograft experiment reporting averaged tumor-volume and Kaplan-Meier survival data as a case study, we reconstruct virtual clones via Bayesian inference, grounded in a minimal modeling framework that uses established ordinary differential equations to simulate tumor growth. A key innovation is the explicit mechanistic linkage between tumor dynamics and individual survival probabilities. The reconstructed clones show excellent agreement with experimental data. We then apply Standing Variations Modeling to generate heterogeneous virtual cohorts not included in the original study. These cohorts accurately recapitulate independent xenograft experiments not used in model calibration, thereby validating our approach. By capturing realistic variability at the preclinical stage, our method offers a practical framework to improve drug development pipelines, reduce costly experimental iterations, and identify rare subpopulations most and least likely to benefit from treatment.

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2.4 Recent Advances of Innovative Numerical Methods for Nonlinear PDEs

MS Abstract. The session aims to highlight recent advances in numerical methods and computational strategies for nonlinear and complex PDE systems, such as those involving evolving geometries, multiscale behavior, and structure-preserving challenges. Topics of interest include recent advances in computational methods designed for these systems, such as model order reduction, structure-preserving methods, adaptive methods, data-driven approaches, and efficient and stable strategies. By bringing together researchers from a broad range of application areas, this forum aims to foster the exchange of ideas and promote collaboration.

- **A Locally Conservative Proximal Galerkin Method for Pointwise Bound Constraints**

Speaker: Guosheng Fu (University of Notre Dame)

Abstract. We introduce the first-order system proximal Galerkin (FOSPG) method, a locally mass-conserving, hybridizable finite element method for solving heterogeneous anisotropic diffusion and obstacle problems. Like other proximal Galerkin methods, FOSPG finds solutions by solving a recursive sequence of smooth, discretized, nonlinear subproblems. We establish the well-posedness and convergence of these nonlinear subproblems. Further, we show stability and error estimates under low regularity assumptions for the linearized equations obtained by solving each subproblem using Newton’s method. The FOSPG method exhibits several advantages, including high-order accuracy, discrete maximum principle or bound-preserving discrete solutions, and local mass conservation. It also achieves prescribed solution accuracy within asymptotically mesh-independent numbers of subproblems and linear solves per subproblem iteration. Numerical experiments on benchmarks for anisotropic diffusion and obstacle problems confirm these attributes.

- **Inverse radiative transfer via goal-oriented adaptive mesh refinement**

Speaker: Shukai Du (Syracuse University)

Co-authors: Samuel Stechmann (University of Wisconsin)

Abstract. The inverse problem in radiative transfer has important applications, including optical tomography and remote sensing, but its numerical solution is still challenging due to the high dimensionality of the radiative transfer equation and the costly iterative solvers required for the inverse problem.

To address these challenges, we propose a goal-oriented hp-adaptive mesh refinement method that naturally integrates the coefficient optimization for the inversion and the mesh adaptivity for error control. By exploiting the link between duality-based mesh refinement and adjoint-based inversion, we introduce a goal-oriented error estimator that can effectively guide adaptive refinement for the inverse problem while remaining inexpensive to compute.

Both the forward and adjoint problems are discretized with discontinuous Galerkin spectral element methods, which provide a convenient framework for mesh adaptivity. Numerical experiments show that this approach accelerates convergence and reduces memory usage, demonstrating its efficiency for solving inverse radiative transfer problems.

- **Simulation of Cascade Gating in Ion Selectivity and Current Regulation**

Speaker: Pei Liu (Florida Institute of Technology)

Abstract. Ion selectivity and current regulation are central to both biological signaling and modern ionic devices. During transport across a hydrophobic region, ions undergo successive stages of hydration, dehydration, and rehydration. We introduce a continuum framework for this cascade-gated transport, combining the Poisson–Nernst–Planck equations for spatial migration with mass-action kinetics for hydration transitions. To capture the separation of time scales between fast hydration reactions and slower ionic flux, we apply time-dependent matching of boundary layers and fast–slow dynamics. High-resolution numerical simulations resolve the coupled dynamics and their voltage dependence. Our results show that the dominant current carrier can switch between ion species under varying applied voltages, demonstrating how cascade gating governs current regulation in both biological and engineered nanopores.

- **Dynamically Regularized Lagrange Multiplier Method for the Incompressible Navier–Stokes Equations: Stability and Convergence**

Speaker: Cao-Kha Doan (Auburn University)

Co-authors: Thi-Thao-Phuong Huang (Auburn University), Lili Ju (University of South Carolina), Rihui Lan (Ocean University of China)

Abstract. We present efficient numerical schemes based on the Lagrange multiplier approach for the Navier–Stokes equations. By introducing a dynamic equation (involving the kinetic energy, the Lagrange multiplier, and a regularization parameter), we form a new system that incorporates the energy evolution process while remaining equivalent to the original equations. Such nonlinear system is then discretized in time using backward differentiation formulas, resulting in a dynamically regularized Lagrange multiplier (DRLM) method. First- and second-order DRLM schemes are derived and shown to be unconditionally energy stable with respect to the original variables. Optimal error estimates for the velocity and pressure of the first-order DRLM scheme are established through a uniform bound on the Lagrange multiplier and mathematical induction. Numerical experiments demonstrate the accuracy, stability, and robustness of the proposed schemes.

- **Energetic Variational Neural Network Discretizations of gradient flows**

Speaker: Yiwei Wang (University of California, Riverside)

Co-authors: Ziqing Hu (University of Notre Dame), Chun Liu (Illinois Institute of Technology), Zhi-liang Xu (University of Notre Dame)

Abstract. Many problems in physics, materials science, biology, and machine learning can be formulated as gradient flows. We introduce structure-preserving algorithms for solving such systems: an Eulerian scheme for L2-gradient flows and a Lagrangian scheme for generalized diffusions, i.e., Wasserstein-type gradient flows. Both approaches employ neural networks for spatial discretization. The Lagrangian scheme offers a computationally efficient realization of the celebrated Jordan–Kinderlehrer–Otto (JKO) variational framework. Unlike conventional numerical methods that rely on discretizing the strong or weak forms of the governing PDEs, our algorithms are constructed directly from the energy-dissipation principle. This guarantees the monotonic decay of the system’s energy, preventing unphysical solution behaviors and ensuring long-term numerical stability. To address challenges posed by the nonlinear nature of neural-network-based discretization, we adopt a temporal-then-spatial discretization strategy specifically designed for variational systems. The resulting schemes are mesh-free and scalable, making them well-suited for solving high-dimensional gradient flows.

- **An Efficient, Decoupled, and Linearly Stabilized Scheme for Phase-Field Models with Variable Mobility**

Speaker: Zhiwei Zhang (Illinois Institute of Technology)

Co-authors: Shuwang Li (Illinois Institute of Technology), Steven M. Wise (University of Tennessee)

Abstract. Phase-field models for multiphysics problems, such as vesicle deformation under osmotic pressure, often result in complex, coupled nonlinear PDEs. A key computational challenge arises in systems with variable mobility, which can preclude the use of the most efficient, high-order implicit schemes that rely on constant-coefficient operators. To address this challenge, we develop and analyze a novel numerical scheme based on the Multiple Scalar Auxiliary Variable (MSAV) method. Our approach introduces a linear stabilization term outside of the chemical potential. This strategy successfully decouples the system into a sequence of linear, constant-coefficient elliptic equations at each time step, which can be solved with high efficiency using fast direct solvers. We present a rigorous numerical verification of the scheme’s second-order accuracy in time and an analysis of its spatial convergence properties. Numerical experiments demonstrate that the proposed scheme is more robust than a baseline nonlinear multigrid (NLMG) solver, remaining stable for significantly larger time steps.

- **Analysis and Computation of a Generalized Ohta-Kawasaki Model**

Speaker: Yanxiang Zhao (George Washington University)

Abstract. In this talk, we present a generalized nonlocal Ohta-Kawasaki model to investigate the nonlocal effects on pattern formation in binary systems with general long-range interactions. In the 1D case, the generalized model exhibits bubble patterns similar to those of the standard Ohta-Kawasaki model. However, through Fourier analysis, we find that the optimal number of bubbles in the generalized model may have an upper bound, regardless of the repulsive strength. This upper bound is determined by the eigenvalues of the nonlocal kernels. To explore the nonlocal effects in the 2D Ohta-Kawasaki model, we develop asymptotically compatible numerical schemes. Furthermore, our numerical studies are extended to disk and spherical domains, uncovering new patterns.

- **Stability and Time-Step Constraints of Exponential Time Differencing Runge–Kutta Discontinuous Galerkin Methods for Advection-Diffusion Equations**

Speaker: Ziyao Xu (Binghamton University)

Abstract. In this paper, we investigate the stability and time-step constraints for solving advection-diffusion equations using exponential time differencing (ETD) Runge-Kutta (RK) methods in time and discontinuous Galerkin (DG) methods in space. We demonstrate that the resulting fully discrete scheme is stable when the time-step size is upper bounded by a constant. More specifically, when central fluxes

are used for the advection term, the schemes are stable under the time-step constraint $\tau \leq \tau_0 d/a^2$, while when upwind fluxes are used, the schemes are stable if $\tau \leq \max\{\tau_0 d/a^2, c_0 h/a\}$. Here, τ is the time-step size, h is the spatial mesh size, and a and d are constants for the advection and diffusion coefficients, respectively. The constant c_0 is the CFL constant for the explicit RK method for the purely advection equation, and τ_0 is a constant that depends on the order of the ETD-RK method. These stability conditions are consistent with those of the implicit-explicit RKDG method. The time-step constraints are rigorously proved for the lowest-order case and are validated through Fourier analysis for higher-order cases. Notably, the constant τ_0 in the fully discrete ETD-RKDG schemes appears to be determined by the stability condition of their semi-discrete (continuous in space, discrete in time) ETD-RK counterparts and is insensitive to the polynomial degree and the specific choice of the DG method. Numerical examples, including problems with nonlinear convection in one and two dimensions, are provided to validate our findings.

- **Efficient optimization-based invariant-domain-preserving limiter for high-order discontinuous Galerkin methods of solving compressible Euler equations**

Speaker: Chen Liu (University of Arkansas)

Co-authors: Xiangxiong Zhang (Purdue University)

Abstract. Research on fluid dynamic simulations has been very active and of interest to both mathematicians and engineers. The PDEs raised in modeling compressible flow, such as the compressible Euler equations are fundamental in gas dynamics with various applications in numerous important areas. Advanced optimization techniques provide powerful tools for finding minimizers when processing large datasets. The flexibility of discontinuous Galerkin (DG) method allows postprocessing numerical solutions by incorporating conservation and invariant domain as constraints. For postprocessing to enforce invariant domains defined by bounds or positivity without affecting conservation and accuracy, a few minimization formulations can be considered. We combine DG and large-scale non-smooth optimization to construct high-order limiters. Our optimization method is efficient and can be further extended to other types of PDEs. Challenging benchmark tests are shown.

- **Structure-preserving reduced order models for thermodynamically consistent reversible-irreversible PDEs**

Speaker: Zengyan Zhang (Pennsylvania State University)

Co-authors: Jia Zhao (University of Alabama)

Abstract. As a powerful data-driven approach for dimensionality reduction, the proper orthogonal decomposition reduced-order model (POD-ROM) has been widely used as a computationally efficient surrogate model for complex, large-scale systems. Given the computational complexity of thermodynamically consistent models, the POD-ROM plays an important role in reducing spatial-temporal complexity. However, the classical POD-ROM can compromise the thermodynamic structure in the reduced-order modeling of these systems. In this talk, we will introduce a numerical platform that systematically derives ROMs for thermodynamically consistent PDEs while preserving their inherent thermodynamic principles and demonstrate its effectiveness through several numerical examples.

- **Recent progress in the analysis of the Poisson-Nernst-Planck system**

Speaker: Rolf Ryham (Fordham University)

Abstract. The Poisson-Nernst-Planck system consists of a coupled system of parabolic and elliptic equations describing the diffusion and electromigration of charges and their electrical potential. While well-posedness and long-term behavior for two-dimensional, bounded domains is well understood, there are significant difficulties in three and higher dimensions where weak solutions are merely found to be locally weakly differentiable. The system, however, enjoys a so-called very weak formulation where, for example, local boundedness follows from minimal assumptions of a weak solution.

- **An integral equation method and an asymptotic analysis approach for erosion in porous media**

Speaker: Szu-Pei Fu (Farmingdale State College)

Co-authors: Pejman Sanaei (Georgia State University)

Abstract. In nature, erosion caused by water or air flow is one of the most prevalent geological and mechanical processes. This phenomenon occurs at the fluid-solid interface when the total shear stress induced by the flow exceeds specific critical threshold that depends on the properties of the solid material. This research project focuses on the mathematical modeling and simulation of erosion process in a porous medium characterized by axisymmetric channels. We employ an integral equation method, which enables efficient and accurate analysis of the erosion process within the porous medium. We present a detailed comparison between the numerical solutions from our model and the reduced mathematical model using asymptotic analysis developed by Kahza and Sanaei [Phys. Rev. Fluids, 9(2024)], providing insights into erosion patterns and validating the proposed approach.

- **Solver-in-the-Loop joint operator learning: fractional Laplace-Beltrami features for interface reconstruction**

Speaker: Shuhao Cao (University of Missouri)

Abstract. In this work, we propose a joint operator learning method for reconstructing images of conductivity coefficients from boundary data. Inspired by the idea of employing partial differential equation (PDE) solvers as preconditioners for this inverse problem, we investigate a “solver-in-the-loop” training mechanism. It allows the interaction of learnable parameters integrated in a PDE solver module and those in neural networks for reconstructing images. Specifically, we employ a fractional Laplace-Beltrami operator with a learnable fractional order, which transforms boundary data into high-dimensional features. These features then serve as input to a neural network, significantly improving reconstruction accuracy.

- **Surface Navier-Stokes Without Inf-Sup Condition**

Speaker: Mansur Shakipov (University of Maryland)

Co-authors: Ricardo Nochetto (University of Maryland)

Abstract. For a sufficiently regular surface without boundary, we show that the surface Navier-Stokes problem can be discretized without the need for the discrete inf-sup condition in a consistent manner. More precisely, by using a nontrivial geometric identity, we reformulate the Navier-Stokes problem as a system of two semilinear problems governed by two Laplacians (one for the velocity and the other one for the pressure). Since the pressure appears explicitly in the second equation of the new system, its discretization no longer requires the validity of a discrete inf-sup condition. We provide numerical experiments confirming that the method is practical.

- **A general framework to derive linear, decoupled and energy-stable schemes for reversible-irreversible thermodynamically consistent models**

Speaker: Jia Zhao (University of Alabama)

Abstract. In this talk, I will present a general numerical platform for designing accurate, efficient, and stable numerical algorithms for incompressible hydrodynamic models that obey thermodynamical laws. The obtained numerical schemes are automatically linear in time. It decouples the hydrodynamic variable and other state variables such that only small-size linear problems need to be solved at each time marching step.

2.5 Computational Thermodynamics: Energy and Energy Landscape

MS Abstract. Thermodynamics is the science concerning the states of a system—whether stable, metastable, or unstable—when interacting with its surroundings. It applies to any systems for which boundary conditions with the surroundings can be defined. Historically, thermodynamics has been studied across distinct domains, each with its own principles: equilibrium thermodynamics, non-equilibrium thermodynamics, quantum mechanics, and statistical mechanics. Despite their differences, these domains are unified by their treatment of energy in relation to boundary conditions. The energy landscape, shaped by internal and external variables, governs the evolution of a system under specific conditions and along specific directions—be they temporal, spatial, configurational, or compositional. This mini symposium invites contributions that explore hypotheses, theories, computation, and artificial intelligence aimed at conjecturing, estimating, predicting, and modeling energy and energy landscapes across diverse systems of interest.

- **Entropy as Information: A unified, trajectory-driven route**

Speaker: Qijun Hong (Arizona State University)

Abstract. Entropy is central to thermodynamics and information theory, yet it remains difficult to evaluate in materials. Conventional workflows partition contributions (configurational, vibrational, electronic, magnetic) with heavy system-dependent machinery and conceptual ambiguity. I will present a single-trajectory, first-principles framework that treats thermodynamic entropy as information carried by atomic motion and structure, delivering accurate results across defect-free solids, mechanically unstable phases, and liquids. The approach combines two complementary ideas. First, we enforce a clean partition between configurational and vibrational entropy by (i) computing S_{conf} as the information entropy of nearest-neighbor environments and (ii) extracting S_{vib} from phonon densities of states obtained via velocity-autocorrelation—explicitly satisfying inclusion (no missing states) and no-double-counting criteria. Second, we introduce a parameter-free, system-agnostic lossy compression of ab initio molecular-dynamics trajectories whose compressed description length equals the thermodynamic entropy, thereby operationalizing the equivalence of Gibbs’ and Shannon’s entropies in this setting.

- **Configurational entropy in solid and liquid silicon**

Speaker: Talid Sinno (University of Pennsylvania)

Co-authors: Jinping Luo (Xian Jiaotong University), Lijun Liu (Xian Jiaotong University), Jack douglas (NIST)

Abstract. Configurational entropy is an important quantity in establishing many properties of a material, such as melting behavior [1], glass dynamics [2], and defect thermodynamics [3]. It is also useful as a scalar metric of the potential energy landscape, and therefore as a target for force field optimization. In this talk, we present an analysis of configurational entropy in both crystalline and liquid silicon as represented by several different empirical interatomic potentials.

In the crystal phase, we focus on the impact of configurational entropy on the formation thermodynamics of intrinsic point defects, i.e., self-interstitials and vacancies, and their clusters. The formation of intrinsic point defects is critical in the silicon crystal growth process, significantly affecting the quality of silicon crystals and, consequently, the performance of semiconductor devices and solar cells. We first describe an efficient computational approach for isolating configurational and vibrational formation entropies for point defects using thermodynamic integration [4, 5]. Using this approach, we demonstrate the role of configurational entropy in setting point defect equilibrium and transport behavior. We find that the configurational entropy associated with point defects increases significantly upon crystal heating, consistent with the hypothesized existence of extended defects [3]. We also perform a detailed comparative analysis across predictions from various potential models.

Next, we consider the temperature dependence of the configurational entropy in the liquid phase. We find that the behavior predicted across the various interatomic potentials falls into two classes—those with high configurational entropy and those with low configurational entropy. We establish a connection

to experimental measurements via crystallization dynamics, which suggest that the low entropy models may be better representations of reality. We also discuss other proxy quantities for the computationally expensive configurational entropy measure, which could be useful for optimization of empirical force fields.

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- **Zentropy**

Speaker: Zi-Kui Liu (Pennsylvania State University)

Abstract. Entropy is a key concept in thermodynamics, and entropy production of an internal process is foundational to kinetics. Thus, the accurate prediction of entropy as a function of internal variables for stable, metastable, and unstable states is necessary for stability and evolution of any systems. Over the last two decades, we developed a multiscale entropy approach (recently termed as zentropy theory) that integrates DFT-based quantum mechanics and Gibbs statistical mechanics with the total energy of individual configurations replaced by their respective free energies. Zentropy theory has demonstrated its capability to predict entropy and Helmholtz energy for stable, metastable, and unstable states, thus Helmholtz energy landscape, of magnetic materials with strongly correlated physics and liquid phases, including negative thermal expansion in Fe₃Pt and melting temperature in elements and compounds. Its limitations and potential applications will be discussed.

- **Energy Landscapes of Electron Hopping in Conductive Polymers: From Single-Chain Dynamics to Device Functionality**

Speaker: Ziyun Miao (Johns Hopkins University)

Co-authors: Tine Curk (Johns Hopkins University)

Abstract. Conductive polymers provide a versatile platform for neuromorphic and adaptive electronic devices. In this work, we use molecular dynamics simulations to investigate how the energy landscape of electron hopping reactions governs the emergent response of single-chain polymer systems. Our approach builds on a custom electron-hopping model, where the hopping barrier is represented by an anisotropic harmonic potential, enabling us to directly connect conformational fluctuations with direction-dependent charge transfer. From the simulations, we extract energy barriers, charge localization patterns, and structural reorganizations, and show how these features map onto an energy landscape representation that captures the stability and accessibility of charge states. This perspective naturally explains why and how our single-chain systems can exhibit qualitatively different device behaviors—acting as a diode, memristor, or transistor—depending on their conformational and energetic organization. By linking simulation-derived hopping energetics with macroscopic device functions, our results demonstrate how energy landscape concepts can be leveraged to design polymer-based electronic materials for neuromorphic engineering.

- **ZENN: A Thermodynamics-Inspired Computational Framework for Heterogeneous Data-Driven Modeling**

Speaker: Shun Wang (Pennsylvania State University)

Abstract. The increasing availability of complex, heterogeneous datasets poses significant challenges for traditional data-driven methods, which often assume data homogeneity and fail to account for internal disparities. Quantifying entropy and its evolution in such settings remains a fundamental problem in digital twins and data science. While traditional entropy-based approaches provide useful approximations, they are limited in handling multi-source, dynamically evolving systems. To address these challenges, I introduce a zentropy-enhanced neural network (ZENN)—a novel framework that extends zentropy theory from quantum and statistical mechanics to data science by assigning intrinsic entropy to each dataset. ZENN simultaneously learns both Helmholtz energy and intrinsic entropy, enabling robust generalization, accurate high-order derivative prediction, and adaptability to heterogeneous, real-world data.

- **Melting of planetary materials determined by machine learning potentials**

Speaker: Jie Deng (Princeton University)

Abstract. Understanding the melting relations of planetary materials is essential for modeling magma oceans, core formation, and long-term planetary evolution. Here, we demonstrate that machine learning potentials (MLPs), trained on density functional theory data, can accurately determine melting phase relations of silicates and oxides under extreme conditions. We employ an iterative learning scheme that integrates enhanced sampling, feature selection, and deep neural networks, enabling efficient and reliable potential development. Using MgSiO_3 and SiO_2 as case studies, we show that large-scale two-phase coexistence simulations with MLPs can robustly resolve melting curves and solid–solid boundaries. We further discuss the impact of exchange–correlation functionals on predicted melting behavior.

- **Designing selective cell targeting with multivalent interactions**

Speaker: Tine Curk (Johns Hopkins University)

Abstract. Multivalent binding consists of multiple simultaneous, but discrete interactions. For example, a nanoparticle decorated with multiple ligands binding to a cell membrane that contains multiple receptors. The (free) energy landscape of such multivalent interaction can be manipulated by tuning individual ligand-receptor bond strengths. I will show that properly designed landscape enables selective targeting of cells depending on the specific profile of membrane receptors, thus enabling selective targeting of arbitrary cell types. I will discuss how statistical mechanics provides general design rules for selective cell targeting. At the end, I will also discuss kinetics of binding and show that maximal selectivity is achieved when the system is out of equilibrium.

- **Zentropy and the Recursive Property of Entropy for the Calculation of Free Energy Landscapes**

Speaker: Luke Myers (Pennsylvania State University)

Co-authors: Nigel Hew (Pennsylvania State University), Shun-Li Shang (Pennsylvania State University), Zi-Kui Liu (Pennsylvania State University)

Abstract. The recursive property of entropy and the chain rule are well-established facts. They are used prominently in the mathematical field of information theory and in the physical field of quantum information theory. However, the chain rule and the recursive property of entropy are rarely used in the field of thermodynamics despite this being the field where the concept of entropy originated. The zentropy method realized the importance of the chain rule in the context of thermodynamics, but previous works treated the chain rule as a physical assumption and did not show its derivation from the definition of entropy. This work shows that the equation for entropy used in the zentropy method is a restatement of the recursion property of entropy, which is a hierarchical form of the chain rule. This work further connects the chain rule of entropy in thermodynamics with Shannon entropy of information theory, and von Neumann entropy of quantum mechanics. Finally, we give examples for the motivation of using the chain rule in the field of thermodynamics.

- **Thermoelasticity and the free energy landscape of H-bond disorder and symmetrization: atomistic simulations of δ -AlOOH at high pressure**

Speaker: Chenxing Luo (Columbia University, Princeton University)

Co-authors: Renata Wentzcovitch (Columbia University)

Abstract. The thermoelastic constants of a material, as second-order derivatives of its free energy, are sensitive probes of complex free energy landscape across phase transitions. The high-pressure hydrous mineral δ -AlOOH provides a compelling case study, exhibiting significant elastic anomalies driven by a complex H-bond disorder and symmetrization. While static ab initio models fail to fully capture this behavior, atomistic simulations with a deep neural network potential succeeded. This approach accurately maps the potential energy surface, demonstrating that thermal motion is essential for navigating the high-pressure, high-temperature thermodynamic landscape. Our results show that the evolution of the free energy landscape not only leads to the onset of H-bond disorder and symmetrization but also serves as the source of the anomalous stiffening observed in the compression curve and thermoelastic tensor. This demonstrates that advanced atomistic simulations provide the crucial link necessary to address the atomistic mechanism that governs experimentally observed phenomena.

- **Ab-initio CALPHAD modeling of NaNH₂BH₃ for solid-state H₂ storage applications**

Speaker: Ricardo Amaral (Pennsylvania State University)

Co-authors: Zi-Kui Liu (Pennsylvania State University)

Abstract. Sodium amidoborane (NaAB) represents a promising solid-state hydrogen storage material, yet fundamental questions about its stability and decomposition mechanisms remain unresolved. This study employs density functional theory and CALPHAD modeling to investigate the thermodynamic properties and decomposition pathways of NaAB and its intermediate, Na₂AB. Our comprehensive analysis reveals that, contrary to previous assumptions regarding dihydrogen bond stabilization, NaAB exists only in a metastable state at room temperature. The compound follows a stepwise decomposition pathway, transitioning to Na₂AB at 89.3° with initial hydrogen release (3.81 wt%), followed by gradual, irreversible decomposition to NaH and BN at temperatures up to 310°. This behavior is governed by the kinetic hindrance of BN formation, which explains the extended hydrogen evolution observed experimentally. Thermodynamic calculations demonstrate that NaH formation is favorable only alongside BN, while gas-phase analysis confirms that borazine and ammonia emissions stem from synthesis impurities rather than intrinsic decomposition. By elucidating these fundamental relationships, this work reconciles conflicting interpretations and provides practical insights for the development of advanced solid-state hydrogen storage materials.

- **Accelerating Energy Solutions with High-Entropy Materials: Leveraging Disorder, Computation, and AI**

Speaker: Corey Oses (Johns Hopkins University)

Abstract. High-entropy materials, complex solids stabilized by configurational disorder, are unlocking new frontiers in energy technology with promising applications spanning clean hydrogen production, waste-heat conversion, energy storage, and nuclear waste immobilization. The Entropy for Energy (S4E) laboratory integrates high-throughput first-principles computation, machine learning, and data-driven design to explore and optimize high-entropy oxides, halides, and alloys. This talk will highlight how harnessing chemical complexity, guided by advanced computational and AI tools within the Materials Genome Initiative framework, accelerates the discovery and development of next-generation energy materials. Join us to learn how these synergistic approaches are streamlining innovation cycles and expanding the landscape of materials for a sustainable energy future.

- **Thermodynamics of Mg₂SiO₄ under extreme pressures: Implications for super-Earths' interiors**

Speaker: Donghao Zheng (Princeton University)

Co-authors: Jie Deng (Princeton University)

Abstract. Understanding the mineralogy of exoplanets is essential for unraveling their interior structures, dynamics and evolution. For large super-Earths, the post-post spinel Mg_2SiO_4 , one of the major mantle phases, undergo the order-disorder transition (ODT) at high temperatures. However, the ODT phase boundary of Mg_2SiO_4 has not been rigorously constrained. Additionally, fundamental thermodynamic properties and melting behavior of the disordered Mg_2SiO_4 remain poorly investigated. Here, we develop a unified machine learning potential (MLP) for solid Mg_2SiO_4 of ab initio accuracy under super-Earth mantle conditions. With the efficient MLP, we extensively calculate the free energy of solid post-post spinel Mg_2SiO_4 via the thermodynamic integration method. The results are used to constrain the ODT phase boundary. Furthermore, we report the P-V-T equation of state and Grüneisen parameters for post-post spinel Mg_2SiO_4 across various degrees of disorder. For liquid Mg_2SiO_4 , we perform ab initio free energy calculation by thermodynamic integration and determine the melting curve of post-post spinel Mg_2SiO_4 . These thermodynamic properties are further applied to update the adiabatic thermal profiles, the mass-radius relation, and viscosity profile of super-Earths.

- **Ferroelastic Hysteresis and Shear-Modulus Softening in CaSiO_3 Perovskite**

Speaker: Tianqi Wan (Lamont-Doherty Earth Observatory)

Co-authors: Chenxing Luo (Princeton University), Zhen Zhang (Iowa State University), Yang Sun (Xiamen University), Renata Wentzcovitch (Lamont-Doherty Earth Observatory)

Abstract. The high likelihood of a tetragonal-cubic phase transition in CaSiO_3 perovskite (CaPv) within both average MORB and cold slab assemblages underscores the significance of this transition in understanding the mineralogy of the mantle and subducting oceanic crust. However, experimental limitations have left insufficient data near the transition to fully resolve velocity changes. In this study, we develop machine-learning interatomic potentials for CaPv , enabling large-scale molecular dynamics (MD) simulations across a broad range of pressure-temperature (P-T) conditions. Using thermodynamic integration, we determine the cubic-tetragonal phase boundary from Gibbs free energy. Our research further examines the compressional behavior and elastic moduli of CaPv across the transition, highlighting the remarkable accuracy of our machine-learning interatomic potentials in predicting equations of state and elastic properties. Importantly, we present the first direct evidence of pronounced ferroelastic hysteresis, along with clear shear-modulus softening across the tetragonal $\leftrightarrow$ cubic transition. These findings represent a major advance in understanding Earth's interior processes and provide a robust framework for future investigations.

- **PyZentropy: Implementing recursive entropy for first-principles thermodynamics in Python**

Speaker: Nigel Hew (Pennsylvania State University)

Co-authors: Luke Myers (Pennsylvania State University), Shun-Li Shang (Pennsylvania State University), Zi-Kui Liu (Pennsylvania State University)

Abstract. Most first-principles methods, such as density functional theory (DFT), typically neglect intra-configurational entropy and consider only inter-configurational contributions when evaluating the total entropy. However, it is well known that each configuration inherently possesses intra-configurational entropy arising from vibrational and electronic degrees of freedom, which can significantly influence finite-temperature properties. To address this limitation, we apply the zentropy method, which extends recursive-entropy concepts from information theory to configurations encountered in DFT calculations. This approach enables more accurate predictions of emergent finite-temperature phenomena, including negative thermal expansion and pressure-temperature or volume-temperature phase diagrams. An open-source Python package, PyZentropy, is being developed to implement this method, and its capabilities are demonstrated through a case study on Fe_3Pt .

2.6 Partial Differential Equations: Theory and Computations

MS Abstract. Partial differential equations (PDEs) are fundamental in describing a wide range of physical, biological, and engineering phenomena. The development of mathematical theory for PDEs continues to advance our understanding of existence, uniqueness, and regularity of solutions, while computational methods are essential for simulating complex systems and tackling large-scale problems. This minisymposium will bring together researchers working on both theoretical and computational aspects of PDEs. Topics will include advances in the analysis of PDEs, the design of efficient numerical methods, and the development of robust algorithms for challenging applications. By combining perspectives from theory and computation, the sessions aim to foster new collaborations and highlight emerging directions in PDE research.

- **Operator Splitting Method for Gradient Flows of Harmonic Maps**

Speaker: Lucas Bouck (Carnegie Mellon University)

Abstract. We study the approximation of gradient flows of harmonic maps, which serve as model problems for applications in micromagnetics, liquid crystals, and nonlinear plate bending. Harmonic maps are vector fields that are critical points of the Dirichlet energy subject to the constraint that the vector field be unit length pointwise. In the literature, most time stepping schemes for gradient flows deal with the constraint by linearizing the unit length constraint every step, which involves solving for the solution increment in the tangent space of the constraint. These schemes lead to robust control over the violation of the constraint, but require solving saddle point systems at every step that may be difficult to precondition. In this talk, we propose a scheme that first computes the unconstrained increment and then projects this increment pointwise onto the tangent space. With an additional stabilization, this scheme is energy stable under mild CFL conditions and provides robust control of the unit length constraint violation. The scheme then comes with the advantage of having to solve symmetric positive definite systems at every step, which can be preconditioned easily. This work is joint work with S. Bartels and C. Palus (Freiburg).

- **Spline-Based Solution Transfer with Potential Applications for Space-Time Methods**

Logan Larose (Pennsylvania State University)

Co-authors: David M. Williams (Pennsylvania State University)

Abstract. This presentation will demonstrate the effectiveness of the Worsey-Farin spline space for interpolation, i.e. solution transfer, between 3-dimensional tetrahedral meshes. The proposed transfer process is especially relevant for slab-based space-time finite element methods. We will show that this transfer method satisfies the following requirements: (i) it maintains high-order accuracy up to 4th order, (ii) it preserves a discrete maximum principle, (iii) it asymptotically enforces mass conservation, and (iv) it constructs a smooth, continuous surrogate solution between space-time slabs. While existing methods meet the first three requirements, the fourth requirement is crucial for enabling visualization and boundary condition enforcement for finite element space-time applications. We will present results of numerical experiments which highlight the conservative nature and order of accuracy of the transfer process, and we will present a qualitative evaluation of the visualization properties of the smoothed solution. Additionally, we provide explicit and comprehensive implementation details for this spline space—which have been lacking since its inception.

- **Error estimates for the interpolation and approximation of gradients and vector fields on protected Delaunay meshes in R^d**

Speaker: David Williams (Pennsylvania State University)

Co-authors: Mathijs Wintraecken (Université Côte d’Azur)

Abstract. One frequently needs to interpolate or approximate gradients on simplicial meshes. Unfortunately, there are very few explicit mathematical results governing the interpolation or approximation

of vector-valued functions on Delaunay meshes in more than two dimensions. Most of the existing results are tailored towards interpolation with piecewise linear polynomials. In contrast, interpolation with piecewise high-order polynomials is not well understood. In particular, the results in this area are sometimes difficult to immediately interpret, or to specialize to the Delaunay setting. In order to address this issue, we derive explicit error estimates for high-order, piecewise polynomial gradient interpolation and approximation on protected Delaunay meshes. In addition, we generalize our analysis beyond gradients, and obtain error estimates for sufficiently-smooth vector fields. Throughout the presentation, we show that the quality of interpolation and approximation often depends (in part) on the minimum thickness of simplices in the mesh. Fortunately, the minimum thickness can be precisely controlled on protected Delaunay meshes in R^d .

- **Fully discrete error analysis of finite element discretizations of time-dependent Stokes equations in a stream-function formulation**

Speaker: Dmitriy Leykekhman (Technical University of Munich)

Co-authors: Boris Vexler (Technical University of Munich), Jacob Wagner (Technical University of Munich)

Abstract. In this talk we present best approximation type a priori error estimates for the fully discrete Galerkin solutions of time-dependent Stokes problem using the stream-function formulation. We use discontinuous Galerkin method of arbitrary degree for the time discretization, whereas we discuss the space discretization in general framework. This makes our result applicable, for example for conformal C1 and for C0 interior penalty methods. The results do not require any additional regularity assumptions beyond the natural regularity given by the domain and data and applicable for example for optimal control problems.

- **L^p -based theory for PDEs on closed manifolds of minimal regularity: A novel and elementary approach**

Speaker: Gonzalo Benavides (University of Maryland)

Co-authors: Ricardo Nochetto (University of Maryland), Mansur Shakipov (University of Maryland)

Abstract. In what sense a PDE is well-posed and what regularity properties it enjoys” is one of the most fundamental questions in the theory of differential equations. In this talk we are concerned with a family of PDEs posed on closed manifolds that are prototypical constituents of a great variety of physical phenomena in thin films. Our approach is elementary and (to a large extent) self-contained that hinges strongly on functional analysis and calculus on manifolds, and thus it circumvents the use of potential theory and Calderón–Zygmund-type estimates on manifolds. Unlike what is typically assumed in differential geometry, our manifolds are not necessarily C^∞ , but we rather specify the minimal regularity for the results to hold. We finish this talk by applying some of our results to the tangent Navier–Stokes and to a novel hydrodynamical model of nematic liquid crystals on surfaces.

- **Surface Stokes Without Inf-Sup Condition**

Speaker: Mansur Shakipov (University of Maryland)

Co-authors: Ricardo Nochetto (University of Maryland)

Abstract. For a d -dimensional hypersurface of class C^3 without boundary, we reformulate the surface Stokes equations as a nonsymmetric indefinite elliptic problem governed by two Laplacians. We then use this elliptic reformulation as a basis for a numerical method based on lifted parametric FEM. Assuming no geometric error for simplicity, we prove its well-posedness, quasi-best approximation in a robust mesh-dependent H^1 -norm for any polynomial degree, as well as an optimal L^2 error estimate for both velocity and pressure. This entails a sufficiently small mesh size that solely depends on the Weingarten map and circumvents the usual discrete inf-sup condition. We present numerical experiments for velocity-pressure pairs with equal and disparate polynomial degrees, demonstrating that the proposed method is both accurate and practical.

- **A priori error analysis of the proximal Galerkin method for variational problems with inequality constraints**

Speaker: Masri Rami (Brown University)

Abstract. The proximal Galerkin (PG) method is a finite element method for solving variational problems with inequality constraints. It has several advantages, including constraint-preserving approximations and mesh independence. This paper presents the first abstract a priori error analysis of PG methods, providing a general framework to establish convergence and error estimates. As applications of the framework, we demonstrate optimal convergence rates for both the obstacle and Signorini problems using various finite element subspaces.

- **Finite element approximation to linear, second order, parabolic equations with L^1 data**

Speaker: Abner Salgado (University of Tennessee)

Abstract. We consider the approximation to the solution of the heat equation with right hand side and initial condition merely in L^1 . Due to the low integrability of the data, to guarantee well-posedness, we must understand solutions in the renormalized sense. We prove that, under an inverse CFL condition, the solution of the standard implicit Euler scheme with mass lumping converges, in $L^\infty(0, T; L^1(\Omega))$ and $L^q(0, T; W_0^{1,q}(\Omega))$, ($q < d + 2/(d + 1)$) to the renormalized solution of the problem.

- **Quasi-neutral limit and the mixer layer problem of Planck-Nernst-Poisson-Navier-Stokes equations for electro-hydrodynamics**

Speaker: Shu Wang (Beijing University of Technology)

Abstract. In this talk we discuss quasi-neutral limit and the small Debye length structure stability problem of PNP-NS equations for electro-hydrodynamics. Quasi-neutrality is one basic assumption in physics such as semiconductors and plasma, which is firstly proposed by W. Van Roosbroeck in Bell System Tech. J., 1950. We prove the small debye length quasi-neutral limit of the initial-boundary value problem for PNP-NS system for physicochemical hydrodynamics with the differential diffusion coefficients for two kinds of charges and the general ill-prepared smooth initial data, and obtain the convergence rate of the approximating solution having the form of the boundary layer, the initial layer and the mixed layer to the exact solution of the system when the Debye length tends to zero, where the mixed layer functions have only the algebraic decay rates with respect to the fast variables. Thus, the rigorous quasineutrality theory of the electric-diffusion of ions in physicochemical hydrodynamics is established.

- **Continuous data assimilation by non-interpolant observables**

Speaker: Vladimir Yushutin (University of Tennessee)

Abstract. Continuous data assimilation approaches a time-dependent PDE with an unknown initial condition by utilizing temporal observations of the evolving system. Typically, the application and the analysis of this methodology rely on observations that approximate the solution in space through an interpolation operator. In this talk, we demonstrate that continuous data assimilation can still yield an effective finite element method even when the data are non-interpolant — for instance, when only boundary values are observed. Another prospect case involves a coupled PDE model with missing initial conditions, where observations are available for only a subset of the system's components.

- **Explicit corrector in homogenization of monotone operators and its application to non-linear dielectric elastomer composites**

Speaker: Yulia Gorb (National Science Foundation)

Co-authors: Thuyen Dang (University of Chicago), Silvia Jimenez-Bolanos (Colgate University)

Abstract. This talk presents recent results on the rigorous periodic homogenization of a weakly coupled electroelastic system, combining a nonlinear electrostatic equation with an elastic equation augmented by electrostriction. Such couplings model the behavior of dielectric elastomers - deformable materials that respond to electric fields. It will be shown that the effective behavior of the composite is governed by a homogenized system of nonlinear PDEs, weakly coupled, whose coefficients depend explicitly on the microstructural geometry, periodicity, and material properties of the original heterogeneous medium. The approach developed for this nonlinear setting yields an explicit corrector result for the homogenization of monotone operators under minimal regularity assumptions.

- **Unified spatiotemporal formulations for time-dependent convection-diffusion problems**

Speaker: Seulip Lee (Tufts University)

Co-authors: James Adler (Tufts University), Xiaozhe Hu (Tufts University)

Abstract. In this talk, we introduce unified spatiotemporal formulations with physics-preserving structure for time-dependent convection-diffusion problems. By treating time as an additional space-like coordinate, the original unsteady problem is recast into a stationary one, enabling the use of well-established tools such as monotone numerical schemes, adaptive strategies, and high-performance linear solvers. Extending this spatiotemporal framework to $H(\text{curl})$ and $H(\text{div})$ convection-diffusion problems raises fundamental challenges, including the definition of four-dimensional curl operators and the extension of spatial vector fields to four-dimensional counterparts. We address these issues through the language of exterior calculus, reformulating the Hodge Laplacian and writing the $H(\text{grad})$, $H(\text{curl})$, and $H(\text{div})$ convection-diffusion equations within a single unified framework. Notably, the resulting spatiotemporal equation naturally incorporates essential physical constraints, such as Gauss's law for magnetism, providing a structure-preserving foundation for applications in magnetohydrodynamics.

- **Reduced Krylov Basis Methods for Parametric Partial Differential Equations**

Speaker: Cheng Zuo (Pennsylvania State University)

Co-authors: Yuwen Li (Zhejiang University), Ludmil Zikatanov (Pennsylvania State University)

Abstract. We present a user-friendly reduced basis method for solving families of parametric partial differential equations. The proposed methods use a preconditioned Krylov subspace method for a high-fidelity discretization of one parameter instance to generate orthogonal basis vectors of the reduced basis subspace. Large-scale discrete parameter-dependent problems are then approximately solved in this low-dimensional Krylov subspace. We prove convergence estimates for the proposed method when the differential operator depends on two parameter coefficients and the preconditioner is chosen as the inverse of the operator at a fixed parameter. Numerical experiments demonstrate that only a small number of Krylov subspace iterations are required to simultaneously generate approximate solutions for a family of high-fidelity and large-scale parametrized systems in the reduced basis subspace.

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2.7 Quantifying and Controlling Uncertainty in Complex Systems

MS Abstract. Uncertainty is an intrinsic feature of complex systems that span various disciplines, such as climate science, engineering, finance, epidemiology, and beyond. These uncertainties may arise due to numerous factors and often manifest in high-dimensional stochastic inputs and quantities of interest. Accurately quantifying uncertainty and designing robust control strategies are essential for making informed decisions and ensuring system reliability. This minisymposium brings together researchers developing mathematical, statistical, and computational frameworks to address uncertainty in complex systems. Topics include uncertainty quantification, stochastic modeling, rare event analysis, optimization under uncertainty, data assimilation, and control of stochastic systems. We also welcome contributions that explore the integration of machine learning with uncertainty-aware modeling, as well as applications in diverse domains. By bridging theory and application, this minisymposium aims to highlight cutting-edge approaches and foster

interdisciplinary collaborations.

- **A Scalable and Extensible Importance Sampling Based Framework for Safety-critical Systems Evaluation**

Speaker: Kostas G. Papakonstantinou (Pennsylvania State University)

Co-authors: Elsayed Eshra (Pennsylvania State University)

Abstract. Accurate and efficient rare event simulation and probability estimation are essential for risk-informed decision-making in safety-critical systems, often relying on computationally expensive models. We present a scalable and extensible sampling framework based on a novel two-stage importance sampling estimator. An unnormalized, flexible sampling target is first constructed, in a general fashion for all cases, intrinsically concentrating probability mass on the domain of interest, while relaxing the optimal yet intractable importance sampling density. This enables effective sampling using diverse MCMC methods, with excellent performance demonstrated by our gradient-based Quasi-Newton mass preconditioned Hamiltonian MCMC (QNp-HMCMC) and gradient-free guided preconditioned Crank-Nicolson (pCN) samplers. The normalizing constant of the approximate target is then estimated using crude density estimators based on the MCMC samples. Neural density estimators can further boost performance, particularly our Score Aligned Neural Density Estimator (SANDE). SANDE aligns the score field of the learned density with that of the unnormalized target, enabling accurate and scalable density estimation, while maintaining competitive computational cost. The proposed framework is validated on challenging test functions and applications of complex engineered systems involving several hundred random variables. Results demonstrate substantial advantages over state-of-the-art methods, particularly in high-dimensional, non-Gaussian, strongly nonlinear, and multimodal settings.

- **Computing Rare Bifurcations in Dynamical Systems**

Speaker: Anirudh Subramanyam (Pennsylvania State University)

Co-authors: Tongtong Jin (University of Southern California), Daniel Maldonado (Argonne National Laboratory)

Abstract. Bifurcations that occur only under extreme fluctuations, such as saddle-node losses of stability, govern the tail risks of many engineered and natural networks. This talk presents an optimization-based framework, grounded in large deviation theory, for efficiently estimating the probabilities of such rare bifurcations and identifying the most likely perturbations that trigger them. Rather than relying on Monte Carlo sampling, we cast rare-event probability estimation as an optimization over uncertain parameters, using a smooth stability metric (i.e., the smallest singular value of the Jacobian) and its gradients. This delivers asymptotically accurate probability estimates and yields interpretable worst-case patterns that illuminate mechanisms of failure. We illustrate the approach on voltage-collapse bifurcations in electric power grids, where it accelerates risk quantification by orders of magnitude while pinpointing vulnerable loading configurations; the methodology is broadly applicable to high-dimensional dynamical systems with parametric uncertainty.

- **Reduced-order moment closure models for uncertainty quantification of multiscale complex systems**

Speaker: Di Qi (Purdue University)

Co-authors: Jian-Guo Liu (Duke University)

Abstract. We present a new strategy for the statistical forecasts of multiscale nonlinear systems involving non-Gaussian probability distributions. The capability of using reduced-order data assimilation models to capture key statistical features is investigated. A closed stochastic-statistical modeling framework is proposed using a high-order statistical closure enabling accurate prediction of leading-order statistical moments and probability density functions of multiscale states. A new ensemble forecast

algorithm is built to efficiently resolve the nonlinear coupling mechanism as a characteristic feature in high-dimensional turbulent systems. Effective nonlinear ensemble filters are then constructed based on the explicit coupling structures in the coupled stochastic and statistical equations, which satisfy an infinite-dimensional Kalman-Bucy filter with conditional Gaussian dynamics. It is demonstrated that crucial principal statistical quantities in the most important large scales can be captured efficiently with accuracy using the new reduced-order model in various dynamical regimes with distinct statistical structures.

- **Conformalized Decision Risk Assessment**

Speaker: Woody Zhu (Carnegie Mellon University)

Abstract. High-stakes decisions in domains such as healthcare, energy, and public policy are often made by human experts using domain knowledge and heuristics, yet are increasingly supported by predictive and optimization-based tools. A dominant approach in operations research is the predict-then-optimize paradigm, where a predictive model estimates uncertain inputs, and an optimization model recommends a decision. However, this approach often lacks interpretability and can fail under distributional uncertainty – particularly when the outcome distribution is multi-modal or complex – leading to brittle or misleading decisions. In this paper, we introduce CREDO, a novel framework that quantifies, for any candidate decision, a distribution-free upper bound on the probability that the decision is suboptimal. By combining inverse optimization geometry with conformal prediction and generative modeling, CREDO produces risk certificates that are both statistically rigorous and practically interpretable. This framework enables human decision-makers to audit and validate their own decisions under uncertainty, bridging the gap between algorithmic tools and real-world judgment.

- **A Class of Interpretable and Decomposable Multi-period Convex Risk Measures**

Speaker: Luhao Zhang (Johns Hopkins University)

Abstract. Multi-period risk measures evaluate the risk of a stochastic process by assigning it a scalar value. A desirable property of these measures is dynamic decomposition, which allows the risk evaluation to be expressed as a dynamic program. However, many widely used risk measures, such as Conditional Value-at-Risk, do not possess this property. In this work, we introduce a novel class of multi-period convex risk measures that do admit dynamic decomposition.

Our proposed risk measure evaluates the worst-case expectation of a random outcome across all possible stochastic processes, penalized by their deviations from a nominal process in terms of both the likelihood ratio and the outcome. We show that this risk measure can be reformulated as a dynamic program, where, at each time period, it assesses the worst-case expectation of future costs, adjusting by reweighting and relocating the conditional nominal distribution. This recursive structure enables more efficient computation and clearer interpretation of risk over multiple periods.

- **How to build a consistency model: Learning flow maps via self-distillation**

Speaker: Boffi Nicholas (Carnegie Mellon University)

Abstract. Flow-based generative models achieve state-of-the-art sample quality, but require the expensive solution of a differential equation at inference time. Flow map models, commonly known as consistency models, encompass many recent efforts to improve inference-time efficiency by learning the *solution operator* of this differential equation. Yet despite their promise, these models lack a unified description that clearly explains how to learn them efficiently in practice. Here, building on the methodology proposed in [?], we present a systematic algorithmic framework for directly learning the flow map associated with a flow or diffusion model. By exploiting a relationship between the velocity field underlying a continuous-time flow and the instantaneous rate of change of the flow map, we show how to convert any distillation scheme into a direct training algorithm via self-distillation, eliminating the need for pre-trained teachers. We introduce three algorithmic families based on different mathematical characterizations of the flow map: Eulerian, Lagrangian, and Progressive methods, which we show encompass and extend all known distillation and direct training schemes for consistency

models. We find that the novel class of Lagrangian methods, which avoid both spatial derivatives and bootstrapping from small steps by design, achieve significantly more stable training and higher performance than more standard Eulerian and Progressive schemes. Our methodology unifies existing training schemes under a single common framework and reveals new design principles for accelerated generative modeling.

- **On Over-Parametrized Models and Sobolev Training**

Speaker: Li Matthew (University of Massachusetts Amherst)

Co-authors: Katharine Fisher (Massachusetts Institute of Technology), Timo Schorlepp (Courant Institute of Mathematical Sciences), Youssef Marzouk (Massachusetts Institute of Technology)

Abstract. With Sobolev training, neural networks are provided data about both the function of interest and its derivatives. This setting is prevalent in scientific machine learning—appearing in molecular dynamics emulators, derivative-informed neural operators, and predictors of summary statistics of chaotic dynamical systems—as well as in traditional machine learning tasks like teacher-student model distillation. However, fundamental questions remain: How does over-parameterization influence performance? What role does the signal-to-noise ratio play? And is additional derivative data always beneficial?

In this work, we study these questions using tools from statistical physics and random matrix theory. In particular, we consider Sobolev training in the proportional asymptotics regime in which the problem dimensionality d , single hidden-layer features p , and training points n grow to infinity at fixed ratios. We focus on target functions modeled as single-index models (i.e., ridge functions with a single intrinsic dimension), providing theoretical insights into the effects of derivative information in high-dimensional learning.

- **Hyperparameter optimization for Gaussian process methods**

Speaker: Nicholas Nelsen (Cornell University)

Abstract. This talk describes new techniques for tackling the central challenge of hyperparameter selection in Gaussian process (GP) methods for scientific computing. The first advance develops a bilevel optimization approach for a GP-based PDE solver. A Gauss–Newton linearization produces inexpensive closed-form updates that bypass repeated PDE solves while retaining accuracy and stability. The second advance addresses randomized algorithms such as random feature regression—a low rank GP approximation—where hyperparameters define sampling distributions but resist direct optimization. Here, a tailored random objective is combined with ensemble Kalman inversion to enable scalable and robust learning of these distributions. Uncertainty quantification arises naturally in both settings through the GP framework, which is showcased in applications ranging from inverse problems to high-dimensional learning tasks.

- **Bridging the Model Hierarchy: A Physics-Guided Machine Learning Framework for High-Resolution Climate Simulation Enhancement**

Speaker: Pouria Behnoudfar (University of Wisconsin)

Co-authors: Charlotte Moser (University of Wisconsin), Marc Bocquet (École Nationale des Ponts), Sibor Cheng (École Nationale des Ponts), Nan Chen (University of Wisconsin)

Abstract. Operational models are widely used to understand and predict natural phenomena. They are high-resolution and contain many crucial variables. Despite numerous successes, biases persist in most of these models, especially in identifying extreme events and reproducing the observed statistics in nature. However, due to the complexity of these models, it is challenging to modify them directly. On the other hand, conceptual and intermediate coupled models accurately characterize certain features of nature. Yet, they contain only a subset of variables within a specific domain and at lower resolutions. By leveraging the strengths of different models, we develop a robust physics-driven machine learning

modeling framework that bridges the model hierarchy through effective latent space data assimilation. It integrates models of varying complexities to capture their respective advantages, enabling simpler models to directly support operational models. The resulting model not only inherits the benefits of the operational models, including their high resolution and comprehensive set of variables, but also globally enhances the accuracy through local dynamical and statistical improvements provided by the simpler models. The latent space technique identifies the dominant nonlinear features of the underlying dynamics, which facilitates effective communication between models. Finally, the machine learning representation of the model significantly enhances simulation efficiency, providing massive, high-quality synthetic data that mimics natural phenomena and advances the study of extreme events with uncertainty quantification. The framework has been applied to enhance the performance of CMIP6 models in characterizing El Niño complexity by utilizing simpler yet statistically accurate models.

- **Spectral Regularized Kernel Two-Sample Tests**

Speaker: Omar Hagrass (Princeton University)

Co-authors: Bharath Sriperumbudur (Princeton University), Bing Li (Princeton University)

Abstract. Over the last decade, an approach that has gained a lot of popularity to tackle nonparametric testing problems on general (i.e., non-Euclidean) domains is based on the notion of reproducing kernel Hilbert space (RKHS) embedding of probability distributions. The main goal of our work is to understand the optimality of two-sample tests constructed based on this approach. First, we show the popular MMD (maximum mean discrepancy) two-sample test to be not optimal in terms of the separation boundary measured in Hellinger distance. Second, we propose a modification to the MMD test based on spectral regularization by taking into account the covariance information (which is not captured by the MMD test) and prove the proposed test to be minimax optimal with a smaller separation boundary than that achieved by the MMD test. Third, we propose an adaptive version of the above test which involves a data-driven strategy to choose the regularization parameter and show the adaptive test to be almost minimax optimal up to a logarithmic factor. Moreover, our results hold for the permutation variant of the test where the test threshold is chosen elegantly through the permutation of the samples. Through numerical experiments on synthetic and real data, we demonstrate the superior performance of the proposed test in comparison to the MMD test and other popular tests in the literature.

- **Large Deviation Theory-Informed Importance Sampling for Rare Event Estimation and Control**

Speaker: Shanyin Tong (University of Pennsylvania)

Abstract. Rare and extreme events like hurricanes, energy grid blackouts, dam breaks, earthquakes, and pandemics are infrequent but have severe consequences. Because estimating the probability of such events can inform strategies that mitigate their effects, scientists must develop methods to study the distribution tail of these occurrences. However, calculating small probabilities is hard, particularly when involving complex dynamics and high-dimensional random variables. In this talk, I will discuss our proposed method for the accurate estimation of rare event or failure probabilities for expensive-to-evaluate numerical models in high dimensions, and its application to rare event control. The proposed approach combines ideas from large deviation theory and adaptive importance sampling. The importance sampler uses a cross-entropy method to find an optimal Gaussian biasing distribution, and reuses all samples made throughout the process for both, the target probability estimation and for updating the biasing distributions. Large deviation theory is used to find a good initial biasing distribution through the solution of an optimization problem. Additionally, it is used to identify a low-dimensional subspace that is most informative of the rare event probability. We compare the method with a state-of-the-art cross-entropy-based importance sampling scheme using examples including a tsunami problem.

- **Extreme event estimation for stochastic differential equations via precise large deviation theory**

Speaker: Timo Schorlepp (Courant Institute of Mathematical Sciences)

Abstract. Estimating the probability of extreme events is an important problem in many scientific and engineering disciplines, as they are often associated with rare system failures or catastrophes. Asymptotically, rare event probabilities can be estimated with a Laplace approximation, also known as precise large deviation theory in this context. The approach involves (i) solving an optimization problem to find the most likely realization of the random parameter leading to a prescribed outcome, and (ii) calculating a determinant to account for Gaussian perturbations around the minimizer.

In this talk, I will discuss how to carry out these steps numerically in a scalable way for extreme events in stochastic differential equations (SDEs) and stochastic partial differential equations (SPDEs) with Brownian noise. In particular, I will highlight the necessity to treat the determinant calculation in step (ii) correctly from an infinite-dimensional point of view to ensure scalability of the numerical method to high dimensions. This leads to either a Fredholm or Carleman-Fredholm determinant computation, depending on whether the second variation of the noise-to-event map is trace-class or only Hilbert-Schmidt.

To illustrate these points, I will consider two examples of extreme event estimates for S(P)DEs: a predator-prey SDE as a toy problem, and a 2D random advection-diffusion problem as a nontrivial SPDE.

The presentation is based on arXiv:2502.20114 (joint work with Tobias Grafke).

- **Randomized Algorithms for Optimal Experimental Design**

Speaker: Vishwas Hebbur Venkata Subba Rao (Argonne National Laboratory)

Abstract. We tackle optimal sensor placement for Bayesian linear inverse problems by establishing connections to the Column Subset Selection Problem (CSSP). We build on the Golub-Klema-Stewart (GKS) approach which involves computing the truncated Singular Value Decomposition (SVD) followed by a pivoted QR factorization on the right singular vectors. We study the effects of using the Federov exchange rule, greedily swapping sensors while improving the objective, after a GKS-style initialization. Theoretical guarantees on the number of swaps are established. Numerical experiments on model inverse problems demonstrate the performance of our approaches.

- **Kernel Density Estimation Adaptive Importance Sampling with Gaussian Processes for Rare-events Probability Estimation**

Speaker: Ashwin Renganathan (Pennsylvania State University)

Co-authors: Annie Booth (Virginia Polytechnic Institute and State University)

Abstract. Estimating rare-event probabilities for expensive black-box models is notoriously difficult because failures are scarce, structured, and a priori unknown. We present an adaptive importance sampling strategy that learns a proposal nonparametrically from data via a kernel density surrogate, allowing it to track multi-modal and anisotropic failure regions without committing to a parametric family. The method interfaces with user-defined input laws and simple domain constraints, and it is designed to be plug-and-play within existing UQ workflows. From a theoretical standpoint, we show that the resulting estimator is unbiased at every iteration and consistent as the design adapts. Under mild regularity conditions, we establish a central limit theorem with an explicit asymptotic variance that contracts toward the oracle variance associated with the ideal failure-tilted density.

- **Scaling Scenario-Based Chance-Constrained Optimization for Rare Events**

Speaker: Jaeseok Choi (Pennsylvania State University)

Co-authors: Anand Deo (Indian Institute of Management), Constantino Lagoa (Pennsylvania State University), Anirudh Subramanyam (Pennsylvania State University)

Abstract. Chance-constrained optimization is a suitable modeling framework for mitigating extreme event risk in many practical settings. The scenario approach is a popular solution method for chance-constrained problems, due to its straightforward implementation and ability to preserve problem structure. However, for safety-critical applications where violating constraints is nearly unacceptable, the scenario approach becomes computationally infeasible due to the excessively large sample sizes it demands. We address this limitation with a new yet straightforward decision-scaling technique. Our method leverages large deviation principles and relies on only mild nonparametric assumptions about the underlying uncertainty distributions.

The method achieves an exponential reduction in sample size requirements compared to the classical scenario approach for a wide variety of constraint structures, while also guaranteeing feasibility with respect to the uncertain constraints. Numerical experiments spanning engineering and management applications show that our decision-scaling technique significantly expands the scope of problems that can be solved both efficiently and reliably.

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2.8 Recent Advances in Scientific Machine Learning Arising from PDEs

MS Abstract. Scientific machine learning (SciML) has rapidly emerged as a transformative paradigm at the intersection of computational science, applied mathematics, and data-driven modeling. In particular, the integration of machine learning techniques with partial differential equations (PDEs) has led to significant advances in modeling, simulation, and prediction for complex physical, biological, and engineering systems. This minisymposium will showcase recent developments in the theory, algorithms, and applications of scientific machine learning methods driven by PDE-based models. Topics will include physics-informed neural networks, operator learning, uncertainty quantification, and hybrid data-model frameworks. Emphasis will be placed on how these methodologies address challenges such as high dimensionality, multiple solution structures, inverse problems, and model interpretability. Through a series of invited talks, the minisymposium aims to foster interdisciplinary dialogue and highlight emerging directions in this rapidly evolving field.

- **Algebraically Precondition a Linear System With Graph Neural Networks**

Speaker: Jie Chen (IBM Research)

Abstract. Preconditioning is at the heart of the iterative solutions of large, sparse linear systems of equations. We consider general-purpose preconditioners applicable to many applications. In this case, the assumed knowledge is only the matrix but not the domain or application. We study the use of graph neural networks (GNNs) as an approximation of the matrix inverse, since a graph is naturally associated with the matrix, just like in algebraic multigrid. We build the GNN architecture, propose a training data generation procedure, and investigate how the preconditioner behaves by vetting a significant portion of the SuiteSparse matrix collection (nearly a thousand matrices). We conclude that GNNs are useful for solving challenging problems and suggest future research directions.

- **Data-driven discovery of conservation laws, Lax pairs, and system integrability**

Speaker: Wei Zhu (Georgia Institute of Technology)

Abstract. In this talk, we present two data-driven approaches for discovering system integrability: conservation law learning via neural deflation and interpretable learning of a Lax pair in Hamiltonian systems. Neural deflation iteratively trains neural networks to identify conserved quantities while ensuring their functional independence. The second approach maximizes compatibility between Lax operators and the system’s Hamiltonian. We demonstrate these methods on various Hamiltonian systems, including harmonic oscillators, the Hénon-Heiles system, discrete lattice equations, and Hamiltonian PDEs such as the Korteweg–de Vries and cubic nonlinear Schrödinger equations.

- **Adaptive sampling and transfer learning for PDE models**

Speaker: Andreas Aristotelous (University of Akron)

Abstract. An adaptive sampling technique applied to the deep Galerkin method (DGM), and separately transfer learning techniques applied to DGM are examined, aimed to improve, and speed up the training of the deep neural network when learning the solution of partial differential equations (PDEs). The proposed algorithms improve the DGM method. The adaptive sampling scheme implementation is natural and efficient. Tests applied to selected PDEs discussing the robustness of our methods are presented.

- **Multiscale Neural Networks for Approximating Green’s Functions**

Speaker: Yahong Yang (Georgia Institute of Technology)

Abstract. Neural networks (NNs) have been widely used to solve partial differential equations (PDEs) in the applications of physics, biology, and engineering. One effective approach for solving PDEs with a fixed differential operator is learning Green’s functions. However, Green’s functions are notoriously difficult to learn due to their poor regularity, which typically requires larger NNs and longer training times. In this paper, we address these challenges by leveraging multiscale NNs to learn Green’s functions. Through theoretical analysis using multiscale Barron space methods and experimental validation, we show that the multiscale approach significantly reduces the necessary NN size and accelerates training.

- **SSBE-PINN: A Sobolev Boundary Scheme Boosting Stability and Accuracy in Elliptic/Parabolic PDE Learning**

Speaker: Chuqi Chen (Hong Kong University of Science and Technology)

Co-authors: Qixuan Zhou (Shanghai Jiao Tong University), Tao Luo (Shanghai Jiao Tong University), Yang Xiang (Hong Kong University of Science and Technology)

Abstract. Physics-Informed Neural Networks (PINNs) have emerged as a powerful framework for solving partial differential equations (PDEs), yet they often fail to achieve accurate convergence in the H^1 norm, especially in the presence of boundary approximation errors. In this work, we propose a novel method called *Sobolev-Stable Boundary Enforcement* (SSBE), which redefines the boundary loss using Sobolev norms to incorporate boundary regularity directly into the training process. We provide rigorous theoretical analysis demonstrating that SSBE ensures bounded H^1 error via a stability guarantee and derive generalization bounds that characterize its robustness under finite-sample regimes. Extensive numerical experiments on linear and nonlinear PDEs—including Poisson, heat, and elliptic problems—show that SSBE consistently outperforms standard PINNs in terms of both relative L^2 and H^1 errors, even in high-dimensional settings. The proposed approach offers a principled and practical solution for improving gradient fidelity and overall solution accuracy in neural network-based PDE solvers.

- **Neural Approximate Inverse Preconditioners**

Speaker: Yuanzhe Xi (Emory University)

Abstract. In this talk, we present a data-driven framework for constructing efficient and accurate approximate inverse preconditioners for solving elliptic partial differential equations (PDEs). The core idea is to train a neural network to approximate the Green’s function of the underlying operator. The architecture exploits the intrinsic multiscale structure of Green’s functions and integrates exact inverse information from a coarse-grid discretization, thereby improving both training efficiency and accuracy. To enable a scalable application, we introduce a data-driven hierarchical matrix construction algorithm that circumvents the prohibitive cost of evaluating all Green’s function entries. This yields an almost linear-cost preconditioner application cost that is naturally suited for parallel architectures. We demonstrate the effectiveness of the approach on a range of challenging elliptic PDE problems, comparing it against state-of-the-art algebraic preconditioners. Numerical experiments show significant reductions in iteration counts and total solution time, highlighting the potential of learning-based preconditioning techniques for large-scale scientific computing.

- **A Natural Deep Ritz Method for Essential Boundary Value Problems**

Speaker: Shuo Zhang (Chinese Academy of Sciences)

Abstract. Implemented for solving elliptic partial differential equations, the deep Ritz method generally does not need the solution bear higher regularities than its variational formulation on proper Sobolev spaces. A main issue, however, lies on the treatment of the essential boundary value conditions, from which the robustness of the method often suffers. We introduce a parameter-free strategy to cope with the essential boundary condition by decomposing the original problem to natural boundary value problems which are still of elliptic type and which are easier to be solved by the deep Ritz method. The mathematical equivalence is proved rigorously based on the underlying structures. Numerical experiments illustrate the improvement of the robustness. This is a joint work with Haijun Yu.

- **Computing ground states of Bose-Einstein condensation by normalized deep neural network**

Speaker: Zhipeng Chang (Pennsylvania State University)

Co-authors: Weizhu Bao (National University of Singapore), Xiaofei Zhao (Wuhan University)

Abstract. We propose a normalized deep neural network (norm-DNN) for computing ground states of Bose-Einstein condensation (BEC) via the minimization of the Gross-Pitaevskii energy functional under unitary mass normalization. Compared with the traditional deep neural network for solving partial differential equations, two additional layers are added in training our norm-DNN for solving this kind of unitary constraint minimization problems: (i) a normalization layer is introduced to enforce the unitary mass normalization, and (ii) a shift layer is added to guide the training to non-negative ground state. The proposed norm-DNN gives rise to an efficient unsupervised approach for learning ground states of BEC. Systematical investigations are first carried out through extensive numerical experiments for computing ground states of BEC in one dimension. Extensions to high dimensions and multi-component are then studied in details. The results demonstrate the effectiveness and efficiency of norm-DNN for learning ground states of BEC. Finally, we extend the norm-DNN for computing the first excited states of BEC and discuss parameter generalization issues as well as compare with some existing machine learning methods for computing ground states of BEC in the literature.

- **Randomized Greedy Algorithms for Neural Network Optimization in Solving PDEs**

Speaker: Ziaofeng Xu (Pennsylvania State University)

Abstract. Greedy algorithms have been successfully analyzed and applied in training neural networks for solving variational problems, ensuring guaranteed convergence orders. In this paper, we extend the analysis of the orthogonal greedy algorithm (OGA) to convex optimization problems arising from the solution of partial differential equations, establishing its optimal convergence rate. This result broadens the applicability of OGA by generalizing its optimal convergence rate from function approximation to convex optimization problems. In addition, we also address the issue regarding practical applicability of greedy algorithms, which is due to significant computational costs from the subproblems that involve an exhaustive search over a discrete dictionary. We propose to use a more practical approach of randomly discretizing the dictionary at each iteration of the greedy algorithm. We quantify the required size of the randomized discrete dictionary and prove that, with high probability, the proposed algorithm realizes a weak greedy algorithm, achieving optimal convergence orders. Through numerous numerical experiments on function approximation, linear and nonlinear elliptic partial differential equations, we validate our analysis on the optimal convergence rate and demonstrate the advantage of using randomized discrete dictionaries over a deterministic one by showing orders of magnitude reductions in the size of the discrete dictionary, particularly in higher dimensions.

- **Randomized subspace correction methods for convex optimization**

Speaker: Jongho Park (King Abdullah University of Science and Technology)

Co-authors: Boou Jiang (King Abdullah University of Science and Technology), Jinchao Xu (King Abdullah University of Science and Technology)

Abstract. This talk introduces an abstract framework for randomized subspace correction methods for convex optimization, which unifies and generalizes a broad class of existing algorithms, including domain decomposition, multigrid, and block coordinate descent methods. We provide a convergence rate analysis ranging from minimal assumptions to more practical settings, such as sharpness and strong convexity. While most existing studies on block coordinate descent methods focus on nonoverlapping decompositions and smooth or strongly convex problems, our framework extends to more general settings involving arbitrary space decompositions, inexact local solvers, and problems with limited smoothness or convexity. The proposed framework is broadly applicable to convex optimization problems arising in areas such as nonlinear partial differential equations, imaging, and data science.

- **Physics-Informed Neural Networks for Solving Two-Phase Flow and Fluid-Structure Interaction Problems with Moving Interfaces**

Speaker: Pengtao Sun (University of Nevada, Las Vegas)

Abstract. In this talk, I will present our recent research work on meshfree/deep neural network (DNN) method for solving two-phase flow problems and fluid-structure interactions (FSI) problems with moving interfaces. We apply the framework of physics-informed neural networks (PINNs) to both moving interface problems by means of a space-time training set as well as arbitrary Lagrangian-Eulerian (ALE) mapping technique, and analyze the convergence property of DNN in terms of number of sampling points in each training subset, which shows that the approximation error of PINNs is bounded above by optimization/training errors and numerical quadrature errors, at the same time, for all loss functions arising from residuals of moving interface PDEs and of interface/boundary/initial conditions. Reynolds transport theorem plays a key role in the analysis. To validate the obtained theoretical results, in this talk I will also illustrate numerical experiments of PINNs for examples of two-phase flow problem with a prescribed moving interface, as well as of dynamic FSI problem, where the ALE mapping is applied to track the solution-dependent moving interface between motions of the fluid and the structure in different coordinate systems: the fluid motion in Eulerian description, and the structural motion in Lagrangian description.

- **Long-Horizon PDE Prediction via Energy-Stable Evolutionary KANs**

Speaker: Guang Lin (Purdue University)

Co-authors: Changhong Mou (Utah State University), Jiahao Zhang (Purdue University)

Abstract. We present *Evolutionary Kolmogorov-Arnold Networks* (EvoKAN), a new framework for solving challenging partial differential equations (PDEs) by blending neural networks with numerical evolution. Unlike conventional approaches that require repeated retraining, EvoKAN learns only from the PDE's initial state; its parameters then evolve dynamically under the same governing equations, enabling accurate long-horizon predictions without additional optimization. Built on spline-based Kolmogorov-Arnold Networks, EvoKAN provides localized multi-scale flexibility while incorporating the Scalar Auxiliary Variable (SAV) method to guarantee unconditional energy stability and computational efficiency. We demonstrate the framework on Allen-Cahn and Navier-Stokes equations, showing that EvoKAN not only matches analytical and benchmark solutions but also robustly captures complex dynamics such as phase-field evolution and turbulent flows. This work highlights EvoKAN as a promising direction for integrating machine learning and numerical PDE solvers to achieve stable, interpretable, and scalable simulations.

- **Operator learning for hyperbolic PDEs**

Speaker: Christopher Wang (Cornell University)

Co-authors: Alex Townsend (Cornell University)

Abstract. We construct the first rigorously justified probabilistic algorithm for recovering the solution operator of a hyperbolic partial differential equation (PDE) in two variables from input-output training pairs. The primary challenge of recovering the solution operator of hyperbolic PDEs is the presence of characteristics, along which the associated Green’s function is discontinuous. Therefore, a central component of our algorithm is a rank detection scheme that identifies the approximate location of the characteristics. By combining the randomized singular value decomposition with an adaptive hierarchical partition of the domain, we construct an approximant to the solution operator using $O(\Psi_\epsilon^{-1}\epsilon^{-7}\log(\Xi_\epsilon^{-1}\epsilon^{-1}))$ input-output pairs with relative error $O(\Xi_\epsilon^{-1}\epsilon)$ in the operator norm as $\epsilon \rightarrow 0$, with high probability. Here, Ψ_ϵ represents the existence of degenerate singular values of the solution operator, and Ξ_ϵ measures the quality of the training data. Our assumptions on the regularity of the coefficients of the hyperbolic PDE are relatively weak given that hyperbolic PDEs do not have the “instantaneous smoothing effect” of elliptic and parabolic PDEs, and our recovery rate improves as the regularity of the coefficients increases. We also include numerical experiments corroborating our theoretical findings.

- **Barron Approximation and locally optimal shallow neural networks**

Speaker: Gerrit Welper (University of Central Florida)

Abstract. By classical results, shallow neural networks can approximate Barron smooth functions with dimension independent convergence rates. While these results are of theoretical nature, much less is understood about the performance of networks that result from practical training algorithms. The talk contains new landscape results for a modified and convex mean-field loss: All local minima satisfy equi-distribution properties similar to classical spline and finite element approximation. As a consequence, all local minima achieve Barron type approximation errors. We obtain practical methods by particle approximations of Wasserstein gradient flow, resulting in gradient descent type methods with dropout regularization.

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2.9 Recent Developments for Numerical Methods for PDEs

MS Abstract. This mini-symposium aims to bring together leading experts and researchers to discuss the latest advancements in computational methods for partial differential equations, which include Transports, Navier-Stokes, Non-Newtonian, Darcy’s Laws and their couplings. This session will explore innovative numerical methods, which leverage either traditional or advanced machine-learning approaches and high-performance computing to address challenges and enhance the accuracy and efficiency. Emphasis will be placed on structure preserving feature of numerical methods and their applications.

- **Subspace correction methods for semicoercive and nearly semicoercive convex variational problems**

Speaker: Jongho Park (King Abdullah University of Science and Technology)

Co-authors: Young Ju Lee (Texas State University)

Abstract. We present new convergence analyses for subspace correction methods for semicoercive and nearly semicoercive convex variational problems, generalizing the theory of singular and nearly singular linear problems to a class of nonlinear problems. For semicoercive problems, we show that the convergence rate can be estimated in terms of a seminorm stable decomposition over the subspaces and the kernel of the problem, aligning with the theory for singular linear problems. For nearly semicoercive problems, we establish a parameter-independent convergence rate, assuming the kernel of the semicoercive part can be decomposed into a sum of local kernels, which aligns with the theory for nearly singular problems. To demonstrate the applicability of our results, we provide domain decomposition and multigrid methods for certain nonlinear partial differential equations.

- **Multiple Solutions of Nonlinear Differential Equations**

Speaker: Sun Lee (Pennsylvania State University)

Abstract. The study of nonlinear partial differential equations (PDEs) has led to significant advancements in fields such as physics, biology, ecology, and quantum mechanics. However, identifying multiple solutions to nonlinear PDEs remains a challenge, particularly when suitable initial guesses are not readily available. To address this issue, we introduce the Companion-Based Multilevel Finite Element Method (CBMFEM), a novel framework that utilizes polynomial-based companion matrices to efficiently generate multiple initial guesses. Our approach employs conforming finite elements on nested meshes to systematically refine and capture diverse solutions for semilinear elliptic equations with polynomial nonlinearities.

- **Greedy algorithm based on localized RBFs for solution of fractional convection-diffusion-reaction equation**

Speaker: Reza Mollapourasl (Farmingdale State College)

Co-authors: Majid Haghi (Farhangian University)

Abstract. Designing an efficient high-order numerical discretization is one of the challenges in numerical solution of fractional differential equations. To overcome the ill-conditioning that often destroys the convergence rate of global RBF methods, a local meshfree method known as radial basis function-generated finite difference (RBF-FD) method equipped with a greedy algorithm is applied to design stable stencil weights and approximate spatial derivatives for parabolic fractional partial differential equations of convection-diffusion-reaction type.

- **Abstract Spectral Approximation Theories and Finite Element Methods for PDE Eigenvalue Problems**

Speaker: Jiguang Sun (Michigan Technological University)

Abstract. We review the abstract spectral approximation theory of linear compact operators. The theory has been used to show the convergence of finite element methods for various eigenvalue problems of PDEs such as the Dirichlet eigenvalue problem, biharmonic eigenvalue problem, and Maxwell's eigenvalue problem. Then we discuss the abstract approximation theory for holomorphic Fredholm operator-valued functions, known as Karma's theory. This theory requires the regular convergence of the discrete approximation operators. We employ the theory to prove the error estimates of the finite element methods for several nonlinear eigenvalue problems including the band structure of dispersive photonic crystals and scattering resonances.

- **Structure-preserving Discretization of the Poisson-Nernst-Planck Equations via the Onsager Principle**

Speaker: Hailiang Liu (Iowa State University)

Co-authors: Qianyi Li (Iowa State University)

Abstract. We propose a variational approach for designing energy-stable and positivity-preserving numerical schemes for the Poisson-Nernst-Planck (PNP) equations. By leveraging the Onsager variational principle, the governing equations are reformulated as a constrained minimization problem. A straightforward time discretization naturally yields a mass-transport formulation and ensures mass conservation and energy dissipation. This structure is preserved under spatial discretization, which transforms the problem into a well-posed minimization problem with linear constraints. We rigorously prove that the scheme guarantees positivity, mass conservation and unconditional energy stability, even in high-dimensional settings. Theoretical results are supported by numerical tests which demonstrate the accuracy, stability, and robustness of the proposed method.

- **Discretization analysis for a convection-diffusion problem**

Speaker: Constantin Bacuta (University of Delaware)

Abstract. For a model convection-diffusion problem, we present new error estimates for a general upwinding finite element discretization based on bubble modification of the test space. The key analysis tool is finding representations of the optimal norms on the trial spaces at the continuous and discrete levels. We analyze and compare three methods: the standard linear discretization, the saddle point least square and the upwinding Petrov-Galerkin methods. We conclude that the bubble upwinding Petrov-Galerkin method is the most performant discretization for the one dimensional model. Our results for the model convection-diffusion problem can be extended for creating new and efficient discretizations for the multidimensional cases.

- **Numerical Approximation for Equations with Line Dirac Sources**

Speaker: Hengguang Li (Wayne State University)

Co-authors: Xiang Wan (Wayne State University), Peimeng Yin (Wayne State University), Lewei Zhao (Wayne State University)

Abstract. We study the elliptic equation with a line Dirac delta function as the source term in a two-dimensional domain. Such a line Dirac measure causes different types of solution singularities in the neighborhood of the line fracture. We establish new regularity results for the solution in a class of weighted Sobolev spaces and propose finite element algorithms that approximate the singular solution at the optimal convergence rate. Numerical tests are presented to justify the theoretical findings.

- **Hierarchical Preconditioning for Stochastic Optimal Control Problems**

Speaker: Zhendong Li (Lehigh University)

Co-authors: Bedřich Sousedík (University of Maryland), Akwum Onwunta (Lehigh University)

Abstract. We develop efficient hierarchical preconditioners for stochastic optimal control problems governed by partial differential equations with random coefficients. Adopting a discretize-then-optimize framework that integrates finite element discretization, stochastic Galerkin approximations, and advanced time discretization schemes, our approach addresses the challenge of large-scale, ill-conditioned linear systems arising in uncertainty quantification. By exploiting the multi-level sparsity inherent in generalized polynomial chaos expansions, we derive hierarchical preconditioners based on truncated stochastic expansions that strike an effective balance between computational cost and preconditioning quality. Comprehensive numerical experiments on benchmark problems demonstrate that our proposed preconditioners significantly accelerate the convergence of iterative solvers compared to traditional mean-based approximations and full-expansion methods, proving robust and efficient for both time-independent and time-dependent optimal control applications.

- **Liquid Crystal Networks preasymptotic energy and its approximation via a Local Discontinuous Galerkin method**

Speaker: Gonzalo Benavides (University of Maryland)

Co-authors: Lucas Bouck (Carnegie Mellon University), Ricardo Nochetto (University of Maryland), Shuo Yang (Beijing Institute of Mathematical Sciences and Applications)

Abstract. Liquid Crystal Networks (LCN) are materials made of elastomeric polymer networks densely cross-linked with Liquid Crystal molecules. They can develop complex shapes upon actuation, and find applications in the design of biomedical devices and robotics. Inspired by the works of Ozenda-Sonnet-Virga (2020) we start from the classical classical Bladon-Warner-Terentjev (1994) 3D trace formula and utilize the Kirchhoff-Love assumption to derive a 2D energy given by the sum of a Stretching energy that measures the deviation from a target metric, and a thickness-scaled Bending energy in terms of, among other geometric quantities, the Second Fundamental Form (SFM). Close to the target metric, the bending energy is roughly equivalent to a properly rescaled squared L^2 -norm

of the Hessian of the deformation, which makes it amenable for computations. Along the lines of Bonito-Guignard-Nochetto-Yang (2020), we propose a Local Discontinuous Galerkin (LDG)-gradient flow to minimize the resulting nonconvex preasymptotic energy. We finish the talk by presenting several numerical experiments. This joint work with Lucas Bouck, Ricardo Nochetto and Shuo Yang, builds upon Lucas' PhD dissertation.

- **High-Accuracy Deep Learning Approaches and Approximation Theory in Scientific Computing**

Speaker: Young Ju Lee (Texas State University)

Co-authors: Jiwei Jia (Jilin University), Ye Lin (Jilin University)

Abstract. In this talk, we present a unified, high-precision framework for scientific computing that leverages the Orthogonal Greedy Algorithm (OGA). First, we tackle fractional Laplacian equations with OGA, yielding provable convergence and superior accuracy over finite element methods (FEMs). Next, we introduce an OGA-based method for second-order elliptic PDEs with Dirichlet boundary conditions, we obtain shallow-network solutions with optimal H^1 -norm error bounds, outperforming standard penalization approaches. We then address indefinite elliptic (Helmholtz-type) problems, providing rigorous a priori error analysis for shallow neural approximations and tailoring OGA to overcome non-coerciveness; extensive numerical quadrature and large-scale experiments confirm OGA's stability and its advantage over FEMs. Building on these advances, we extend OGA to linear operator learning by estimating kernel functions and Green's operators, achieving order-of-magnitude improvements in inference speed and generalization error compared to benchmarks like DeepONet.

- **Quantum algorithms for solving PDEs**

Speaker: Xiantao Li (Pennsylvania State University)

Abstract. I will present some quantum algorithms for solving PDEs, by mapping them to the Schrodinger equation. We will explain the potential speedup compared to classical numerical methods and existing issues.

- **Advanced Numerical Methodologies for Fluid-Structure Interactions**

Speaker: Pengtao Sun (University of Nevada, Las Vegas)

Abstract. The interaction of a flexible structure with a flowing fluid in which it is submersed or by which it is surrounded gives rise to a rich variety of physical phenomena with applications in many fields of engineering, named as fluid-structure interactions (FSI). To understand these phenomena, we need to find an effective way to model and simulate both fluid and structure, simultaneously, by investigating the interaction between them. In general, FSI problems require the fluid and the structure fields at the common interface to share not only the same velocity but also the common traction force. There are currently several major approaches classified with respect to the numerical treatment how the interfacial conditions of FSI are dealt with on the moving interface. In my talk, I will focus on the body-fitted mesh/arbitrary Lagrangian-Eulerian finite element methods for solving FSI problems, and study their optimal convergence properties in theory as well as apply them to hydrodynamic and hemodynamic FSI problems in practice.

- **Adaptive Preconditioning of Sparse Linear Systems using Successive Over-Relaxation with Reinforcement Learning**

Speaker: Soha Yusuf (Rensselaer Polytechnic Institute)

Co-authors: Shaowu Pan (Rensselaer Polytechnic Institute), Jason Hicken (Rensselaer Polytechnic Institute)

Abstract. We study sparse linear systems arising from advection-dominated partial differential equations and propose a data-driven strategy to accelerate their solution. Specifically, we use a dynamic successive-over-relaxation (SOR) preconditioner inside FGMRES in which the relaxation parameter is chosen at each Krylov iteration by a reinforcement-learning agent, enabling per-iteration tuning of the preconditioner. In our framework, the reinforcement-learning agent is implemented as a deep Q-network (DQN) that applies multiplicative actions to scale the current relaxation factor. Compared with a standard SOR preconditioner that uses a fixed relaxation parameter, our framework requires fewer Krylov iterations on benchmark diffusion, advection, and advection–diffusion problems. The experiments show that reinforcement learning can serve as a robust, generalizable auto-tuner for classical linear solvers.

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2.10 Computational and Probabilistic Methods: From Theory to Practice

MS Abstract. This mini-symposium explores the computational and probabilistic aspects of modern mathematical modeling, with a focus on the deep connections between applied mathematics and computer science. As complex systems in physics, biology, engineering, and finance present increasing analytical and numerical challenges, the need for rigorous, efficient, and reliable modeling frameworks has become paramount. Emphasis will be placed on the mathematical foundations of relevant methods, as well as their implementation and performance in computational environments. By bringing together theoretical and applied perspectives, the symposium aims to advance the understanding and practical utility of mathematical models in solving real-world problems through the combined lens of probability, computation, algebra, and applied analysis.

- **A criterion for crystallization in hard-core lattice particle systems**

Speaker: Ian Jauslin (Rutgers University)

Co-authors: Qidong He (Rutgers University), Joel L. Lebowitz (Rutgers University)

Abstract. As is well known, many materials freeze at low temperatures. Microscopically, this means that their molecules form a phase where there is long range order in their positions. Despite their ubiquity, proving that these freezing transitions occur in realistic microscopic models has been a significant challenge, and it remains an open problem in continuum models at positive temperatures. In this talk, I will focus on lattice particle models, in which the positions of particles are discrete. In contrast to the continuum case, there are many examples of lattice particle systems for which crystallization has been proved (in particular in an impressive series of papers by Mazel, Stuhl and Suhov, which cover hard discs on various lattices). In this talk, I will present a general criterion under which crystallization can be proved to occur. The class of models that the criterion applies to are those in which there is *no sliding*, that is, particles are largely locked in place when the density is large. The tool used in the proof is Pirogov-Sinai theory and cluster expansions. I will present the criterion in its general formulation, and discuss some concrete examples. This is joint work with Qidong He and Joel L. Lebowitz.

- **Hydrodynamic limits for interacting particles with two spatial scales**

Speaker: Daniel Chen (Brown University)

Co-authors: Kavita Ramanan (Brown University)

Abstract. From wireless communication to social dynamics, interacting agents (or particles) are driven by heterogeneous information from various sources. Many such phenomena are appropriately modeled as a system of randomly evolving particles with direct interactions at two distinct spatial scales: locally with neighbors on a sparse graph as well as globally through the empirical measure of all particles. For a large class of such interacting jump processes, we establish hydrodynamic limits that capture the asymptotic evolution of macroscopic observables, as the underlying graph sequence converges in a suitable local sense. We autonomously characterize the limit in terms of a certain

generalized "local-field equation" (LFE). We also show that for a certain subclass of dynamics, the LFE describes a Markovian process. Lastly, we numerically demonstrate the efficacy of the asymptotic theory on moderate-sized systems.

- **Antithetic Noise in Diffusion Models**

Speaker: Guanyang Wang (Rutgers University)

Abstract. We initiate a systematic study of antithetic initial noise in diffusion models. Across unconditional models trained on diverse datasets, text-conditioned latent-diffusion models, and diffusion-posterior samplers, we find that pairing each initial noise with its negation consistently yields strongly negatively correlated samples. To explain this phenomenon, we combine experiments and theoretical analysis, leading to a symmetry conjecture that the learned score function is approximately affine anti-symmetric (odd symmetry up to a constant shift), and provide evidence supporting it. Leveraging this negative correlation, we enable two applications: (1) enhancing image diversity in models like Stable Diffusion without quality loss, and (2) sharpening uncertainty quantification (e.g., up to 90% narrower confidence intervals) when estimating downstream statistics. Building on these gains, we extend the two-point pairing to a randomized quasi-Monte Carlo estimator, which further improves estimation accuracy. Our framework is training-free, model-agnostic, and adds no runtime overhead.

- **Random weights of DNNs and emergence of fixed points**

Speaker: Oleksii Krupchytskyi (Pennsylvania State University)

Abstract. In this talk we consider a special class of deep neural networks (DNNs) where the input and the output vectors have the same dimension. Such DNNs are widely used in applications, e.g., autoencoders. The training of such networks can be characterized by their fixed points (FPs). We are concerned with the dependence of the FPs number and their stability on the distribution of randomly initialized DNNs' weight matrices.

Specifically, we consider the i.i.d. random weights with heavy and light-tail distributions. Our objectives are twofold. First, the dependence of FPs number and stability of FPs on the type of the distribution tail. Second, the dependence of the number of FPs on the DNNs' architecture. We perform extensive simulations and show that for light tails (e.g., Gaussian), which are typically used for initialization, a single stable FP exists for broad types of architectures. In contrast, for heavy tail distributions (e.g., Cauchy), which typically appear in trained DNNs, a number of FPs emerge. We further observe that these FPs are stable attractors and their basins of attraction partition the domain of input vectors. Finally, we observe an intriguing non-monotone dependence of the number of fixed points $Q(L)$ on the DNNs' depth L .

This is a joint work with my PhD advisor Prof. L. Berlyand (PSU) and Prof. V. Slavin (ILTPE, Kharkiv) (arXiv preprint 2025). This work has been supported by NSF grant MPRESS-U: N2401227.

- **Cutoff for the Swendsen-Wang dynamics on the complete graph**

Speaker: Blanca Antonio (Pennsylvania State University)

Co-authors: Zhezheng Song (Carnegie Mellon University)

Abstract. We provide new results concerning the speed of convergence of the Swendsen-Wang (SW) dynamics for the q -state ferromagnetic Potts model on the n -vertex complete graph, also known as the mean-field setting. The SW dynamics was introduced as an attractive alternative to the local Glauber dynamics, often offering faster convergence rates in a variety of settings. A series of works characterized the asymptotic mixing time of the mean-field SW dynamics for all $q \geq 2$ and all values of the inverse temperature parameter $\beta > 0$. In particular, it is known that when $\beta > q$, the mixing time of the SW dynamics is $\theta(\log n)$. We strengthen this result by showing that for all $\beta > q$, there exists a constant $c(\beta, q) > 0$ such that the mixing time of the SW dynamics is $c(\beta, q) \log n + \theta(1)$. This implies that the mean-field SW dynamics exhibits the cutoff phenomenon in this regime, demonstrating that it undergoes a sharp transition from "far from stationarity" to "well-mixed" within a narrow $\theta(1)$ time window.

- **Spin system dynamics beyond worst-case initialization**

Speaker: Gheissari Reza (Northwestern University)

Abstract. Glauber dynamics for spin systems like the Ising and Potts models are Markov chains that model their physical time-evolutions in statistical physics, and also serve as natural MCMC sampling algorithms from complex high-dimensional distributions. Classical Markov chain analysis is focused on mixing times (times to approximate stationarity) from worst-case initialization, but tools for understanding mixing times from natural (e.g., uniform-at-random, or higher temperature) initializations are far more limited. We describe some recent results on low-temperature regimes where spin system dynamics are exponentially slow to equilibrate from worst-case, but where mixing from random or special initializations can be analyzed and shown to be significantly faster.

- **Facilitating Efficiency of Deep Neural Networks using Marchenko-Pastur Distribution**

Speaker: Mariia Kiyashko (Pennsylvania State University)

Abstract. In this talk we present several aspects of Random Matrix Theory (RMT) and its applications to Deep Neural Networks (DNNs). We begin with a short overview of RMT, focusing on the Marchenko-Pastur (MP) spectral approach. We consider the weight layer W of a DNN being of the form $W=R+S$, where R is a random matrix, S is of small rank, and the size of W goes to infinity. First, we present recent analytical results on enhancing DNN efficiency through MP-based pruning techniques in the case when the rank of S is fixed ([1]). Next, we present numerical results showing that in practice, the rank of S may grow. We conclude with the recent RMT results necessary for relaxing the fixed rank condition and discuss how they may be applied to analytically prove the efficiency of the MP-pruning in the general setting ([2]).

This is a joint work with my PhD advisor Prof. L. Berlyand (PSU), I. Afanasiev (ILTPE, Kharkiv, Ukraine), and with Y. Shmalo (Hebrew University).

(1) Leonid Berlyand, et al. “Enhancing accuracy in deep learning using random matrix theory.” *Journal of Machine Learning*. (2024).

(2) Ievgenii Afanasiev, Leonid Berlyand, Mariia Kiyashko “Asymptotic behavior of eigenvalues of large rank perturbations of large random matrices”, arXiv:2507.12182v2.

This work has been partially supported by the NSF Grant IMPRESS-U: N2401227.

- **Percolation and Criticality in Hyperuniform Networks**

Speaker: Yongyi Wang (Pennsylvania State University)

Co-authors: Yang Jiao (Arizona State University), Jaekuk Kim (Princeton University), Salvatore Torquato (Princeton University), Reka Albert (Pennsylvania State University)

Abstract. Hyperuniformity provides a general framework for studying point configurations with suppressed density fluctuations on macroscopic scales, encompassing both lattices and certain exotic disordered systems with quasi-long-range correlations. Percolation, in turn, is a classic continuous phase transition model in statistical physics that probes transport in disordered media. We study distance-based bond percolation on Delaunay triangulation networks derived from stealthy hyperuniform and Poisson (uncorrelated) point configurations. Using the Newman–Ziff Monte Carlo algorithm and finite-size scaling analysis, we estimate critical thresholds and exponents across a range of system sizes. Our results show clear differences between hyperuniform and Poisson embeddings: hyperuniform networks percolate more readily and display distinctive universality-class characteristics, with the stealthiness parameter providing a natural knob to tune the critical point. These findings suggest that hyperuniformity, beyond its structural definition, manifests as an emergent property in macroscopic critical phenomena. This perspective opens new pathways for designing network architectures with tailored transport properties, linking structural order, phase transitions, and applied network design.

- **Markov chain resetting: a general view**

Speaker: Yuri Suhov (Pennsylvania State University)

Abstract. We explore a general framework for Markov chain resetting and its applications.

- **Computational and probabilistic methods to understand the dynamics of biological networks**

Speaker: Reka Albert

Abstract. Modeling the dynamics of biological systems requires an approach that captures the individuality and specific interactions of each element. Due to the high-dimensional state space, this requirement poses an extraordinary computational and cognitive challenge. My group developed concepts and methods that simplify the exploration of state spaces, focusing on the regions where irreversible decisions occur. This approach enables more efficient identification of key dynamic behaviors, decision points, and control strategies. I will highlight a coarse-grained Markov chain method, which distills complex system dynamics into a compact, parameterized summary. This research offers new pathways for both prediction and intervention, with potential applications ranging from cellular processes to ecological systems.

- **Probabilistic Analysis of Gaussian Elimination**

Speaker: Konstantin Tikhomirov (Carnegie Mellon University)

Abstract. Gaussian Elimination with partial pivoting is a classical method of solving systems of linear equations. A seminal work of Wilkinson established upper bounds on the forward and backward errors of the computational procedure in terms of the growth factor, defined as the ratio of largest absolute values of elements of the intermediate matrices and the original coefficient matrix. While it is known that in the worst case the growth factor is exponential in the matrix dimension, empirical evidence suggests that the Gaussian elimination tends to be numerically stable on typical (random) inputs. In this talk, I will discuss estimates on the growth factor for random coefficient matrices, and present some open problems. Based on joint work with Han Huang.

- **Random sphere-packing on lattices**

Speaker: Izabella Stuhl (Pennsylvania State University)

Abstract. We explore sphere-packings on lattices and their connection to the behavior of lattice systems with hard-core exclusion, emphasizing their role in understanding the structure of the phase diagram.

2.11 Physics-Guided Generative AI for Scientific Computing: Theory, Algorithms and Applications

MS Abstract. This minisymposium highlights advances in physics-guided and generative AI for scientific computing across theory, methods, and applications. We focus on methods that encode physical structure within operator-learning and generative frameworks; on analysis that studies approximation, stability, generalization and optimization in scientific machine learning (ML); and on applications that realize calibrated uncertainty quantification, robust data assimilation, multi-fidelity inference, and trustworthy deployment. Through an interdisciplinary forum, the minisymposium bridges theory and practice and highlights open problems essential to trustworthy AI in science.

Topics include (but not limited to): physics-informed operator learning and generative models; advanced optimization for scientific ML; theoretical guarantees in scientific machine learning; multiscale/multi-fidelity inference and data assimilation; and foundation models for scientific computing.

- **Unsupervised Neural Operators for Optimal Control: Scaling Laws and Applications**

Speaker: Wezhe Xu (Purdue University)

Abstract. Optimal control provides a principled framework for transforming dynamical system models into intelligent decision-making, yet classical computational approaches are often too expensive for real-time deployment in dynamic or uncertain environments. In this work, we propose a neural operator learning framework designed for optimal control problems. It offers a new paradigm by directly approximating the mapping from system conditions to optimal control strategies, enabling instantaneous inference across diverse scenarios once trained. We investigate both the promise and limitations of neural operators for optimal control. Theoretically, we establish scaling laws that quantify how sample and model complexity depend on the intrinsic dimension and regularity of the optimal control function, thus clarifying the price to pay for efficiency. Numerically, we demonstrate case studies where neural operators achieve remarkable gains in real-time performance, as well as regimes where complexity barriers persist. Together, these results provide a balanced perspective: neural operators represent a powerful new tool for high-performance control when hidden low-dimensional structure can be exploited, yet remain fundamentally constrained by dimensional complexity in more challenging settings.

- **Learning Hyperbolic Conservation Laws from Data**

Speaker: Lizuo Liu (Dartmouth College)

Abstract. We propose a neural entropy-stable conservative flux form neural network (NESCOFN) for learning hyperbolic conservation laws and their associated entropy functions directly from solution trajectories, without requiring any predefined numerical discretization. While recent neural network architectures have successfully integrated classical numerical principles into learned models, most rely on prior knowledge of the governing equations or assume a fixed discretization. Our approach removes this dependency by embedding entropy-stable design principles into the learning process itself, enabling the discovery of physically consistent dynamics in a fully data-driven setting. By jointly learning both the numerical flux function and a corresponding entropy, the proposed method ensures conservation and entropy dissipation, critical for long-term stability and fidelity in the system of hyperbolic conservation laws. Numerical results demonstrate that the method achieves stability and conservation over extended time horizons and accurately captures shock propagation speeds, even without oracle access to future-time solution profiles in the training data.

- **From Equations to Insights: Unraveling Symbolic Structures in PDEs with LLMs**

Speaker: Ling Liang (University of Tennessee)

Co-authors: Rohan Bhatnagar (University of Maryland), Krish Patel (University of Maryland), Haizhao Yang (University of Maryland)

Abstract. Motivated by the remarkable success of artificial intelligence (AI) across diverse fields, the application of AI to solve scientific problems, often formulated as partial differential equations (PDEs), has garnered increasing attention. While most existing research concentrates on theoretical properties (such as well-posedness, regularity, and continuity) of the solutions, alongside direct AI-driven methods for solving PDEs, the challenge of uncovering symbolic relationships within these equations remains largely unexplored. In this paper, we propose leveraging large language models (LLMs) to learn such symbolic relationships. Our results demonstrate that LLMs can effectively predict the operators involved in PDE solutions by utilizing the symbolic information in the PDEs both theoretically and numerically. Furthermore, we show that discovering these symbolic relationships can substantially improve both the efficiency and accuracy of symbolic machine learning for finding analytical approximation of PDE solutions, delivering a fully interpretable solution pipeline. This work opens new avenues for understanding the symbolic structure of scientific problems and advancing their solution processes.

- **Variationally stable reduced basis neural operator**

Speaker: Yuan Qiu (Georgia Institute of Technology)

Co-authors: Wolfgang Dahmen (University of South Carolina), Peng Chen (Georgia Institute of Technology)

Abstract. Minimizing PDE-based residual losses is a common way to softly enforce physical consistency in neural operators. However, the link between small residuals and small solution errors is often unclear. We show with two canonical examples, Poisson and linear elasticity, how to construct variationally correct first-order least-squares residuals that are provably equivalent to errors in PDE-compliant energy norms rather than in a generic L2 norm. This yields training objectives that directly control accuracy and naturally accommodate mixed Dirichlet/Neumann data via variational lifts. To alleviate optimization challenges and reduce training costs, we apply proper orthogonal decomposition (POD) to high-fidelity snapshots, training the neural operator to predict only the POD coefficients. This approach preserves residual-error equivalence while enabling efficient evaluation of the quadratic loss in the reduced space. Numerical studies compare this approach with pointwise training- and evaluation-based neural operators and, importantly, show that the proposed variationally correct loss serves as a reliable a posteriori error estimator, exhibiting a tight correlation with the solution error in the appropriate PDE energy norms.

- **Error Analysis of Operator Learning on the Space of Probability Measures**

Speaker: Frank Cole (University of Minnesota)

Co-authors: Dixi Wang (Purdue University), Yineng Chen (Purdue University), Rongjie Lai (Purdue University), Yulong Lu (University of Minnesota)

Abstract. Variational problems on the space of probability measures arise frequently in scientific modeling and computation, but many existing methods demand extensive computational time and are limited to solving single instances of the problem. In contrast, operator learning provides an alternative approach to develop efficient surrogate solvers. In this talk, we consider the operator learning approach to solve optimal transport, a classical problem in many areas of science and math. We specialize our analysis to two concrete settings: nonparametric learning, where the measures live on a low-dimensional manifold, and parametric learning, where the measures are assumed to be Gaussian. We theoretically analyze how the performance depends on various sources of error, such as the sample size, discretization level, and complexity of the architecture, and we present numerical experiments to validate our methodology. This is joint work with Dixi Wang, Yineng Chen, Rongjie Lai, and Yulong Lu.

- **Constrained Policy Optimization for Large Language Model Alignment**

Speaker: Dongsheng Ding (University of Tennessee)

Abstract. Large Language Models (LLMs) hold great promise for high-stakes applications such as robotics and healthcare, but ensuring they meet requirements like safety and fairness remains a core challenge. This talk presents a constrained policy optimization framework for aligning LLMs with explicit policy constraints. We first introduce the constrained alignment problem in the LLM policy space and discuss its optimization properties, such as convexity and duality, enabling a reduction to an unconstrained problem. Building on this insight, we present an iterative dual-based alignment method that alternates between Lagrangian maximization and dual descent. For the resulting LLM policies, we show approximate optimality with respect to both the objective and the constraints, with suboptimality bounded by the LLM parameterization gap. We illustrate improved constraint satisfaction and more favorable trade-offs between the objective and the constraints in a safety alignment task.

- **On exploration of an interior mirror descent flow for stochastic nonconvex constrained problem**

Speaker: Kuangyu Ding (Purdue University)

Co-authors: Toh Kim-Chuan (National University of Singapore)

Abstract. We study a nonsmooth nonconvex optimization problem defined over nonconvex constraints, where the feasible set is given by the intersection of the closure of an open set and a smooth manifold. By endowing the open set with a Riemannian metric induced by a barrier function, we obtain a Riemannian subgradient flow formulated as a differential inclusion, which remains strictly within the interior of the feasible set. This continuous dynamical system unifies two classes of iterative optimization methods, namely the Hessian barrier method and mirror descent scheme, by revealing that these methods can be interpreted as discrete approximations of the continuous flow. We explore the long-term behavior of the trajectories generated by this dynamical system and show that the existing deficient convergence properties of the Hessian barrier and mirror descent schemes can be more insightfully interpreted through the lens of continuous trajectories. For instance, the notorious spurious stationary points [Chen, 2024] observed in mirror descent scheme are interpreted as stable equilibria of the dynamical system that do not correspond to real stationary points of the original optimization problem. We provide two sufficient conditions such that these spurious stationary points can be avoided. In the absence of these regularity conditions, we propose a novel random perturbation strategy that ensures the trajectory converges (subsequentially) to an approximate stationary point. Building on these insights, we introduce two iterative Riemannian subgradient methods, form of interior point methods, that generalizes the existing Hessian barrier method and mirror descent scheme for solving nonsmooth nonconvex optimization problems.

- **LoDAdaC: a unified local training-based decentralized framework with Adam-type updates and compressed communication**

Speaker: Yangyang Xu (Rensselaer Polytechnic Institute)

Abstract. In the decentralized distributed learning, achieving fast convergence and low communication cost is essential for scalability and high efficiency. Despite extensive research, existing decentralized methods can either have fast convergence or enjoy low communication cost but cannot achieve both goals simultaneously. This disadvantage causes significant inefficiency (either in computation or communication) in solving large-scale decentralized learning problems, e.g., in large language model training.

To address this limitation, we propose LoDAdaC, a unified **Local Training (MLT) Decentralized** framework with **Adam-type updates** and **Compressed communication (CC)**. LoDAdaC accommodates a broad class of optimizers for its local adaptive updates, including AMSGrad, Adam, and AdaGrad; it is compatible with standard (possibly biased) compressors such as low-bit quantization and sparsification. MLT and CC enable LoDAdaC to achieve multiplied reduction of communication cost, while the technique of adaptive updates enables fast convergence. We rigorously prove the combined advantage through complexity analysis. In addition, experiments on image classification and large language model training validate our theoretical findings and show that LoDAdaC significantly outperforms existing decentralized algorithms in terms of convergence speed and communication efficiency.

- **FunDiff: Diffusion models over function spaces for physics-informed generative modeling**

Speaker: Lu Lu (Yale University)

Abstract. Recent advances in generative modeling – particularly diffusion models and flow matching – have achieved remarkable success in synthesizing discrete data such as images and videos. However, adapting these models to physical applications remains challenging, as the quantities of interest are continuous functions governed by complex physical laws. Here, we introduce FunDiff, a novel framework for generative modeling in function spaces. FunDiff combines a latent diffusion process with a function autoencoder architecture to handle input functions with varying discretizations, generate continuous functions evaluable at arbitrary locations, and seamlessly incorporate physical priors. These priors are enforced through architectural constraints or physics-informed loss functions, ensuring that generated samples satisfy fundamental physical laws. We theoretically establish minimax optimality guarantees for density estimation in function spaces, showing that diffusion-based estimators achieve optimal convergence rates under suitable regularity conditions. We demonstrate the practical effectiveness of FunDiff across diverse applications in fluid dynamics and solid mechanics. Empirical results show that

our method generates physically consistent samples with high fidelity to the target distribution and exhibits robustness to noisy and low-resolution data.

- **Quantitative Clustering in Mean-Field Transformer Models**

Speaker: Shi Chen (Massachusetts Institute of Technology)

Co-authors: Zhengjiang Lin (Massachusetts Institute of Technology), Yury Polyanskiy (Massachusetts Institute of Technology), Philippe Rigollet (Massachusetts Institute of Technology)

Abstract. Transformers are at the core of large language models, yet their internal dynamics remain poorly understood. Recent work suggests that token evolution in deep transformers resembles an interacting particle system, exhibiting clustering behavior similar to synchronization in Kuramoto models. In this talk, we study the long-time behavior of a mean-field transformer model and prove exponential convergence to a clustered state under suitable assumptions. Our results offer new mathematical perspectives on the emergent dynamics of deep transformers with long context.

- **A supervised learning scheme for the Hamilton-Jacobi equation via density coupling**

Speaker: Haomin Zhou (Georgia Institute of Technology)

Abstract. In this talk, I will present a supervised learning scheme for the first-order Hamilton-Jacobi PDEs in high dimensions. The scheme is designed by using the geometric structure of Wasserstein Hamiltonian flows via a density coupling strategy. It can be equivalently posed as a regression problem using the Bregman divergence, which provides the loss function in learning. The data is generated through the particle formulation of Wasserstein Hamiltonian flow. We prove a posterior estimate on the L^1 residual of the proposed scheme based on the support of the coupling density. Several numerical examples with different Hamiltonians are provided to support our findings. This presentation is based on joint work with Jianbo Cui (HK PolyU) and Shu Liu (Florida State).

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2.12 Optimal Transport in Biological Sciences

MS Abstract. Optimal transport (OT) theory has emerged as a powerful mathematical framework for comparing probability distributions and analyzing structured data. In recent years, it has found increasing applications in the biological sciences, ranging from single-cell transcriptomics and developmental biology to neuroscience and imaging. This minisymposium brings together researchers working at the interface of OT and biology to showcase recent advances of OT in both theoretical developments and practical applications. The talks will feature models, computational methods, and cross-disciplinary efforts that use OT to gain insights from complex biological data. The goal is to foster dialogue between mathematicians and biologists interested in the role of OT on addressing challenges in modern biology.

- **Optimal transport reveals dynamic gene regulatory networks via gene velocity estimation**

Speaker: Ritambhara Singh (Brown University)

Abstract. Inferring gene regulatory networks from gene expression data is an important and challenging problem in the biology community. We propose OTVelo, a methodology that takes time-stamped single-cell gene expression data as input and predicts gene regulation across two time points. It is known that the rate of change of gene expression, which we will refer to as gene velocity, provides crucial information that enhances such inference; however, this information is not always available due to the limitations in sequencing depth. Our algorithm overcomes this limitation by estimating gene velocities using optimal transport. We then infer gene regulation using time-lagged correlation and Granger causality via regularized linear regression. Instead of providing an aggregated network across all time points, our method uncovers the underlying dynamical mechanism across time points. We validate our algorithm on 13 simulated datasets with both synthetic and curated networks and demonstrate its efficacy on 9 experimental data sets.

- **Optimal Transport based metrics and statistics for quantifying cell shape heterogeneity**

Speaker: Wenjun Zhao (Wake Forest University)

Abstract. Recent advances in experimental methodologies and community efforts have led to a surge in large cell image datasets, that require the developments of new methods to analyze them and extract meaningful information. In this context, I will describe our recent efforts to leverage optimal transport theory, with the introduction of metrics inspired by Wasserstein/Gromov-Wasserstein distances for 2D and 3D cell shapes, that are efficient to compute and can be used for a variety of tasks, including Dimensionality reduction, statistical testing and machine learning. Real data applications will focus on analyzing 2D contour of cancer cells, and 3D images of nucleus and cell shapes under different stages of development.

- **Efficient Trajectory Inference in Wasserstein Space Using Consecutive Averaging**

Speaker: Amartya Banerjee (University of North Carolina at Chapel Hill)

Abstract. Capturing data from dynamic processes through cross-sectional measurements is seen in many fields, such as computational biology. Trajectory inference deals with the challenge of reconstructing continuous processes from such observations. In this work, we propose methods for B-spline approximation and interpolation of point clouds through consecutive averaging that is intrinsic to the Wasserstein space. Combining subdivision schemes with optimal transport-based geodesic, our methods carry out trajectory inference at a chosen level of precision and smoothness, and can automatically handle scenarios where particles undergo division over time. We prove linear convergence rates and rigorously evaluate our method on cell data characterized by bifurcations, merges, and trajectory splitting scenarios like supercells, comparing its performance against state-of-the-art trajectory inference and interpolation methods. The results not only underscore the effectiveness of our method in inferring trajectories but also highlight the benefit of performing interpolation and approximation that respect the inherent geometric properties of the data.

- **Generative Particle Flows with Force-Matching for Reconstructing Nonlinear Cellular Dynamics**

Speaker: Hyemin Gu (University of Massachusetts Amherst)

Co-authors: Yu-Chen Cheng (Dana-Farber Cancer Institute), Yannis Pantazis (Foundation for Research and Technology - Hellas), Markos Katsoulakis (University of Massachusetts Amherst)

Abstract. Single-cell RNA sequencing provides high-dimensional snapshots of cell states but does not directly capture continuous dynamics. To address this, we developed PROFET (Particle-based Reconstruction Of generative Force-matched Expression Trajectories), a computational framework that reconstructs continuous, nonlinear trajectories from static distributions.

PROFET combines two innovations: (i) a Lipschitz-regularized gradient flow of f-divergences, which generates stable particle flows between time-stamped distributions, and (ii) a novel neural force-matching procedure that reconstructs a global, time-dependent vector field from these flows. Together, these steps yield a continuous-time dynamical system capable of modeling out-of-equilibrium and nonlinear evolution.

This formulation departs from optimal transport geodesics and continuous normalizing flows by constructing explicit potentials from f-divergences and by decoupling trajectory generation from vector field learning, improving both stability and efficiency. Applications to synthetic benchmarks and high-dimensional single-cell datasets illustrate the ability of PROFET to uncover heterogeneous trajectories that equilibrium-based OT methods fail to capture.

- **Synchronized Optimal Transport for Trajectory Inference in Biological Systems**

Speaker: Jingfeng Wang (North Carolina State University)

Abstract. Trajectory inference is a central task in computational biology, particularly for uncovering cellular dynamics from high-dimensional and multimodal data. However, existing methods often fail to coherently integrate information across primary and secondary modalities, leading to suboptimal representations of biological processes. To address this challenge, we propose a neural network-based framework that incorporates Synchronized Optimal Transport (SyncOT) for trajectory inference. By jointly optimizing across primary and auxiliary spaces, our method achieves synchronized modeling of cellular dynamics while minimizing the aggregated cost across modalities. This enables more consistent and biologically meaningful trajectory reconstruction. Experimental results on biological datasets demonstrate that SyncOT provides a robust and effective approach for multimodal optimization, yielding more accurate and interpretable trajectories of cellular processes.

- **Cryo-EM as a Stochastic Inverse Problem**

Speaker: Diego Balam Sanchez Espinosa (Cornell University)

Co-authors: Erik Thiede (Cornell University), Yunan Yang (Cornell University)

Abstract. Cryo-electron microscopy (Cryo-EM) enables high-resolution imaging of biomolecules, but structural heterogeneity remains a major challenge in 3D reconstruction. Traditional methods assume a discrete set of conformations, limiting their ability to recover continuous structural variability. In this work, we formulate cryo-EM reconstruction as a stochastic inverse problem (SIP) over probability measures, where the observed images are modeled as the push-forward of an unknown distribution over molecular structures via a random forward operator. We pose the reconstruction problem as the minimization of a variational discrepancy between observed and simulated image distributions, using statistical distances such as the KL divergence and the Maximum Mean Discrepancy. The resulting optimization is performed over the space of probability measures via a Wasserstein gradient flow, which we numerically solve using particles to represent and evolve conformational ensembles. We validate our approach using synthetic examples, including a realistic protein model, which demonstrates its ability to recover continuous distributions over structural states. We analyze the connection between our formulation and Maximum A Posteriori (MAP) approaches, which can be interpreted as instances of the discretize-then-optimize (DTO) framework. We further provide a consistency analysis, establishing conditions under which DTO methods, such as MAP estimation, converge to the solution of the underlying infinite-dimensional continuous problem. Beyond cryo-EM, the framework provides a general methodology for solving SIPs involving random forward operators.

- **Robust Molecular Structure Comparison via Optimal Transport**

Speaker: Xiaoqi Wei (North Carolina State University)

Abstract. Root-mean-square deviation (RMSD) is widely used to assess structural similarity in systems ranging from flexible ligand conformers to complex molecular cluster configurations. Despite its wide utility, RMSD calculation is often challenged by inconsistent atom ordering, indistinguishable configurations in molecular clusters, and potential chirality inversion during alignment. These issues highlight the necessity of accurately establishing atom-to-atom correspondence as a prerequisite for meaningful alignment. Traditional approaches often rely on heuristic cost matrices combined with the Hungarian algorithm, yet these methods underutilize the rich intra-molecular structural information and may fail to generalize across chemically diverse systems. In this work, we introduce OTMol, a novel method that formulates the molecular alignment task as a fused supervised Gromov-Wasserstein (fsGW) optimal transport problem. By leveraging the intrinsic geometric and topological relationships within each molecule, OTMol eliminates the need for manually defined cost functions and enables a principled, data-driven matching strategy. Importantly, OTMol preserves key chemical features such as molecular chirality and bond connectivity consistency. We evaluate OTMol across a wide range of molecular systems, including Adenosine triphosphate, Imatinib, lipids, small peptides, water clusters, and demonstrate that it consistently achieves low RMSD values while preserving computational efficiency. Importantly, OTMol maintains molecular integrity by enforcing one-to-one mappings between entire molecules, thereby avoiding erroneous many-to-one alignments that often arise in clustering

scenarios. Our results underscore the utility of optimal transport theory for molecular alignment and offer a generalizable framework applicable to structural comparison tasks in cheminformatics, molecular modeling, and related disciplines.

- **Machine-Learning Interatomic Potentials for Long-Range Systems**

Speaker: Yajie Ji (Yale University)

Co-authors: Jiuyang Liang (Flatiron Institute), Zhenli Xu (Shanghai Jiao Tong University)

Abstract. Machine-learning interatomic potentials have emerged as a revolutionary class of force-field models in molecular simulations, delivering quantum-mechanical accuracy at a fraction of the computational cost and enabling the simulation of large-scale systems over extended timescales. However, they often focus on modeling local environments, neglecting crucial long-range interactions. We propose a Sum-of-Gaussians Neural Network (SOG-Net), a lightweight and versatile framework for integrating long-range interactions into machine learning force field. The SOG-Net employs a latent-variable learning network that seamlessly bridges short-range and long-range components, coupled with an efficient Fourier convolution layer that incorporates long-range effects. By learning sum-of-Gaussians multipliers across different convolution layers, the SOG-Net adaptively captures diverse long-range decay behaviors while maintaining close-to-linear computational complexity during training and simulation via non-uniform fast Fourier transforms. The method is demonstrated effective for a broad range of long-range systems.

- **Optimal Transport Modeling of Cellular Differentiation: From Low-Rank Structure to Temporal Dynamics**

Speaker: Peter Halmos (Princeton)

Co-authors: Julian Gold (Princeton), Xinhao Liu (Princeton) Benjamin J. Raphael (Princeton)

Abstract. Optimal transport (OT) provides a principled framework for coupling probability distributions by minimizing transport cost. Yet classical OT remains computationally prohibitive for large scale data, with quadratic complexity in the number of samples. Low-Rank OT addresses this challenge by introducing a rank constraint on the coupling, reducing the complexity of OT to linear. Low-Rank OT also generalizes K-means clustering for a pair of datasets and provides a natural formulation for co-clustering. Building on this perspective, we introduce an alternative parametrization of Low-Rank OT based on the latent-coupling (LC) factorization (Lin ‘21), which decomposes the transport into two clusterings linked by a non-square transition matrix. We derive a coordinate mirror-descent based algorithm, Factor Relaxation with Latent Coupling (FRLC), which solves Low-Rank OT with Sinkhorn sub-problems. This construction naturally leads to a multi-marginal extension of Low-Rank OT to sequential data, which we call Hidden-Markov OT (HM-OT). We demonstrate that HM-OT is a powerful and scalable tool for single-cell and spatial transcriptomics, capable of co-clustering cell-trajectories across time and revealing interpretable differentiation maps across cell states.

2.13 Low-Rank Adaptation for Efficient Fine-Tuning in Foundation Models

MS Abstract. Low-rank adaptation (LoRA) has become a cornerstone for efficient fine-tuning of large-scale models, enabling parameter efficiency and deployment flexibility. Recent advances go beyond the original formulation by incorporating optimization-based improvements such as gradient approximation and spectral initialization, leveraging random projection techniques to enhance stability and expressiveness. Besides, within the context of federated learning, low-rank adaptation also raises a lot of attention for efficiency and flexibility. This session will provide an overview of these developments, highlight both theoretical insights and empirical results, and discuss emerging opportunities for combining low-rank adaptation with current foundation models.

- **Bridging Model Heterogeneity via LoRA-Based Knowledge Distillation in Federated Learning**

Speaker: Yujia Wang (Pennsylvania State University)

Abstract. Federated learning (FL) enables collaborative model training and fine-tuning across distributed clients without sharing raw data. However, it faces significant challenges due to heterogeneous client computational capacities when fine-tuning large-scale foundation models. In practice, some resource-limited clients may be unable to load such models at all, forcing them to fine-tune smaller alternatives. This disparity naturally introduces model heterogeneity, as clients participate with foundation models of varying sizes or even distinct architectures. To address this issue, we propose a LoRA-based knowledge distillation framework that bridges heterogeneous client models in FL. In our approach, strong clients fine-tune large-scale models while resource-limited clients adapt smaller models, and their LoRA modules are aligned through cross-architecture knowledge distillation. We leverage synthetic data generation, where clients contribute privacy-preserving few-shot prompts and the server synthesizes queries for consistent supervision. Experimental results demonstrate that our method effectively enables scalable and efficient federated fine-tuning across diverse foundation models.

- **Non-Convex Tensor Recovery from Tube-Wise Sensing**

Speaker: Tongle Wu (Pennsylvania State University)

Abstract. In this paper, we propose a novel tube-wise local tensor compressed sensing (CS) model, where sensing operators are independently applied to each tube of a third-order tensor. To recover the low-rank ground truth tensor, we minimize a non-convex objective via Burer–Monteiro factorization and solve it using gradient descent with spectral initialization. We prove that this approach achieves exact recovery with a linear convergence rate. Notably, our method attains provably lower sample complexity than existing TCS methods. Our proof leverages the leave-one-out technique to show that gradient descent generates iterates implicitly biased towards solutions with bounded incoherence, which ensures contraction of optimization error in consecutive iterates. Empirical results validate the effectiveness of GD in solving the proposed local TCS model.

- **Federated Fine-tuning of Large Language Models under Heterogeneous Tasks and Client Resources**

Speaker: Jiamu Bai (Pennsylvania State University)

Co-authors: Daoyuan Chen (Alibaba Group), Bingchen Qian (Alibaba Group), Liuyi Yao (Alibaba Group), Yaliang Li (Alibaba Group)

Abstract. Federated Learning (FL) has recently been applied to the parameter-efficient fine-tuning of Large Language Models (LLMs). While promising, it raises significant challenges due to the heterogeneous resources and data distributions of clients. This study introduces FlexLoRA, a simple yet effective aggregation scheme for LLM fine-tuning, which mitigates the "buckets effect" in traditional FL that restricts the potential of clients with ample resources by tying them to the capabilities of the least-resourced participants. FlexLoRA allows for dynamic adjustment of local LoRA ranks, fostering the development of a global model imbued with broader, less task-specific knowledge. By synthesizing a full-size LoRA weight from individual client contributions and employing Singular Value Decomposition (SVD) for weight redistribution, FlexLoRA fully leverages heterogeneous client resources. Involving thousands of clients performing heterogeneous NLP tasks and client resources, our experiments validate the efficacy of FlexLoRA, with the federated global model achieving consistently better improvement over SOTA FL methods in downstream NLP task performance across various heterogeneous distributions. FlexLoRA's practicality is further underscored by our theoretical analysis and its seamless integration with existing LoRA-based FL methods, offering a path toward cross-device, privacy-preserving federated tuning for LLMs.

- **FLoRA: Federated Fine-Tuning Foundation Models with Heterogeneous Low-Rank Adaptations**

Speaker: Ziyao Wang (University of Maryland)

Abstract. The rapid development of Large Language Models (LLMs) has been pivotal in advancing AI, with pre-trained LLMs being adaptable to diverse downstream tasks through fine-tuning. Federated learning (FL) further enhances fine-tuning in a privacy-aware manner by utilizing clients' local data through in-situ computation, eliminating the need for data movement. However, fine-tuning LLMs, given their massive scale of parameters, poses challenges for clients with constrained and heterogeneous resources in FL. Previous methods employed low-rank adaptation (LoRA) for efficient federated fine-tuning but utilized traditional FL aggregation strategies on LoRA adapters. This approach led to mathematically inaccurate aggregation noise, reducing fine-tuning effectiveness and failing to address heterogeneous LoRAs. In this work, we first highlight the mathematical incorrectness of LoRA aggregation in existing federated fine-tuning methods. We introduce a new approach called FLoRA that enables federated fine-tuning on heterogeneous LoRA adapters across clients through a novel stacking-based aggregation method. Our approach is noise-free and seamlessly supports heterogeneous LoRAs. Extensive experiments demonstrate FLoRA's superior performance in both homogeneous and heterogeneous settings, surpassing state-of-the-art methods. We envision this work as a milestone for efficient, privacy-preserving, and accurate federated fine-tuning of LLMs.

- **PrunedLoRA: Efficient and Robust Gradient-Based Structural Pruning for Low-rank Adaptation in Fine-tuning**

Speaker: Xin Yu (Pennsylvania State University)

Abstract. Low-rank adaptation has become a widely used paradigm for parameter-efficient fine-tuning of large language models, yet its representational capacity often lags behind full fine-tuning. Within the context of low-rank adaptation, how to obtain the representational low-rank adapter from the high-parameter space is an open question. In this paper, we introduce *PrunedLoRA*, a new framework that leverages structural pruning to obtain highly representative low-rank adaptations from an overparameterized initialization. Without requiring a fixed rank budget like prior works, our method dynamically removes less important components and avoids reactivation. For the pruning criteria, inspired by Optimal Brain Surgeon, we propose a new gradient-based pruning method for the weight matrix with fine-grained pruning and recovery updates. In the theoretical aspect, we provably show that under the impact of weight perturbation, gradient-based pruning methods are more robust than activation-based pruning for prediction error. Empirically, *PrunedLoRA* outperforms LoRA and its variant on supervised fine-tuning across mathematical reasoning, code generation capabilities and natural language understanding tasks. With different levels of sparsity, PrunedLoRA also exceeds the established baseline of structural pruning approaches.

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2.14 Nonlinear Waves in Fluids

MS Abstract. This minisymposium explores recent advances in models for the complex behavior of fluid flow. The main focus is given to various models where nonlinearity, dispersion, and other effects are important. Recent theoretical, numerical, and experimental advances based on linear and nonlinear systems will be presented.

- **Exact solution and integrability of ballistic motion of fluid with free surface**

Speaker: Pavel Lushnikov (University of New Mexico)

Abstract. A fully nonlinear dynamics for potential flow of ideal incompressible fluid with a free surface is considered in two dimensional geometry. A fluid is assumed to be moving at large distances either towards or away from the origin which can be considered as a version of ballistic motion. An infinite set of exact solution is found including formation of droplets and cusps on a free surface. These solutions are characterized by motion of complex singularities outside of fluid and can be obtained from fully integrable exact reductions of fluid dynamics.

- **Instabilities of steep Stokes waves**

Speaker: State University of New York at Buffalo

Abstract. We explore various instabilities that affect steep Stokes waves in exact 1D equations governing the motion of a free surface of deep water subject to gravity forces. We show new results for stability spectra computed via numerical modeling of large eigenvalue problem and compare them to asymptotic models.

- **Well-posedness and stability of the Benjamin-Ono equation with quasiperiodic initial data**

Speaker: Sultan Aitzhan (Drexel University)

Abstract. We consider the Benjamin-Ono equation in the spatially quasiperiodic setting. We establish local well-posedness of the initial value problem with initial data in quasiperiodic Sobolev spaces. This requires developing some of the fundamental properties of Sobolev spaces and the energy method for quasiperiodic functions. We then discuss prospects for global existence as well as the existence of quasiperiodic traveling waves.

- **Riemann problems, rarefaction waves, dispersive shocks and soliton refraction in the stationary Kadomtsev-Petviashvili and good Boussinesq equations**

Speaker: Lin Haodong (State University of New York at Buffalo)

Co-authors: Gino Biondini (State University of New York at Buffalo), Mark Hoefer (University of Colorado at Boulder), Gennady El (Northumbria University)

Abstract. We consider the stationary reduction of the Kadomtsev-Petviashvili II (KP-II) equation as well as that of its system of genus-one Whitham modulation equations, together with their relation with the good Boussinesq equation and its own genus-one Whitham modulation system. We use the corresponding dispersionless systems and genus-one Whitham modulation systems to study Riemann problems for the stationary KP-II equation and the good Boussinesq equation. We classify the Riemann problems that give rise to rarefaction waves or two-dimensional dispersive shock waves (DSWs) in terms of the input data. We quantitatively characterize the rarefaction waves using self-similar solutions of the dispersionless system, and we quantitatively describe the DSW, using the DSW fitting method as well as the analysis of the full genus-one modulation system. Finally, we study the soliton refraction by oblique rarefaction waves and dispersive shocks. We compare the analytical predictions with the results obtained by direct numerical simulations of the corresponding PDEs, showing excellent agreement.

- **Recent progress on soliton gases in two spatial dimensions**

Speaker: Gino Biondini (State University of New York at Buffalo)

Abstract. The mathematical description of soliton gases has been well developed for systems in one spatial dimension. In this talk, I will discuss ongoing work aimed at generalizing these tools to systems in two spatial dimensions, focusing in particular on the Kadomtsev-Petviashvili equation.

- **Stokes Waves and Their New Secondary Bifurcations**

Speaker: Anastassiya Semenova (Rochester Institute of Technology)

Abstract. The study of surface gravity waves is crucial for understanding the formation of rogue waves and whitecaps in ocean swell. Waves originating from the epicenter of a storm can often be approximated as unidirectional. In this presentation, we will explore periodic traveling waves on the free surface of an ideal, infinitely deep, two-dimensional fluid. We will focus on surface waves of permanent shape, and present new families of Stokes waves with two crests per wavelength.

- **Breather interactions in the discrete Manakov system**

Speaker: Nicholas Ossi (State University of New York at Buffalo)

Co-authors: Vincent Caudrelier (University of Leeds), Barbara Prinari (State University of New York at Buffalo)

Abstract. The discrete Manakov system is the vector generalization of the Ablowitz-Ladik model, which is an integrable spatial discretization of the nonlinear Schrödinger equation. This system admits a variety of discrete vector soliton solutions, referred to as fundamental solitons, fundamental breathers, and composite breathers. In this talk, a full characterization of the interactions of these solitons and breathers, including the explicit forms of their polarization vectors before and after the interaction, will be given. Additionally, the results will be interpreted in terms of a Yang-Baxter refactorization property for the transmission coefficients associated with the interacting solitons.

- **Generalized Constantin-Lax-Majda Equation with Dissipation**

Speaker: Denis Silantyev (University of Colorado Colorado Springs)

Co-authors: Pavel Lushnikov (University of New Mexico), Michael Siegel (New Jersey Institute of Technology), David Ambrose (Drexel University)

Abstract. We consider the generalized Constantin-Lax-Majda equation with dissipation $\omega_t = -a\omega\omega_x + \omega\mathcal{H}\omega - \nu\Lambda^\sigma(\omega)$, $u_x = \mathcal{H}\omega$, where $\widehat{\Lambda^\sigma} = |k|^\sigma$, both for the problem on the circle $x \in [-\pi, \pi]$ and the real line, and summarize known and new results for global-in-time existence of the solutions and collapsing solutions. We also point out the gaps and parameter regions that are worthy of investigation.

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2.15 Recent advances in quantum machine learning

MS Abstract. Quantum computing is offering the possibility of solving problems that are intractable for classical methods. Among its most active directions, quantum machine learning leverages quantum resources to explore the potential quantum advantage in speed, accuracy, and scalability of machine learning algorithms. However, quantum machine learning faces challenges such as noisy hardware and training instability on near term devices. This minisymposium presents recent studies that have progressed in tackling the problems. This minisymposium covers a wide range of algorithmic and theoretical achievements in quantum machine learning, including novel hybrid quantum-classical frameworks, exploration of quantum computing for scientific machine learning, optimization methods for variational models under noise, cutting-edge quantum algorithms for nonconvex optimization, hardware-efficient circuit designs, etc.

- **Derivative-Free Quasi-Newton Optimization for Variational Quantum Algorithms**

Speaker: Dongwei Shi (Lehigh University)

Co-authors: Yunfan Zeng (Arizona State University), Baoyu Zhou (Arizona State University), Xiu Yang (Lehigh University)

Abstract. Variational Quantum Algorithms (VQAs) like QAOA promise NP-hard solutions such as Max-Cut but depend on costly, noisy evaluations. We explore applying a noise-aware, derivative-free quasi-Newton optimizer (limited-memory BFGS with a relaxed Armijo line-search and Hessian damping) to VQA training. On two-layer bipartite Max-Cut benchmarks, this approach converges faster and reaches higher cut values than Powell's, Nelder-Mead, and COBYLA under equal function-evaluation budgets across 20 trials. These findings highlight the practical benefits of noise-aware quasi-Newton methods for improving VQA performance in noisy, resource-limited quantum environments.

- **Operator-Level Quantum Acceleration of Non-Logconcave Sampling**

Speaker: Jiaqi Leng (University of California, Berkeley)

Abstract. Sampling from probability distributions of the form $\sigma \propto e^{-\beta V}$, where V is a continuous potential, is a fundamental task across physics, chemistry, biology, computer science, and statistics. However, when V is non-convex, the resulting distribution becomes non-logconcave, and classical methods such as Langevin dynamics often exhibit poor performance. We introduce the first quantum algorithm that provably accelerates a broad class of continuous-time sampling dynamics. For Langevin dynamics, our method encodes the target Gibbs measure into the amplitudes of a quantum state, identified as the kernel of a block matrix derived from a factorization of the Witten Laplacian operator. This connection enables Gibbs sampling via singular value thresholding and yields up to a quartic quantum speedup over best-known classical methods in the non-logconcave setting. Building on this framework, we further develop the first quantum algorithm that accelerates replica exchange Langevin diffusion, a widely used method for sampling from complex, rugged energy landscapes.

- **Recent Progress in Quantum Eigenvalue Problems**

Speaker: Ruizhe Zhang (Purdue University)

Abstract. Computing the eigenvalues of a matrix is a fundamental task in numerical linear algebra. Kitaev’s Quantum Phase Estimation (QPE) algorithm, when implemented on a quantum computer, enables the efficient solution of the eigenvalue problem for exponentially large matrices under specific conditions. This advancement has the potential to provide significant quantum advantages in fields like quantum chemistry and quantum machine learning. Recent research has focused on reducing the quantum resources needed for Kitaev’s original protocol, leading to the development of “post-Kitaev” or early fault-tolerant QPE schemes. In this talk, I will present some of the recent progress made in this area. Specifically, I will first introduce the QMEGS algorithm, which enables the estimation of multiple dominant eigenvalues simultaneously using a single ancilla and shorter circuits. Next, I will discuss our recent work on estimating ground state degeneracy and exploring topological properties using a quantum computer.

- **On the practical boundary of quantum computing advantages**

Speaker: Junyu Liu (University of Pittsburgh)

Abstract. Quantum computing is one of the most exciting future computing technologies based on the fundamental law of matrix mechanics. However, the scope of quantum algorithms, and when they could offer potential advantages over classical counterparts in practical applications, is highly obscure. In this talk, we will try to help illustrate the boundary of practical quantum advantages through novel methods provided by advanced tools developed in computer science. First, we will introduce GroverGPT v1 and v2, a large language model simulating quantum searching with 8 billion training parameters. On certain metrics, we could also show that it can outperform existing general-purpose models. Moreover, especially with advanced tools like Chain-of-Thought and quantum-native tokenizer, we show that the model has significant generalization capabilities and can simulate the results of Grover’s quantum circuit in experiments with up to 20 qubits, with evidence that the model can partially “learn” the nature of quantum algorithms, which helps illustrate the boundary of classical simulability of quantum Turing machines. Second, we show an end-to-end pipeline for the practical noiseless and fault-tolerant resource estimations of the HHL algorithm, a famous quantum algorithm for linear system equations with provable quantum speedups and which is BQP-complete. For a given quantum error correction code setup, we explicitly perform the resource count and identify the space, time, and energy costs for performing HHL algorithms fault-tolerantly, and illustrate when it will outperform classical counterparts for a general setup of condition numbers, row sparsity, precision, and matrix size. Our work indicates that it is possible to illustrate a practical boundary between quantum and classical computing using the most advanced tools in high-performance computing and large language models.

- **Critical Perspectives on Quantum Computing for Power System Computational Problems**

Speaker: Masoud Barati (University of Pittsburgh)

Abstract. This talk examines the emerging interface between quantum computing and modern power system analysis, with particular emphasis on the AC Power Flow (ACPF) and AC Optimal Power Flow (ACOPF) problems. These formulations lie at the core of power system planning and operation but are notoriously large-scale, nonlinear, and nonconvex, posing persistent computational challenges. We will discuss how quantum algorithms—despite present hardware constraints and theoretical uncertainties—may open new avenues for addressing these challenges. Some methods remain largely exploratory, lacking firm performance guarantees, while others build on established quantum subroutines that could deliver meaningful progress even in the pre-fault-tolerant era. The talk aims to bridge practical modeling needs in power engineering with algorithmic innovations in quantum computing, offering both a critical perspective and cautious optimism for what lies ahead.

- **Quantum DeepONet: Neural operators accelerated by quantum computing**

Speaker: Pengpeng Xiao (Yale University)

Abstract. In the realm of computational science and engineering, constructing models that reflect real-world phenomena requires solving partial differential equations (PDEs) with different conditions. Recent advancements in neural operators, such as deep operator network (DeepONet), which learn mappings between infinite-dimensional function spaces, promise efficient computation of PDE solutions for a new condition in a single forward pass. However, classical DeepONet entails quadratic complexity concerning input dimensions during evaluation. Given the progress in quantum algorithms and hardware, here we propose to utilize quantum computing to accelerate DeepONet evaluations, yielding complexity that is linear in input dimensions. Our proposed quantum DeepONet integrates unary encoding and orthogonal quantum layers. We benchmark our quantum DeepONet using a variety of PDEs, including the antiderivative operator, advection equation, and Burgers’ equation. We demonstrate the method’s efficacy in both ideal and noisy conditions. Furthermore, we show that our quantum DeepONet can also be informed by physics, minimizing its reliance on extensive data collection. Quantum DeepONet will be particularly advantageous in applications in outer loop problems which require exploring parameter space and solving the corresponding PDEs, such as uncertainty quantification and optimal experimental design.

- **Quantum Machine Learning Applications in High Energy Physics and Beyond**

Speaker: Konstantin Matchev (University of Alabama)

Co-authors: Sergei Gleyzer (University of Alabama), Kyounghul Kong (University of Kansas), Katia Matcheva (University of Alabama)

Abstract. This talk will review recent applications of quantum machine learning to problems in high energy particle physics motivated by the analysis of data from the Large Hadron Collider at CERN, Geneva. Typical tasks include the classifications of jets as quarks or gluons; the classification of calorimeter clusters as electrons or photons; generative modelling of fragmentation and hadronization in jets; and representation learning. The explored hybrid quantum architectures include: quantum equivariant deep neural networks, quantum equivariant graph neural networks, quantum transformers, quantum diffusion models, quantum GANs, etc.

- **Quantum-Assisted Machine Learning for Physics AI and Surrogate Modeling**

Speaker: Alex Khan (BQP)

Abstract. Physics-Informed Neural Networks (PINNs) have emerged as powerful surrogates for modeling nonlinear partial differential equations in fluid dynamics and multiphysics applications. However, their utility is constrained by poor generalizability and the high cost of training large networks. We explore recent advances in **Quantum-Assisted PINNs (QA-PINNs)**—hybrid quantum-classical architectures that replace select hidden layers with variational quantum circuits to reduce trainable parameters and enhance learning efficiency. We first benchmark QA-PINNs on canonical forward problems in computational fluid dynamics, demonstrating up to **20% parameter reduction** while

retaining predictive accuracy. We then extend QA-PINNs to **inverse problems**, such as phase-change modeling in ice accretion, where quantum layers enable a **30–35% reduction** in parameters without loss of fidelity in estimating critical thermodynamic coefficients. Finally, we present a novel integration of **transfer learning** with QA-PINNs, tested across 90 spring–mass–damping systems, where quantum transfer learning achieves **over 60% fastest convergence cases**, highlighting improved generalization over classical methods. Together, these studies outline a pathway for scalable, generalizable, and efficient surrogate modeling that leverages quantum machine learning to address long-standing challenges in physics-informed simulation.

- **Quantum-Inspired Hamiltonian Descent for LLM Sparsification**

Speaker: Yuxiang Peng (Purdue University)

Abstract. Modern large language models (LLMs) rely on deep stacks of dense matrix multiplications for feature extraction, demanding enormous computational resources and energy consumption—comparable to that of small towns. To reduce model size without sacrificing performance, SparseGPT introduces sparsification techniques that approximate dense matrices with sparse matrices. However, identifying these sparse matrices involves solving large-scale mixed-integer optimization problems, which are computationally prohibitive.

Recent advances in quantum optimization, such as Quantum Hamiltonian Descent (QHD), offer promising pathways for accelerating such problems, but the limited scalability of current quantum hardware constrains their practical use. Inspired by QHD, we propose Quantum-Inspired Hamiltonian Descent (QIHD)—a classical algorithm that natively exploits GPU acceleration while partially recovers quantum behaviors to gain advantages at scale. Moreover, QIHD shows great scalability that can handle large-scale optimization problems in model sparsification.

In this talk, I will present the design and implementation of QIHD for language model sparsification. Empirical results demonstrate that QIHD achieves superior trade-offs between solution quality and runtime, outperforming existing solvers such as Gurobi and SparseGPT across various model sizes. As a landmark example of quantum-inspired methods achieving real-world benefits, QIHD sheds light on explorations of broader quantum-inspired applications.

- **PolarGrad: A Class of Matrix-Gradient Optimizers from a Unifying Preconditioning Perspective**

Speaker: Weijie Su (University of Pennsylvania)

Abstract. The ever-growing scale of deep learning models and datasets underscores the critical importance of efficient optimization methods. While preconditioned gradient methods such as Adam and AdamW are the de facto optimizers for training neural networks and large language models, structure-aware preconditioned optimizers like Shampoo and Muon, which utilize the matrix structure of gradients, have demonstrated promising evidence of faster convergence. In this talk, we introduce a unifying framework for analyzing "matrix-aware" preconditioned methods, which not only sheds light on the effectiveness of Muon and related optimizers but also leads to a class of new structure-aware preconditioned methods. A key contribution of this framework is its precise distinction between preconditioning strategies that treat neural network weights as vectors (addressing curvature anisotropy) versus those that consider their matrix structure (addressing gradient anisotropy). This perspective provides new insights into several empirical phenomena in language model pre-training, including Adam’s training instabilities, Muon’s accelerated convergence, and the necessity of learning rate warmup for Adam. Building upon this framework, we introduce PolarGrad, a new class of preconditioned optimization methods based on the polar decomposition of matrix-valued gradients. As a special instance, PolarGrad includes Muon with updates scaled by the nuclear norm of the gradients. We provide numerical implementations of these methods, leveraging efficient numerical polar decomposition algorithms for enhanced convergence. Our extensive evaluations across diverse matrix optimization problems and language model pre-training tasks demonstrate that PolarGrad outperforms both Adam and Muon.

2.16 Advances in Modeling and Computation of Transport Problems

MS Abstract. This minisymposium highlights recent progress in modeling and simulating transport phenomena across kinetic theory, fluid dynamics, radiative transfer, and data-driven dynamical systems. The talks feature reduced basis methods, low-rank and adaptive-rank solvers for high-dimensional kinetic equations, and conservative, positivity-preserving discretizations for population balance and shallow water models. Complementing these advances in traditional PDE-based approaches, we also include emerging data-informed strategies, such as neural operator-based forecasting, invariant-measure techniques for system identification, and spectral methods for chaotic dynamics, showing how modern numerical analysis and machine learning together are reshaping the computation of complex multiscale transport processes.

- **Reduced Basis Methods for Parametric Steady-State Radiative Transfer Equation**

Speaker: Fengyan Li (Rensselaer Polytechnic Institute)

Abstract. The radiative transfer equation (RTE) is a fundamental mathematical model to describe physical phenomena involving the propagation of radiation and its interactions with the host medium, and it arises in many applications. Deterministic methods can produce accurate solutions without any statistical noise, yet often at a price of expensive computational costs originating from the intrinsic high dimensionality of the model. This is more prominent in multi-query tasks when the RTE needs to be solved repeatedly. This motivates the developments of model order reduction techniques for such transport models.

With this work, we present the first systematic investigation of projection-based reduced order models (ROMs) following the reduced basis method (RBM) framework to simulate the parametric steady-state RTE. The use of RBM compared to standard proper orthogonal decomposition (POD) is well motivated, especially considering that a large number of degrees of freedom is needed by full order models to solve high dimensional transport models like RTE. Four ROMs are designed, with each defining a nested family of reduced surrogate solvers of different resolution/fidelity. Two of them are certified in the setting when the absorption cross section is positively bounded below uniformly. One technical focus and contribution lie in the proposed implementation strategies under the affine assumption of the parameter dependence of the model. These broadly applicable strategies not only ensure the efficiency and accuracy of the offline training stage and the online prediction of reduced surrogate solvers, they also take into account the conditioning of the reduced systems as well as the stagnation-free residual evaluation for numerical robustness. Numerical experiments will be presented to demonstrate and accuracy, robustness, and efficiency the proposed reduced surrogate solvers. It is observed that four to six orders of magnitude speedup is achieved by our ROMs for some 2D2v examples.

- **A Nodal Discontinuous Galerkin Method with Low-Rank Velocity Space Representation for the Multi-Scale BGK Model**

Speaker: Joseph Nakao (Swarthmore College)

Co-authors: Andres Galindo-Olarte (Oden Institute for Computational Engineering and Sciences), Mirjeta Pasha (Virginia Polytechnic Institute and State University), Jing-Mei Qiu (University of Delaware), William Taitano (Los Alamos National Laboratory)

Abstract. Solving the Boltzmann-BGK comes with several numerical challenges, including the curse of dimensionality, structure preservation, and controlling spurious oscillations that can occur with discontinuous profiles. In this talk, we present a novel hybrid algorithm in which a low-rank decomposition is applied in the velocity subspace, while a full-rank nodal discontinuous Galerkin representation is used in the physical (position) space. To handle the limit of vanishing collision time, a multiscale implicit integrator based on an auxiliary moment equation is utilized. The result is an efficient, structure-preserving algorithm whose framework can be extended to higher dimensions. The algorithm's order of accuracy, reduced computational complexity, and robustness will be demonstrated on a suite of canonical gas kinetics problems.

- **A Conservative and Positivity-Preserving Discontinuous Galerkin Method for the Population Balance Equation**

Speaker: Ziyao Xu (Binghamton University)

Abstract. We develop a conservative, positivity-preserving discontinuous Galerkin (DG) method for the population balance equation (PBE), which models the distribution of particle numbers across particle sizes due to growth, nucleation, aggregation, and breakage. To ensure number conservation in growth and mass conservation in aggregation and breakage, we design a DG scheme that applies standard treatment for growth and nucleation, and introduces a novel discretization for aggregation and breakage. The birth and death terms are discretized in a symmetric double-integral form, evaluated using a common refinement of the integration domain and carefully selected quadrature rules. Beyond conservation, we focus on preserving the positivity of the number density in aggregation-breakage. Since local mass corresponds to the first moment, the classical Zhang-Shu limiter, which preserves the zeroth moment (cell average), is not directly applicable. We address this by proving the positivity of the first moment on each cell and constructing a moment-conserving limiter that enforces nonnegativity across the domain. To our knowledge, this is the first work to develop a positivity-preserving algorithm that conserves a prescribed moment. Numerical results verify the accuracy, conservation, and robustness of the proposed method.

- **Adaptive-Rank Methods for the Multi-Scale BGK Equation via Greedy Sampling**

Speaker: William Sands (University of Delaware)

Co-authors: Jing-Mei Qiu (University of Delaware), Daniel Hayes (University of Delaware), Nanyi Zheng (University of Delaware)

Abstract. Simulating multi-scale kinetic equations is challenging because of their high dimensionality and the need to capture both kinetic and fluid regimes. In this talk, I will present a new adaptive-rank method for the BGK model, which builds upon our earlier work for the Vlasov–Poisson system. The key idea is a greedy sampling strategy that adaptively selects and evolves the most important information from the kinetic solution. An advantage of the proposed framework is that it avoids the need to construct low-rank decompositions of nonlinear terms, which may not be separable. A conservative correction technique is introduced to enforce mass, momentum, and energy conservation while preserving the correct asymptotic behavior in the fluid limit. The method also leverages a local semi-Lagrangian solver, which enables large time steps and is coupled to the self-consistent macroscopic system. I will show how this framework accurately captures shocks and remains robust across a wide range of Knudsen numbers, offering a promising approach for multiscale kinetic simulations.

- **Invariant Measures for Data-Driven Dynamical System Identification**

Speaker: Jonah Botvinick-Greenhouse (Cornell University)

Co-authors: Yunan Yang (Cornell University)

Abstract. In this talk, we propose a novel approach for performing dynamical system identification, based upon the comparison of simulated and observed physical invariant measures. While standard methods directly treat time-trajectories as inference data, we instead seek models fitting the observed global time-invariant statistics. With this change in perspective, we gain robustness against pervasive challenges in system identification including noise, chaos, and slow sampling. In the first half of the talk, we pose the system identification task as a partial differential equation (PDE) constrained optimization problem, in which synthetic stationary solutions of the Fokker-Planck equation, obtained as fixed points of a finite-volume discretization, are compared to physical invariant measures extracted from observed trajectory data. In the latter half, we use Takens’ embedding theory to introduce a critical data-dependent coordinate transformation which can guarantee unique system identifiability from the invariant measure alone. This contribution resolves a major challenge of system identification through invariant measures, as systems exhibiting distinct transient behaviors may still share the same

time-invariant statistics in their state-coordinates. Throughout, we present comprehensive numerical tests which highlight the effectiveness of our approach on a variety of challenging system identification tasks.

- **Data Completion for Electrical Impedance Tomography by Conditional Diffusion Models**

Speaker: Ke Chen (University of Delaware)

Abstract. Data scarcity is a fundamental barrier in Electrical Impedance Tomography (EIT) since undersampled Dirichlet-to-Neumann (DtN) measurements degrade conductivity reconstructions. We address this bottleneck via diffusion-based completion of partially observed DtN data. Specifically, we train a diffusion model that learns the distribution of DtN data and infers full measurements conditioned on the partial observations. Our method accommodates flexible source–receiver configurations and outperforms baselines such as matrix completion under extreme undersampling (1%). Moreover, the completion approach is compatible with off the shelf EIT solvers as a preprocessing step. When coupled with our completion method, a deep learning inverse solver achieves much better reconstruction than the same solver without completion. Under mild assumptions on conductivity and measurement distributions, we derive nonasymptotic bounds on the distributional discrepancy between the completed and true DtN data. Beyond EIT, our diffusion-based completion applies broadly to PDE-based inverse problems with sparse measurements.

- **Fast Algorithms for A Linear Four-Field Thermo-Poroelastic Model**

Speaker: Mingchao Cai (Morgan State University)

Abstract. Thermo-poroelastic models capture the interplay between elastic porous material deformation, fluid flow, and thermal effects under non-isothermal conditions. This talk presents a four-field formulation for the linear thermo-poroelastic model and introduces two novel algorithms. The first focuses on constructing parameter-robust preconditioners for the resulting linear system, proposing two approaches: one reorganizes variables into a 2-by-2 block structure, while the other directly addresses the 4-by-4 coupled operator. Both preconditioners exhibit robustness to parameter variations and mesh refinement. The second algorithm is a decoupled iterative finite element method, for which stability and optimal convergence are rigorously proven. Numerical experiments are provided to validate the effectiveness and efficiency of the proposed methods.

- **Binned Spectral Power Loss for Improved Prediction of Chaotic Systems**

Speaker: Dibyajyoti Chakraborty (Pennsylvania State University)

Co-authors: Arvind T. Mohan (Pennsylvania State University), Romit Maulik (Pennsylvania State University)

Abstract. Forecasting multiscale chaotic dynamical systems with deep learning remains a formidable challenge due to the spectral bias of neural networks, which hinders the accurate representation of fine-scale structures in long-term predictions. This issue is exacerbated when models are deployed autoregressively, leading to compounding errors and instability. In this work, we introduce a novel approach to mitigate the spectral bias which we call the Binned Spectral Power (BSP) Loss. The BSP loss is a frequency-domain loss function that adaptively weighs errors in predicting both larger and smaller scales of the dataset. Unlike traditional losses that focus on pointwise misfits, our BSP loss explicitly penalizes deviations in the energy distribution across different scales, promoting stable and physically consistent predictions. We demonstrate that the BSP loss mitigates the well-known problem of spectral bias in deep learning. We further validate our approach for the data-driven high-dimensional time-series forecasting of a range of benchmark chaotic systems which are typically intractable due to spectral bias. Our results demonstrate that the BSP loss significantly improves the stability and spectral accuracy of neural forecasting models without requiring architectural modifications. By directly targeting spectral consistency, our approach paves the way for more robust deep learning models for long-term forecasting of chaotic dynamical systems.

- **Moment-enhanced shallow water equations for non-slip boundary conditions**

Speaker: Shiping Zhou (Michigan State University)

Co-authors: Juntao Huang (University of Delaware), Andrew Christlieb (Michigan State University)

Abstract. The shallow water equations often assume a constant velocity profile along the vertical axis. However, this assumption does not hold in many practical applications. To better approximate the vertical velocity distribution, models such as the shallow water moment expansion models have been proposed. Nevertheless, under non-slip bottom boundary conditions, both the standard shallow water equation and its moment-enhanced models struggle to accurately capture the vertical velocity profile due to the stiff source terms. In this work, we propose modified shallow water equations and corresponding moment-enhanced models that perform well under both non-slip and slip boundary conditions. The primary difference between the modified and original models lies in the treatment of the source term, which allows our modified moment expansion models to be readily generalized, while maintaining compatibility with our previous analysis on the hyperbolicity of the model. To assess the performance of both the standard and modified moment expansion models, we conduct a comprehensive numerical comparison with the incompressible Navier–Stokes equations—a comparison that is absent from existing literature.

- **Data-driven Whitney forms for structure preserving models**

Speaker: Benjamin Shaffer (University of Pennsylvania)

Co-authors: Brooks Kinch (University of Pennsylvania), Elizabeth Armstrong (Sandia National Laboratories), Michael Meehan (Sandia National Laboratories), John Hewson (Sandia National Laboratories), Nathaniel Trask (University of Pennsylvania, Sandia National Laboratories)

- **Abstract.** We present a framework for constructing real-time digital twins based on structure-preserving reduced finite element models conditioned on a latent variable. The approach uses conditional attention mechanisms to learn both a reduced finite element basis and a nonlinear conservation law within the framework of finite element exterior calculus (FEEC). This guarantees numerical well-posedness and exact preservation of conserved quantities, regardless of data sparsity or optimization error. The conditioning mechanism supports real-time calibration to parametric variables, allowing the construction of digital twins which support closed loop inference and calibration to sensor data. The framework interfaces with conventional finite element machinery in a non-invasive manner, allowing treatment of complex geometries and integration of learned models with conventional finite element techniques.

2.17 Scientific Machine Learning with Robust Computation

MS Abstract. This minisymposium brings together researchers at the intersection of scientific machine learning, and robust computational methods to address emerging challenges in modeling, simulation, numerical analysis and data-driven discovery across the physical and engineering sciences and applications. As machine learning increasingly augments traditional numerical approaches, key questions arise regarding stability, interpretability, and reliability of learning-based solvers for differential equations, multiscale modeling, and uncertainty quantification. The invited talks will showcase recent advances in the development of structure-preserving algorithms, physics-informed learning, and hybrid methods that integrate data-driven models with rigorous numerical analysis. The goal is to foster interdisciplinary dialogue and promote the development of robust, efficient, and theoretically sound methodologies for scientific computing in the era of high-performance and data-intensive applications.

- **An efficient algorithm for computing the stationary statistical solution of some geophysical fluid systems**

Speaker: Daozhi Han (State University of New York at Buffalo)

Abstract. We introduce a highly efficient, second-order time-marching scheme for infinite-dimensional nonlinear geophysical fluid models, designed to accurately approximate invariant measures—that is, the stationary statistical properties (or “climate”) of the underlying dynamical system. Beyond second-order accuracy in time, the scheme is particularly well suited for long-time simulations due to two key features: (i) it requires solving only a fixed symmetric positive-definite linear system with constant coefficients at each step, and (ii) it guarantees long-time stability, producing uniformly bounded solutions in time for any bounded external forcing, regardless of initial data. We rigorously prove convergence of both global attractors and invariant measures of the discrete system to those of the continuous model in the vanishing time-step limit. Applications to the Lorentz 96 model, the 2D Navier-Stokes and the continuously stratified QG model will be discussed.

- **Uncertainty in Uncertainty and Rockafellian Relaxation**

Speaker: Sean Carney (Union College)

Abstract. A critical aspect of PDE constrained optimization is to account for uncertainty in the underlying physical models, for example in model coefficients, boundary conditions, and initial data. Uncertainty in physical systems is modeled with random variables, however, in practice there may be some nontrivial ambiguity in the underlying probability distribution from which they are sampled. As stochastic optimal control problems are known to be ill-conditioned to perturbations in the sampling distribution, we describe an analytic framework that is better conditioned to such “meta-uncertainties” and conclude with numerical examples.

- **Scientific machine learning for blood glucose regulation in type 1 diabetes**

Speaker: Yixiang Deng (Brown University, University of Delaware)

Co-authors: Kevin Arao (BIDMC, Harvard Medical School), Christos Mantzoros (BIDMC, Harvard Medical School), George Karniadakis (Brown University)

Abstract. Due to insufficient insulin secretion, patients with type 1 diabetes mellitus (T1DM) are prone to blood glucose fluctuations ranging from hypoglycemia to hyperglycemia. While dangerous hypoglycemia may lead to coma immediately, chronic hyperglycemia increases patients’ risks for cardiorenal and vascular diseases in the long run. In principle, an artificial pancreas – a closed-loop insulin delivery system requiring patients to manually input insulin dosage according to the upcoming meals – could supply exogenous insulin to control the glucose levels and hence reduce the risks from hyperglycemia. However, insulin overdosing in some type 1 diabetic patients, who are physically active, can lead to unexpected hypoglycemia beyond the control of the common artificial pancreas. Therefore, it is important to take into account the glucose decrease due to physical exercise when designing the next-generation artificial pancreas. In this work, we develop a framework integrating systems biology-informed neural networks (SBINN), deep reinforcement learning (RL) algorithms, and T1DM data collected from wearable devices, to automate insulin dosing for patients. In particular, we build patient-specific computational models using SBINN to mimic the glucose-insulin dynamics for a few patients from the dataset, by simultaneously considering patient-specific carbohydrate intake and physical exercise intensity. Our patient-specific artificial pancreas, based on two deep RL algorithms, provided better insulin dosage, leading to safer glucose levels compared to those in the original dataset.

- **A numerical method for PDEs via stochastic particle trajectories**

Speaker: Jihun Han (University of Albany)

Abstract. I will present a numerical method for solving PDEs based on a stochastic representation of the solution. This approach captures the underlying particle dynamics associated with the physical processes described by the PDE. By aggregating information from the particles’ collective exploration, the method iteratively reinforces the approximation toward the solution. I will highlight its effectiveness across a broad class of problems, including elliptic equations with interfaces, multiscale structures, and perforated domains, as well as hyperbolic-type problems such as the Eikonal and Burgers equations.

- **Data-Driven Modeling with the Koopman Operator**

Speaker: Andrew Horning (Rensselaer Polytechnic Institute)

Abstract. Koopman operator theory provides an elegant way to learn nonlinear dynamics from data. In Koopman-based methods, a linear model of the dynamics in a high-dimensional feature space is computed directly from data with simple tools from numerical linear algebra. The eigenfunctions of the Koopman operator, approximated via the linear model, rigorously encode highly interpretable information about the state-space dynamics: fixed points, basins of attraction, periodic orbits, isoclines, phase reductions, and much more. In this talk, we identify several key challenges for the future of robust Koopman-based modeling and describe how ideas from approximation theory are improving the state-of-the-art.

- **Data Uniformity Improves Training Efficiency and More, with a Convergence Framework Beyond the NTK Regime**

Speaker: Yuqing Wang (Johns Hopkins University)

Co-authors: Shangding Gu (University of California, Berkeley)

Abstract. Data selection plays a crucial role in data-driven decision-making, including in large language models (LLMs), and is typically task-dependent. Properties such as data quality and diversity have been extensively studied and are known to enhance model performance. However, it remains unclear whether there exist other quantitative and general principles of data selection that can consistently improve performance, especially for complex tasks with limited prior knowledge. In this talk, I will demonstrate that selecting more uniformly distributed data can improve training efficiency while enhancing performance. Specifically, we establish that more uniform (less biased) distribution leads to a larger minimum pairwise distance between data points, denoted by $h_{\min}$, and prove that a smaller $h_{\min}$ can slow down the training dynamics of gradient descent (GD). Moreover, we theoretically show that the approximation error of neural networks decreases as $h_{\min}$ increases. Our analysis introduces a convergence framework for GD beyond the Neural Tangent Kernel (NTK) regime, applicable to a broad class of architectures, including transformers, without requiring Lipschitz smoothness. This framework further provides theoretical justification for the use of residual connections and function compositions in deep neural architectures. In the end, we conduct comprehensive experiments for supervised fine-tuning across various settings, including different optimization strategies, model sizes, and training datasets. The results consistently demonstrate that selecting data by maximizing pairwise distance accelerates training and achieves comparable or better performance in LLMs across diverse datasets. Code and Datasets are available at the link: <https://github.com/SafeRL-Lab/data-uniformity>.

- **Neural Correction Operator: solving EIT with operator learning and conditional diffusion model**

Speaker: Ke Chen (University of Delaware)

Abstract. Electrical Impedance Tomography (EIT) is a non-invasive medical imaging method that reconstructs electrical conductivity mediums from boundary voltage-current measurements, but its severe ill-posedness renders direct operator learning with neural networks unreliable. We propose the neural correction operator framework, which learns the inverse map as a composition of two operators: a reconstruction operator using L-BFGS optimization with limited iterations to obtain an initial estimate from measurement data and a correction operator implemented with deep learning models to reconstruct the true media from this initial guess. We explore convolutional neural network architectures and conditional diffusion models as alternative choices for the correction operator. We evaluate the neural correction operator by comparing with L-BFGS methods as well as neural operators and conditional diffusion models that directly learn the inverse map over several benchmark datasets. Our numerical experiments demonstrate that our approach achieves significantly better reconstruction quality compared to both iterative methods and direct neural operator learning methods with the same architecture. The proposed framework also exhibits robustness to measurement noise while achieving

substantial computational speedup compared to conventional methods. The neural correction operator provides a general paradigm for approaching neural operator learning in severely ill-posed inverse problems.

2.18 Computational Dynamics

MS Abstract. This session will discuss recent advanced in computational dynamics on the topic ranging from Synchronization, Arnold Tongues for Coupled Stochastic Oscillators, kernel regression of dynamical systems, weak Neural Ordinary Differential Equations, computational geometry for solving free boundary problems, and hybrid method for kinetic equations.

- **MSE Culpa - Why the mean-squared-error is not enough for machine learning of chaotic dynamical systems**

Speaker: Romit Maulik (Pennsylvania State University)

Co-authors: Dibyajyoti Chakraborty (Pennsylvania State University), Seung Whan Chung (Lawrence Livermore National Laboratory), Troy Arcomano (Allen Institute for AI)

Abstract. Predicting the long-term behavior of chaotic systems is notoriously difficult because of their sensitivity to initial conditions and the shortcomings of standard mean-squared error based optimization of data-driven models. In this work, we introduce a new training strategy for data-driven modeling of chaotic dynamical systems that overcomes issues of non-convexity and exploding gradients. The idea is to divide training trajectories into non-overlapping time windows and add a penalty that enforces continuity across these windows. We demonstrate that this technique improves the smoothness of the loss surface for an optimization and leads to machine learning models that can recover the invariant properties of high-dimensional chaotic dynamical systems. Our approach is demonstrated on canonical problems such as the Kuramoto Sivashinsky equations as well as for the forecasting of atmospheric dynamics from reanalysis data.

- **Modal Analysis of Quasi-Periodic Systems via Multi-variate Gaussian Process Regression**

Speaker: Jiwoo Song (Pennsylvania State University)

Co-authors: Daning Huang (Pennsylvania State University)

Abstract. Quasi-periodic systems that exhibit discrete frequencies (e.g., integer multiples of a fundamental tone) are frequently observed in science and engineering, including in aeroelastic flutter, vortex-induced vibrations, and other fluid–structure interaction problems. Accurate modal analysis of such systems is essential for uncovering the underlying dynamics, yet it poses challenges for standard tools such as dynamic mode decomposition (DMD) or spectral proper orthogonal decomposition (SPOD). While these methods effectively capture coherent structures, they rely on assumptions such as uniform sampling. Furthermore, they may suffer from spectral pollution and numerical discretization, limiting their robustness and accuracy in practical experimental and computational settings, especially in low-data limit. In this work, we extend multivariate Gaussian process regression (MVGPR) as a probabilistic framework for modal analysis of spatiotemporal data. By designing kernel functions tailored for harmonic processes, the proposed approach enforces conjugacy of modal conjugate pairs, thereby improving the reliability of phase and amplitude characterization. We establish the theoretical connection of MVGPR to system identification, DMD, and SPOD, and demonstrate its capability to handle temporally irregular data while mitigating spectral pollution. Representative examples are provided to demonstrate the advantages of the MVGPR approach over conventional modal analysis methods. The results illustrate the advantages of MVGPR over the conventional methods, showing that it can accurately capture the SPOD modes even when the data are temporally irregular without causing spectral pollution or numerical discretization error.

- **Koopman Eigenfunctions, Synchronization, and Arnold Tongues for Coupled Stochastic Oscillators**

Speaker: Maxwell Kreider (Pennsylvania State University)

Abstract. Phase reduction is an effective theoretical and numerical tool for studying synchronization of coupled deterministic oscillators, but stochastic oscillators require new definitions of asymptotic phase. The Q-function, i.e. the slowest decaying complex eigenmode of the stochastic Koopman operator (SKO), was proposed as a means of phase reduction for stochastic oscillators. Here, we show that the Q-function approach also leads to a novel definition of "synchronization" for coupled stochastic oscillators. A system of coupled oscillators in the synchronous regime may be viewed as a single (higher-dimensional) oscillator. Therefore, we investigate the relation between the Q-functions of the uncoupled oscillators and the higher-dimensional Q-function for the coupled system. We propose a definition of synchronization between coupled stochastic oscillators in terms of the eigenvalue spectrum of Kolmogorov's backward operator (the generator of the Markov process, or the SKO) of the higher dimensional coupled system. We observe a novel type of bifurcation reflecting the relationship between the leading eigenvalues of the SKO for the coupled system, and qualitative changes in the cross-spectral density of the coupled oscillators. Using our proposed definition, we observe synchronization domains for symmetrically-coupled stochastic oscillators that are analogous to Arnold tongues for coupled deterministic oscillators.

- **Geometric local parameterization for solving Hele-Shaw problems with surface tension**

Speaker: Zengyan Zhang (Pennsylvania State University)

Co-authors: Wenrui Hao (Pennsylvania State University), John Harlim (Pennsylvania State University)

Abstract. With broad applications in biology, physics, and materials science, including tumor growth and fluid interface dynamics, the Hele-Shaw problem with surface tension provides a canonical model for studying the dynamics of evolving interfaces. Solving such problems requires precise treatment of sharp boundaries. However, constructing a global parameterization for complicated surfaces and explicitly tracking boundary motion is challenging. In this work, we present a geometric local parameterization approach for efficiently solving the two-dimensional Hele-Shaw problems, where the boundary is identified only from randomly sampled data. Through convergence and error analysis, as well as numerical experiments, we demonstrate the capability and effectiveness of our approach in resolving complex interface evolution.

- **A Fully Implicit Hybrid Method for Kinetic Equations: Efficient Time Integration via Coarse-Fine Velocity Grid Coupling**

Speaker: Evan Habbershaw (Pennsylvania State University)

Abstract. Fully implicit solvers for kinetic equations permit large stable time steps, but their cost scales poorly with the size of the velocity grid, limiting practical simulations. We present a fully implicit hybrid strategy that couples fine and coarse velocity grids: the fine-grid component is advanced with an implicit sweeping solver tailored to linear advection-relaxation subproblems, while the coarse-grid component is updated implicitly using an iterative solver that captures the remaining nonlinear coupling. On representative $2x2v$ tests, the method reduces CPU wall time significantly relative to a baseline fully implicit approach, with even greater gains on GPUs as velocity-grid size grows. We discuss algorithmic design (split formulation, grid communication, solver details), verification against standard tests, and outline ongoing work toward $3x3v$ cases where cubic growth in velocity degrees of freedom further amplifies the savings. The approach provides a practical path to stable, accurate, and faster kinetic simulations within a fully implicit framework.

2.19 Recent Advances in Numerical Scheme-Inspired Data-driven Methods

MS Abstract. This mini-symposium highlights recent progress at the intersection of scientific computing, numerical analysis, and machine learning. We bring together researchers developing data-driven methods for learning operators, embedding physical laws and wisdoms from numerical methods into machine learning architectures, and advancing the theory of physics-informed and scientific machine learning. Applications include mathematical modeling, inverse problems, and uncertainty quantification, illustrating the growing impact of these methods across applied mathematics.

- **Convergence and Performance of Finite-Difference-Based Methods for Noisy Black-Box Optimization**

Speaker: Dat Tran (Rowan University)

Abstract. In this talk we discuss recent advances in derivative-free optimization for challenging nonconvex problems where only function evaluations, possibly noisy, are available. We present finite difference based methods that balance gradient approximation accuracy with step sizes. In the noiseless case, we establish convergence of gradients to zero and global convergence rates under broad assumptions. In the noisy case, our algorithms reach near stationary points without prior knowledge of the noise level, and we provide explicit complexity guarantees. We also introduce two new strategies for functions with locally Lipschitz continuous gradients: one based on backtracking line search and another based on a dynamic step line search that remains effective under noise. Finally, numerical experiments on a variety of test problems demonstrates the robustness and efficiency of our new methods in comparison with widely used solvers such as those in SciPy.

- **Neural Networks with Trainable Matrix Activation Functions**

Speaker: Zhengqi Liu (Pennsylvania State University)

Co-authors: Ludmil Zikatanov (Pennsylvania State University), Shuhao Cao (University of Missouri), Yuwen Li (Zhejiang University)

Abstract. The training process of neural networks usually optimize weights and bias parameters of linear transformations, while nonlinear activation functions are pre-specified and fixed. This work develops a systematic approach to constructing matrix-valued activation functions. The activation is based on linear operators whose matrix representations depend non-linearly on the data. Such operators are defined using only scalar multiplications and comparisons. The proposed activation functions depend on parameters that are trained along with the weights and bias vectors. Neural networks based on this approach are simple and efficient and are shown to be robust in numerical experiments.

- **The Measure Theoretic Koopman Operator**

Speaker: Maria Oprea (Cornell University)

Abstract. The Stochastic Koopman (SKO) operator has been associated in literature with dynamical systems that exhibit stochastic behaviour. However, the SKO can only recover the expectation of an observable along the trajectory and requires tracking data for its computation. In this work, the Distributional Koopman Operator (DKO) is introduced as a novel framework for analyzing stochastic dynamical systems where only aggregate distribution data is available, avoiding the need for particle tracking. Our DKO framework extends the Koopman operator to act on observables of probability distributions, leveraging the transfer operator to propagate these distributions forward in time. We analyse the properties of this new operator, and show how one can recover information about higher order moments from this formulation. Lastly, we design an algorithm to compute the DKO from data.

- **Fine-tuning Spatiotemporal Operator Learning for Turbulent Flows**

Speaker: Shuhao Cao (University of Missouri)

Co-authors: Yuanzhe Xi (Emory University), Ruipeng Li (Lawrence Livermore National Laboratory), Francesco Brarda (Emory University)

Abstract. Recent advancements in operator-type neural networks have shown promising results in approximating the solutions of spatiotemporal Partial Differential Equations (PDEs). However, these neural networks often entail considerable training expenses, and may not always achieve the desired accuracy required in many scientific and engineering disciplines. In this paper, we propose a new learning framework to address these issues. To better exploit this capacity, a new paradigm is proposed to refine the commonly adopted end-to-end neural operator training and evaluations with the help from the wisdom from traditional numerical PDE theory and techniques. Specifically, in the learning problems for the turbulent flow modeled by the Navier-Stokes Equations (NSE), the proposed paradigm trains an FNO only for a few epochs. Then, only the newly proposed spatiotemporal spectral convolution layer is fine-tuned without the frequency truncation. Numerical experiments on commonly used NSE benchmarks demonstrate significant improvements in both computational efficiency and accuracy, compared to end-to-end evaluation and traditional numerical PDE solvers under certain conditions. The source code is publicly available at <https://github.com/scaomath/torch-cfd>.

2.20 Scientific Machine Learning for Dynamical Systems and Inverse Problems

MS Abstract. Scientific Machine Learning (SciML) has emerged as a transformative paradigm for modeling, simulating, and understanding complex dynamical systems across science and engineering. This minisymposium brings together researchers at the intersection of machine learning and science to discuss recent advances in data-driven and hybrid modeling techniques for dynamical systems and inverse problems. Topics include physics-informed learning, operator learning, uncertainty quantification, data assimilation, and structure-preserving algorithms. The sessions will highlight both theoretical developments and practical applications in areas such as chaotic systems and turbulence dynamics. The goal is to foster cross-disciplinary dialogue and identify future directions for robust, interpretable, and efficient SciML methods in the study of dynamical systems and the solution of inverse problems.

• Physics-scaling informed data-driven turbulent inflow generation

Speaker: Xiang Yang (Pennsylvania State University)

Abstract. The specification of turbulent inflow requires not only accurate mean flow profiles but also realistic turbulent fluctuations. Generative AI, with its ability to synthesize high-fidelity data, offers promising new avenues for this longstanding challenge. While recent generative-AI-based methods have achieved realistic inflow fields, their applicability remains limited by stability concerns and, critically, by poor generalization beyond the Reynolds numbers used in training. This work introduces a physics-scaling-informed generative framework that achieves both realism and Reynolds number generalization. A variational autoencoder (VAE) compresses turbulent boundary-layer fields at $Re_\theta = 750$ into an $O(10)$ -dimensional latent space, while a long short-term memory (LSTM) network models temporal evolution. Generalization across Reynolds numbers is enabled by a rescaling-recycling strategy based on inner and outer scaling laws from boundary-layer theory, a procedure that can also extend to other generative-AI methods. In addition to proposing this new VAE-LSTM framework, we conduct a systematic comparative study of turbulent inflow generation methods, including the generative-AI-enabled ConField and widely adopted synthetic methods such as DF and DFSEM. Results show that AI-based methods produce more realistic inflow fields and shorter development lengths at the training Reynolds number than synthetic approaches, but all methods—AI-based and synthetic—require comparable development lengths ($\sim 10\delta$) when extrapolating beyond the training regime. Between the two AI-based methods, VAE-LSTM achieves accuracy comparable to ConField while requiring significantly less training data and computational cost. To promote adoption and reproducibility, our implementations of the VAE-LSTM and all benchmarked methods are released openly within OpenFOAM.

- **Bayesian Inversion for Elliptic PDEs on unknown manifolds**

Speaker: John Harlim (Pennsylvania State University)

Abstract. In this talk, I will discuss recent efforts in solving Bayesian inverse problems involving elliptic PDEs on unknown domains identified with point cloud data that lie on a Riemannian compact embedded manifold. Particularly, I will discuss graph-Laplacian-based methods for designing Matern-type priors and solving mesh-free PDE solvers. When the manifolds have Dirichlet boundary conditions, we consider a prior represented by linear superpositions of Dirichlet Laplacian eigenfunctions and solutions of harmonic functions with appropriate boundary conditions. If time permitted, I would demonstrate how to extend this approach in the neural operator setting to speed up the Bayesian inference.

- **Multimodal Atmospheric Super-Resolution With Deep Generative Models**

Speaker: Haiwen Guan (Pennsylvania State University)

Abstract. Score-based diffusion modeling is a generative machine learning algorithm that can be used to sample from complex distributions. They achieve this by learning a score function, i.e., the gradient of the log-probability density of the data, and reversing a noising process using the same. Once trained, score-based diffusion models not only generate new samples but also enable zero-shot conditioning of the generated samples on observed data. This promises a novel paradigm for data and model fusion, wherein the implicitly learned distributions of pretrained score-based diffusion models can be updated given the availability of online data in a Bayesian formulation. In this article, we apply such a concept to the super-resolution of a high-dimensional dynamical system, given the real-time availability of low-resolution and experimentally observed sparse sensor measurements from multimodal data. Additional analysis on how score-based sampling can be used for uncertainty estimates is also provided. Our experiments are performed for a super-resolution task that generates the ERA5 atmospheric dataset given sparse observations from a coarse-grained representation of the same and/or from unstructured experimental observations of the IGRA radiosonde dataset. We demonstrate accurate recovery of the high dimensional state given multiple sources of low-fidelity measurements. We also discover that the generative model can balance the influence of multiple dataset modalities during spatiotemporal reconstructions.

- **Hyperbolic machine learning moment closures for kinetic equations**

Speaker: Juntao Huang (University of Delaware)

Abstract. In this talk, we take a data-driven approach and apply machine learning to the moment closure problem for kinetic equations. Instead of learning the unclosed high order moment, we propose to directly learn the gradient of the high order moment using neural networks, called the gradient-based moment closure. Moreover, we introduce two approaches to enforce the hyperbolicity of our gradient-based machine learning moment closures. A variety of benchmark tests, including the variable scattering problem, the Gaussian source problem and the two material problem, show both good accuracy and generalizability of our machine learning closure model.

- **Parametrizing Contact Diffeomorphisms**

Speaker: George Kevrekidis (Johns Hopkins University)

Abstract. The study of contact geometry, the “odd-dimensional” analogue of symplectic geometry, is an important sub-field of Differential Geometry that has attracted significant interest from both theoretical *and* applied perspectives. It is central in our understanding of dissipative systems and lies at the heart of differential equivalence problems, but can be used as a theoretical framework in many other fields as well, such as optimization theory or thermodynamics; This is also suggested by the recent (over the past 5 years) surge of publications in the area. In this presentation, we consider the possibility of parametrizing contact flows, i.e. one-parameter families of *contact* diffeomorphisms, by

composing exact contact maps with prolonged diffeomorphisms of the first jet space. This arises as a natural extension of pre-existing work for symplectic systems. This approach has advantages from an applied perspective (e.g. producing contact integrators amenable to back-propagation) but also has interesting theoretical aspects, in particular whether the approach could be universal. We further discuss with several computational examples.

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2.21 Recent Developments in Applied Inverse Problems and Imaging

MS Abstract. Inverse problems for Partial Differential Equations (PDEs) are common in practical fields such as non-destructive testing, medical imaging, photonics, optics, geophysical exploration, and radar technology. These problems typically involve identifying unknown information about the PDEs, like coefficients, initial conditions, or domain shapes, using the solution data. Theoretical and computational studies of these inverse problems have garnered considerable interest across mathematics, engineering, and physics. Over the past several decades, this research area has rapidly expanded, achieving significant progress in mathematical theory, computational methods, and applications. This mini-symposium aims to gather researchers from various subfields to share recent findings, exchange ideas, and explore future collaborative opportunities.

- **Extending Qualitative Methods to Biharmonic Scattering**

Speaker: Isaac Harris (Purdue University)

Abstract. In this talk, we will discuss extending the direct sampling method (DSM) to inverse shape problems for biharmonic scattering. This method is a computationally simple and analytically rigorous way to define an imaging function to recover the scatterer. Here, we will focus on the case of scattering by a clamped region by an incident plane wave. Using the far-field data, we will analyze the DSM and prove its a stable reconstruction method. The techniques for analyzing the DSM are similar to the standard Helmholtz equation with a few interesting surprises we will discuss how to tackle. Numerical examples are given to show the applicability of the imaging functionals. We will also discuss the associated transmission eigenvalue problem.

- **All-at-once alternating minimization method for an inverse medium scattering problem**

Speaker: Thanh Nguyen (Rowan University)

Co-authors: Luca Barone (Rowan University), Dat Tran (Rowan University)

Abstract. We present a numerical method for solving an inverse medium scattering problem using the all-at-once approach. In this approach, the inverse scattering problem is converted into an optimization problem in which both the medium parameter and the state variable are considered as unknown variables. The resulting optimization problem is solved by an alternating minimization algorithm. We will discuss the convergence of the proposed algorithm and illustrate its performance with numerical examples.

- **Identifying defective units in infinite periodic arrays of sources**

Speaker: Nhung Nguyen (Kansas State University)

Abstract. This talk focuses on detecting defective units in unbounded periodic arrays of radiating sources, motivated by nondestructive evaluation of large-scale source systems. A key challenge is that defects break the periodicity of the structure, which leads us to employ the Floquet–Bloch transform to recover it. Combining this approach with our stable imaging function, we develop a numerical method capable of identifying defective sources. The method determines not only the number of defects but also their locations and intensities. Numerical experiments confirm its robustness, accuracy, and effectiveness. This is joint work with Dinh-Liem Nguyen and Thi-Phong Nguyen.

- **Statistical Inversion using Deep Network and Level Set Methods for Diffuse Optical Imaging**

Speaker: Taufiqar Khan (University of North Carolina at Charlotte)

Abstract. In this talk, we provide an overview of the ill-posed inverse problem in Diffuse Optical Tomography (DOT). Then we present the Bayesian inversion using deep learning and level sets for image reconstruction which is significantly faster than inversion using finite element method. The results of image reconstruction is demonstrated using synthetic data for the recently proposed algorithm. This is joint work with Sudeb Majee (UNC Charlotte), Anuj Abhisekh (Case Western Reserve University) and Thilo Strauss (Xi'an Jiaotong-Liverpool University).

- **Inside-out duality for scattering poles**

Speaker: Jiguang Sun (Michigan Technological University)

Co-authors: Xiaodong Liu (Chinese Academy of Sciences), Lei Zhang (Zhejiang University of Technology)

Abstract. Scattering poles correspond to non-trivial scattered fields in the absence of incident waves and play a crucial role in the study of wave phenomena. These poles are complex wavenumbers with negative imaginary parts. In this paper, we prove two generalized Rellich's lemmas for scattered fields associated with complex wavenumbers. These lemmas are then used to establish uniqueness results for inverse scattering problems. We further explore the inside-out duality, which characterizes scattering poles through the linear sampling method applied to interior scattering problems. Notably, we demonstrate that exterior Dirichlet/Neumann poles can be identified without prior knowledge of the actual sound-soft or sound-hard obstacles. Numerical examples are provided to validate the theoretical results.

- **Integral equations for linear flexural-gravity waves**

Speaker: Jeremy Hoskins (University of Chicago)

Abstract. Flexural waves, the propagation of waves in thin elastic sheets, arise in a number of contexts, and, particularly, in the study of ice shelves. In the frequency domain, they are commonly modeled as a fourth order PDE in two dimensions with clamped plate, free plate, or supported plate boundary conditions. Here, we review existing approaches for solving boundary value problems of this type, and discuss some limitations. Building on this, for the supported plate and free plate problems, we propose novel representations which ultimately reduce the problems to second kind integral equations. Moreover, the resulting integral equations are amenable to standard high order discretization approaches and fast algorithms. Several numerical examples will be presented which illustrate the properties of these integral equations. Finally, generalizations to other wave phenomena will be discussed.

- **Super-resolution Imaging in Disordered Media**

Speaker: Alexei Novikov (Pennsylvania State University)

Abstract. High-resolution imaging in complex media, such as turbulent air, underwater environments, or biological tissues, faces challenges due to wavefront distortion caused by scattering from inhomogeneities. I will describe an approach for imaging point-like sources in scattering media when large and diverse datasets are available. We use algorithms derived from computer science and statistics, diverging from traditional imaging techniques. Specifically, we first employ a dictionary learning algorithm to accurately estimate signals from all possible positions of the sources. Then, we apply a Multi-Dimensional Scaling algorithm to convert information about correlations of the estimated signals into the corresponding positions of their sources.

- **A fast reconstruction method for radiating sources in Maxwell's equations**

Speaker: Thu Le (University of Wisconsin)

Co-authors: Dinh-Liem Nguyen (Kansas State University), Isaac Harris (Purdue University)

Abstract. This talk presents a fast and robust numerical method for reconstructing point-like sources in the time-harmonic Maxwell's equations, given Cauchy data at a fixed frequency. This electromagnetic inverse source problem arises in applications such as antenna synthesis and pollution source tracing. We introduce a new boundary-integral-based method and a computational algorithm to recover unknown sources, supported by theoretical analysis and stability results. Even in the presence of noise, our method accurately and efficiently localizes electromagnetic sources. It also estimates the moment vectors of point sources and the directions of these vectors for small-volume sources with low relative error, demonstrating the robustness of the approach. In addition, the method enables imaging at arbitrary distances from the measurement boundary and offers easy implementation with low computational cost. Numerical examples in three dimensions are presented to demonstrate the performance of our method.

- **Learning Surrogates and Operator-to-Function Maps for Imaging Inverse Problems**

Speaker: Anuj Abhishek (Case Western Reserve University)

Abstract. Inverse problems in imaging often involve reconstructing unknown quantities from indirect and noisy measurements, and their solution is typically hindered by expensive forward computations and ill-posedness. Recent advances in operator learning provide new perspectives on how to address these challenges. In this talk, we will discuss how neural operator architectures can be used both to accelerate classical Bayesian inference methods and to learn novel operator-to-function mappings arising in imaging applications. Along the way, we will highlight theoretical approximation guarantees and illustrate these ideas through examples from medical imaging.

- **A nonlocal boundary value method for fractional parabolic equations**

Speaker: Thi-Phong Nguyen (New Jersey Institute of Technology)

Co-authors: Nguyen Van Duc (Vinh University), Nguyen Van Thang (Quan Hanh Secondary School)

Abstract. Fractional-derivative models, which capture anomalous transport by incorporating time-based memory effects and nonlocal spatial influences, are applicable in various fields, including physics, engineering, geoscience, and finance. Backward time-space-fractional parabolic equations arise in inverse problems of anomalous diffusion or transport models, where the goal is to recover the initial state from data at a later time. As is typical, such problems are highly ill-posed. In this talk, we discuss a nonlocal boundary value method for regularizing the problem. A Hölder-type error estimate is also derived using both a priori and a posteriori parameter choice rules. The efficiency of the method is demonstrated through numerical examples.

2.22 Mathematical modelling for infectious diseases and interventions

MS Abstract. Societies are shaped by the effects of both emerging and returning infectious diseases. For example, the bubonic plague killed as many as 50% of the 14th century European population, and more recently, consider the societal shifts surrounding COVID-19, a pandemic responsible directly and indirectly for the deaths of over 20 million people worldwide. Diseases once nearly eliminated from regions with quality healthcare, such as measles and tuberculosis, have resurged due to behavioral changes, rising antimicrobial resistance, and other compounding factors. These trends highlight the global importance of studying and deploying interventions such as vaccines and antimicrobial treatments as well as their effects. In this minisymposium, we will explore the interplay between infection and intervention at in-host, hospital, and epidemic scales with an emphasis on bacterial infections. This minisymposium showcases many different mathematical modeling approaches, including ODE models, statistical models, and game theoretic models.

- **A General Analytic Approach to Predicting the Best Antibiotic Dosing Regimen**

Speaker: Leah Childers (Pennsylvania State University)

Abstract. Determining optimal antibiotic dosing strategies is complex. Clinically, some antibiotics work best in continuous low doses, while others require high repeated pulses. However, the best approach for any antibiotic and bacterial infection remains unclear. Using mathematical models, we analyze bacterial populations under two strategies – constant concentration and repeated dosing – given fixed pharmacodynamic and pharmacokinetic properties. Our results reveal that the shape of the dose-response curve, which measures bacterial net growth rate against antibiotic concentration, is crucial. Specifically, its concavity determines the optimal dosing strategy. In cases where the curve exhibits multiple concavities, additional factors such as desired or tolerable dosing range influence the regimen. These findings challenge the universal application of “hit hard and hit early,” as some recommended schedules include lower, constant doses.

- **Inference of asymptomatic carriers of antimicrobial-resistant organisms in healthcare settings using multimodal observations**

Speaker: Sen Pei (Columbia University)

Co-authors: Dwayne Seeram (Columbia University), Seth Blumberg (University of California San Francisco), Bo Shopsis (New York University), Anne-Catrin Uhlemann (Columbia University), Jeffrey Shaman (Columbia University)

Abstract. Asymptomatic carriers of antimicrobial-resistant organisms (AMROs) can unwittingly transmit these pathogens in healthcare systems, contributing to the burden of healthcare-associated infections (HAIs). Surveillance in hospitals can involve different types of observations to monitor AMRO spread; however, a framework to coherently synthesize these datasets to identify AMRO carriers is lacking. Here, we develop a new inference framework combining a data-driven mechanistic transmission model and multimodal observations from clinical cultures, electronic health records, patient mobility, and genomic sequence data. Using extensive simulated outbreaks, we validate the inference framework for AMROs with various levels of community importation and hospital transmission and evaluate the utility of different combinations of data sources. Inference results show that using multimodal observations consistently improves the accuracy in identifying AMRO carriers. We apply the inference framework to carbapenem-resistant *Klebsiella pneumoniae* (CRKP) at an urban quaternary care hospital and find that the addition of even sparsely sampled genome sequence data to patient characteristics supports more accurate identification of CRKP carriers. Model simulations suggest that inference-guided targeted isolation leads to a greater reduction of AMRO burdens compared to alternative, heuristic approaches. Thus, the synergistic effect of utilizing multimodal observations for estimating AMRO carriage risk may inform improved interventions in hospital settings.

- **Multiple Rational Behaviors in a Cholera Intervention Game**

Speaker: Connor Olson (Pennsylvania State University)

Abstract. Human behavior is central to the unfolding of an epidemic. The classic theory of mathematical epidemiology does not parameterize human behavior and correcting this oversight has been a major research effort over the last half century. In this talk, we present an adaptation of the social distancing game (SDG) to a disease inspired by Cholera that has an environmental reservoir that contributes to infection risk, which we coin the Environmental Distancing Game (EDG). As opposed to SDGs, which are proven to have unique Nash strategies in the SI case, we reveal that EDGs possess multiple subgame perfect equilibrium strategies even in the simplest models. We then explore the structure of these rational strategies and explain how unexpected behaviors can arise in certain parameter regimes. To conclude, we discuss why our results are indicative of similarly complicated strategies in EDGs built upon more complex epidemic models.

- **Modeling PrEP-on-demand strategies to prevent HIV transmission**

Speaker: Jessica Conway (Pennsylvania State University)

Abstract. In 2010, analysis of the iPrEx study results demonstrated that daily dosing with antiretroviral therapy (ART) in advance of exposure to HIV, termed pre-exposure prophylaxis (PrEP), can significantly reduce the risk of HIV transmission and population spread. However, daily adherence to a drug regimen can be difficult to maintain and may come with side-effects. In contrast, the IPERGAY study published in 2015 suggested that short-term use around the time of exposure may be just as effective at reducing HIV risk as daily use. Here we investigate short-term use, termed "on-demand" or "event-based" PrEP. We aim to make model-based predictions of effective on-demand drug regimen. Focusing on transmission through sexual exposure, we incorporate a deterministic model of tissue-level pharmacokinetics and pharmacodynamics (PK/PD) of Truvada into a branching-process model of early HIV infection. Thus, we predict the risk of HIV transmission and risk reduction associated with dose size and timing relative to exposure. To evaluate effectiveness of dosing strategies, we simulate strategies by sampling a virtual population and performing extensive sensitivity analyses. Hence, we aim to identify practical dosing strategies that most effectively reduce risk of HIV transmission through sexual exposure.

- **Stochastic Models of Viral Replication Dynamics: Extinction of Virus and Host**

Speaker: Rahnuma Islam (University of Pittsburgh)

Co-authors: David Swigon (University of Pittsburgh)

Abstract. Although viral dynamics is typically modeled using ordinary differential equations, a natural way to address the phenomena of viral persistence and host cell survival is to use stochastic models of viral reproduction. Here we present a study of viral and substrate cell extinction and their dependence on viral production rate for two simple stochastic models of viral reproduction that differ in the method of viral release: one accounts for viral bursting, in which the release of viruses is instantaneous after cell lesion, the other for viral budding, in which new viral particles are released from infected cells gradually. We show that for both viral release mechanisms, simulation of continuous-time Markov chain versions of the stochastic models is the most accurate but also time-consuming way to obtain the results, and that traditional diffusion approximation methods lead to serious discrepancies in extinction probabilities and mean times. We then propose a modified stochastic differential equation approach that achieves a significant improvement in simulation speed while maintaining accuracy.

2.23 AI for Math

MS Abstract. The AI for Math minisymposium explores the intersection of artificial intelligence and mathematical research, with a focus on how large language models and related techniques can advance mathematical reasoning, discovery, and education. Speakers will present recent developments in AI-assisted theorem proving, symbolic computation, and applications of machine learning to mathematical problem solving. The session aims to foster dialogue between researchers in mathematics, computer science, and AI, highlighting opportunities for collaboration and the future of AI-driven mathematical exploration.

- **Can Large Language Models Adequately Perform Symbolic Reasoning Over Time Series?**

Speaker: Zewen Liu (Emory University)

Co-authors: Juntong Ni (Emory University), Xianfeng Tang (Amazon), Max S.Y. Lau (Emory University), Wenpeng Yin (Pennsylvania State University), Wei Jin (Emory University)

Abstract. Uncovering hidden symbolic laws from time series data, as an aspiration dating back to Kepler's discovery of planetary motion, remains a core challenge in scientific discovery and artificial intelligence. While Large Language Models show promise in structured reasoning tasks, their ability

to infer interpretable, context-aligned symbolic structures from time series data is still underexplored. To systematically evaluate this capability, we introduce SymbolBench, a comprehensive benchmark designed to assess symbolic reasoning over real-world time series across three tasks: multivariate symbolic regression, Boolean network inference, and causal discovery. Unlike prior efforts limited to simple algebraic equations, SymbolBench spans a diverse set of symbolic forms with varying complexity. We further propose a unified framework that integrates LLMs with genetic programming to form a closed-loop symbolic reasoning system, where LLMs act both as predictors and evaluators. Our empirical results reveal key strengths and limitations of current models, highlighting the importance of combining domain knowledge, context alignment, and reasoning structure to improve LLMs in automated scientific discovery.

- **Derivation of physical equations for high-speed laser welding using large language models**

Speaker: Zhengxiao Yu (Pennsylvania State University)

Abstract. It is challenging to formulate complex physical phenomena that occur in a manufacturing process, particularly when the available data are limited, rendering conventional data-driven approaches ineffective. This study aims to predict humping onset in high-speed laser welding by introducing a novel framework, namely text-to-equations generative pre-trained transformer (T2EGPT). This method leverages the capabilities of large language models (LLMs), in combination with sparse experimental data and enriched literature data, to derive an interpretable and generalizable equation for predicting humping initiation. By capturing key correlations among physical parameters, T2EGPT generates a compact and dimensionless expression that accurately predicts hump formation. The equation reveals that humping arises from the interplay between inertia-driven backward melt flow and capillary-driven surface stabilization, where inertial forces drive molten metal backward and capillary forces resist surface deformation. Compared to traditional data-driven models, T2EGPT demonstrates enhanced predictive accuracy and cross-material transferability. More broadly, this study highlights the potential of LLMs to integrate textual information with data-driven discovery, enabling the extraction of physical laws in data-scarce scientific domains.

- **FoVer: Training Step-Level Reasoning Verifiers with Formal Verification Tools**

Speaker: Ryo Kamoi (Pennsylvania State University)

Abstract. Process Reward Models (PRMs), which provide step-level feedback on the reasoning generated by Large Language Models (LLMs), are receiving increasing attention. However, two key research gaps remain: creating training data for PRMs that includes accurate step-level error labels typically requires costly human annotation, and existing PRMs are limited to math reasoning problems. In response to these gaps, this work aims to enable automatic synthesis of training data for PRMs with accurate error labels and the generalization of PRMs to diverse reasoning tasks. We propose FoVer, an approach to create training data for PRMs using step-level error labels automatically annotated by formal verification tools, such as Z3 and Isabelle, which provide automatic and accurate verification for symbolic tasks like formal theorem proving. Using this approach, we synthesize training data for PRMs that includes accurate step-level error labels on LLM responses for formal logic and theorem proving tasks without relying on human annotation. Although this data synthesis is feasible only for tasks compatible with formal verification, we observe that LLM-based PRMs trained on our dataset exhibit cross-task generalization, improving verification across diverse reasoning tasks. Specifically, PRMs trained with FoVer significantly outperform baseline PRMs based on the original LLMs and achieve competitive or superior results compared to state-of-the-art PRMs, as measured by step-level verification on ProcessBench and Best-of-K performance across 12 reasoning benchmarks, including MATH, AIME, ANLI, MMLU, and BBH.

- **The Quest for Open-Source Olympiad AI**

Speaker: Hamed Mahdavi (Pennsylvania State University)

Abstract. Less than a year ago, our work, "Brains vs. Bytes," highlighted a significant weakness in even the most advanced Large Language Models: a failure to produce logically sound proofs for complex mathematical problems. We showed that models were adept at finding answers. However, they lacked the rigorous, sound reasoning that is the hallmark of human mathematics. At the time, the prospect of an AI achieving top-tier performance in a competition like the International Mathematical Olympiad seemed distant.

That entire landscape was upended in July 2025. At the IMO, frontier proprietary models from Google and OpenAI demonstrated a stunning breakthrough, achieving a performance equivalent to a gold medal. This landmark event proved that machine-based mathematical reasoning at the highest level is possible. However, the methods for this success remained inaccessible to the broader research community.

In light of this achievement, our research program has pivoted to a new and ambitious goal: to replicate this remarkable result using entirely open-source models. This talk will detail our strategy, which focuses on using **agentic** workflows to intelligently generate synthetic data that improves LLMs mathematical proof writing capabilities. We will explain how we use agents to guide proprietary models to "show their work." This generates not just final proofs, but also strategic plans, critiques of flawed attempts, and high-level explanations. This process creates a rich, targeted dataset designed to teach smaller, open models the advanced problem-solving techniques that were previously out of reach. Our ultimate aim is to democratize this new frontier of AI, making elite mathematical reasoning a transparent and reusable capability for researchers and educators everywhere.

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2.24 Foundation Models: From Theory to Practice

MS Abstract. This minisymposium aims to bring together researchers that work on advancing the state of the art of foundation models. Foundation models are designed to learn common patterns from vast datasets, allowing them to be adapted for a wide range of downstream tasks in a zero-shot or few-shot manner, rather than being built from scratch for each application. In recent years, foundation models have achieved substantial advance in modeling, mathematical analysis, and computational practices. This minisymposium focuses on recent developments in Transformer, Mamba, Mixture of Experts (MoE), and other foundation models.

- **Towards Interpretable Time Series Foundation Models**

Speaker: Tengfei Ma (Stony Brook University)

Abstract. Time series data prevail in a broad spectrum of domains such as healthcare, finance, and climate research. In recent years foundation models have been reshaping the AI research, however, there are intrinsic challenges for building foundation models for time series. In this talk, I will discuss about these challenges and present our recent work on a shape-based time series foundation model that achieves both generalizability and interpretability. I will further discuss how the shape-based model can be integrated with complementary architectures, as well as approaches aligning heterogeneous pretrained time series models via latent graphs.

- **Sparse and Low-Dimensional Structures in Deep Networks**

Speaker: Akshay Rangamani (New Jersey Institute of Technology)

Abstract. In this talk I will describe recent progress in characterizing low dimensional structure that emerges in deep networks. First we explore the phenomenon of Neural Collapse where top-layer feature embeddings of samples from the same class tend to concentrate around their means, and the top layer's weights align with those features. We first show how it emerges when training deep networks with weight decay and normalization. We then investigate these properties in intermediate layers and explore its implications for generalization in deep learning. Next we show how to extend the basic tool

of decomposing covariances to uncover low-dimensional structures in deep regression models. Finally we investigate a toy model for modular addition through Fourier representations to show how language models might learn low-dimensional structures.

- **A Foundation Model Approach for Learning Causal Graphs**

Speaker: Naiyu Yin (Lehigh University)

Co-authors: Yue Yu (Lehigh University)

Abstract. Due to its human-interpretability and invariance properties, Directed Acyclic Graph (DAG) has been a foundational tool across various areas of AI research, leading to significant advancements. However, DAG learning remains highly challenging, due to its super-exponential growth in computational cost and identifiability issues, particularly in small-sample regimes. To address these two challenges, in this work we leverage the recent success of linear transformers and develop a foundation model approach for discovering multiple order-consistent DAGs across tasks. In particular, we propose Attention-DAG (ADAG), a novel attention-mechanism-based architecture for learning multiple linear Structural Equation Models (SEMs). ADAG learns the mapping from observed data to both graph structure and parameters via a nonlinear attention-based kernel, enabling efficient multi-task estimation of the underlying linear SEMs. By formulating the learning process across multiple tasks as a continuous optimization problem, the pre-trained ADAG model captures the common structural properties as a shared low-dimensional prior, thereby reducing the ill-posedness of downstream DAG learning tasks in small-sample regimes.

We evaluate our proposed approach on benchmark synthetic datasets and find that ADAG achieves substantial improvements in both DAG learning accuracy and zero-shot inference efficiency. To the best of our knowledge, this is the first practical approach for pre-training a foundation model specifically designed for DAG learning, representing a step toward more efficient and generalizable downstream applications in causal discovery.

- **PDE Foundation Model: Generalization, Learning to Learn and more**

Speaker: Jingmin Sun (Johns Hopkins University)

Co-authors: Yuxuan Liu (University of California, Los Angeles), Zecheng Zhang (University of Notre Dame), Hayden Schaeffer (University of California, Los Angeles)

Abstract. This talk explores the path toward foundation models for scientific computing, focusing on learning solution operators for parametric partial differential equations (PDEs). The core of the presentation showcases our contributions to overcoming these limitations: (1) A multi-modal transformer framework (PROSE) that achieves zero-shot generalization to new PDE families by jointly processing input functions and symbolic equations; and (2) A meta-learning strategy (LeMON) that enables a single pre-trained neural operator to rapidly adapt to new physical systems with minimal data. Together, these advances bridge the gap between specialized, single-task solvers and a flexible, multi-operator foundation model capable of real-time simulation and design.

- **Toward Universal Foundation Model for Neuroimaging**

Speaker: Huang Haoxu (New York University)

Abstract. Recent advances in self-supervised learning have enabled data-driven approaches to building generalist models by leveraging massive amounts of unlabeled data. In this talk, I will present our work on developing 3D imaging foundation models for neuroimaging. I will highlight how our approach achieves notable gains in both efficiency and performance compared to existing 3D imaging foundation models, and discuss its potential for advancing large-scale neuroimaging research.

- **Hierarchical Mamba Meets Hyperbolic Geometry: A New Paradigm for Structured Language Embeddings**

Speaker: Mengjia Xu (New Jersey Institute of Technology)

Co-authors: Sarang Patil (New Jersey Institute of Technology), Ashish Pandey (New Jersey Institute of Technology), Ionnis Koutis (New Jersey Institute of Technology)

Abstract. Selective state-space models excel at long-sequence modeling, but their capacity for language representation – in complex hierarchical reasoning – remains underexplored. Most large language models rely on *flat* Euclidean embeddings, limiting their ability to capture latent hierarchies. To address this, we propose Hierarchical Mamba (HiM), integrating efficient Mamba2 with hyperbolic geometry to learn hierarchy-aware language embeddings for deeper linguistic understanding. Mamba2-processed sequences are projected to the Poincaré ball or Lorentzian manifold with “learnable” curvature, optimized with a hyperbolic loss. Our HiM model facilitates the capture of relational distances across varying hierarchical levels, enabling effective long-range reasoning for tasks like mixed-hop prediction and multi-hop inference in hierarchical classification. Experimental results show both HiM effectively capture hierarchical relationships across four linguistic and medical datasets, surpassing Euclidean baselines, with HiM-Poincaré providing fine-grained distinctions with higher h-norms, while HiM-Lorentz offers more stable, compact, and hierarchy-preserving embeddings-favoring robustness.

- **Robust Feature Selection for Trustworthy AI**

Speaker: Anton Xue (University of Texas at Austin)

Abstract. From vision models in self-driving cars that fail to identify pedestrians to LLMs that hallucinate fallacious reasoning, modern AI systems can be hard to trust. At the heart of this unreliability is a fundamental challenge: robust feature selection. Whether selecting pixels to explain a prediction or prior statements to justify a logical step, the core task is to identify input features that reliably determine the output.

Towards reliable models, we introduce a general, model-agnostic framework for providing rigorous statistical guarantees on the robustness of any feature selection method. Our mechanism treats selected features as a probabilistic set and efficiently certifies an output’s stability by sampling its robustness to perturbations in feature choice.

This approach provides practical guarantees for feature attributions in explainable AI and extends to certifying LLM reasoning. By treating prior claims in a chain-of-thought as features for the next step, our method inductively certifies each successive claim. This yields a quantitative reliability measure and a diagnostic that identifies the source of logical errors, thereby making robust feature selection a more tractable strategy for achieving trustworthy AI.

- **Surya FM: A foundation model in heliophysics**

Speaker: Spiridon Kasapis (Princeton University)

Co-authors: Sujit Roy (University of Alabama in Huntsville, NASA Marshall Space Flight Center), Johannes Schmude (IBM Research), Rohit Lal (University of Alabama in Huntsville), Vishal Gaur (University of Alabama in Huntsville), Marcus Freitag (IBM Research), Julian Kuehnert (IBM Research), Theodore Van Kessel (IBM Research), Dinesha Hegde (University of Alabama in Huntsville), Andrés Muñoz-Jaramillo (Southwest Research Institute), Johannes Jakubik (IBM Research), Etienne Vos (IBM Research), Kshitiz Mandal (University of Alabama in Huntsville), Ata Akbari Asanjan (Universities Space Research Association), Joao Lucas De Sousa Almeida (IBM Research), Amy Lin (University of Alabama in Huntsville), Talwinder Singh (Georgia State University), Kang Yang (Georgia State University), Chetraj Pandey (Georgia State University), Jinsu Hong (Georgia State University), Berkay Aydin (Georgia State University), Thorsten Kurth (NVIDIA Corporation), Ryan McGranaghan (NASA Jet Propulsion Laboratory), Vishal Upendran (SETI Institute), Shah Bahauddin (University of Colorado Boulder), Daniel Da Silva (NASA Goddard Space Flight Center), Nikolai Pogorelov (University of Alabama in Huntsville), Anne Spalding (Trillium Tech Inc.), Campbell Watson (IBM Research), Manil Maskey (NASA Marshall Space Flight Center), Madhulika Guhathakurta (NASA Science Mission Directorate), Juan Bernade-Moreno (IBM Research), Rahul Ramachandran (NASA Marshall Space Flight Center)

Abstract. Heliophysics is central to understanding and forecasting space weather events and solar activity. Despite decades of high-resolution observations from the Solar Dynamics Observatory (SDO), most models remain task-specific and constrained by scarce labeled data, limiting their capacity to generalize across solar phenomena. We introduce Surya, a 366M parameter foundation model for heliophysics designed to learn general-purpose solar representations from multi-instrument SDO observations, including eight Atmospheric Imaging Assembly (AIA) channels and five Helioseismic and Magnetic Imager (HMI) products. Surya employs a spatiotemporal transformer architecture with spectral gating and long-short range attention, pretrained on high-resolution solar image forecasting tasks and further optimized through autoregressive rollout tuning. Zero-shot evaluations demonstrate its ability to forecast solar dynamics and flare events, while downstream fine-tuning with parameter-efficient Low-Rank Adaptation (LoRA) shows strong performance on solar wind forecasting, active region segmentation, solar flare forecasting, and EUV spectra. Surya is the first foundation model in heliophysics that uses time advancement as a pretext task on full-resolution SDO data. Its novel architecture and performance suggest that the model is able to learn the underlying physics behind solar evolution.

- **In-Context Operator Learning on the Space of Probability Measures**

Speaker: Dixi Wang (Purdue University)

Co-authors: Frank Cole (University of Minnesota), Yineng Chen (Purdue University), Yulong Lu (University of Minnesota), Rongjie Lai (Purdue University)

Abstract. We introduce in-context operator learning on probability measure spaces for optimal transport (OT). The goal is to learn a single solution operator that maps a pair of distributions to the OT map, using only few-shot samples from each distribution as a prompt and without gradient updates at inference. We parameterize the solution operator and develop scaling-law theory in two regimes. In the nonparametric setting, when tasks concentrate on a low-intrinsic-dimension manifold of source-target pairs, we establish generalization bounds that quantify how in-context accuracy scales with prompt size, intrinsic task dimension, and model capacity. In the parametric setting (e.g., Gaussian families), we give an explicit architecture that recovers the exact OT map in context and provide finite-sample excess-risk bounds. Our numerical experiments on synthetic transports and generative-modeling benchmarks validate the framework.

- **Multimodal Foundation Model for Accelerating Numerical Simulation of Differential Equations via Error Correction**

Speaker: Jiaxin Yuan (University of Maryland)

Abstract. Fast and accurate simulation of dynamical systems is a fundamental challenge across scientific and engineering domains. Traditional numerical integrators often face a trade-off between accuracy and computational efficiency, while existing neural network-based approaches typically require training a separate model for each case.

To overcome these limitations, we introduce two novel multi-modal foundation models for large-scale simulation of differential equations: FMint (Foundation Model based on Initialization) for ordinary differential equations (ODEs), and FMint-SDE for stochastic differential equations (SDEs). Based on a decoder-only transformer with in-context learning, FMint leverages numerical and textual modalities to learn a universal error-correction scheme. It is trained using prompted sequences of coarse solutions generated by conventional solvers, enabling broad generalization across diverse systems. We evaluate our models on a suite of challenging ODE and SDE benchmarks spanning applications in molecular dynamics, mechanical systems, finance, and biology. Experimental results show that our approach achieves superior accuracy and efficiency compared to classical solvers, underscoring the potential of FMint and FMint-SDE as general-purpose simulation tools for dynamical systems.

2.25 New Algorithms and Theory for Reinforcement Learning

MS Abstract. We have five active speakers who will present their recent works on the new algorithms and theory for reinforcement learning. Below are the names and institutions for these five speakers: Wenbo Jing (NYU), Jiadong Liu (U Penn), Laixi Shi (JHU), Haochen Zhang (Penn State), and Zhong Zheng (U Penn).

- **Explainable reinforcement learning from human feedback to improve language model alignment**

Speaker: Shicheng Liu (Pennsylvania State University)

Abstract. A common and effective strategy for humans to improve an unsatisfactory outcome in daily life is to find a cause of this outcome and correct the cause. In this paper, we investigate whether this human improvement strategy can be applied to improving reinforcement learning from human feedback (RLHF) for alignment of language models (LMs). In particular, it is observed in the literature that LMs tuned by RLHF can still output unsatisfactory responses. This paper proposes a method to improve the unsatisfactory responses by correcting their causes. Our method has two parts. The first part proposes a post-hoc explanation method to explain why an unsatisfactory response is generated to a prompt by identifying the training data that lead to this response. We formulate this problem as a constrained combinatorial optimization problem where the objective is to find a set of training data closest to this prompt-response pair in a feature representation space, and the constraint is that the prompt-response pair can be decomposed as a convex combination of this set of training data in the feature space. We propose an efficient iterative data selection algorithm to solve this problem. The second part proposes an unlearning method that improves unsatisfactory responses to some prompts by unlearning the training data that lead to these unsatisfactory responses and, meanwhile, does not significantly degrade satisfactory responses to other prompts. Experimental results demonstrate that our algorithm can improve RLHF.

- **Data-Driven Knowledge Transfer in Batch Q^* Learning**

Speaker: Wenbo Jing (New York University)

Co-authors: Elynn Chen (New York University), Xi Chen (New York University)

Abstract. In data-driven decision-making across marketing, healthcare, and education, leveraging large datasets from existing ventures is crucial for navigating high-dimensional feature spaces and addressing data scarcity in new ventures. We investigate knowledge transfer in dynamic decision-making by focusing on batch stationary environments and formally defining task discrepancies through the framework of Markov decision processes (MDPs). We propose the Transfer Fitted Q-Iteration algorithm with general function approximation, which enables direct estimation of the optimal action-state function Q^* using both target and source data. Under sieve approximation, we establish the relationship between statistical performance and the MDP task discrepancy, highlighting the influence of source and target sample sizes and task discrepancy on the effectiveness of knowledge transfer. Our theoretical and empirical results demonstrate that the final learning error of the function is significantly reduced compared to the single-task learning rate.

- **Federated Online Reinforcement Learning**

Speaker: Zhong Zheng (University of Pennsylvania)

Abstract. Federated reinforcement learning (FRL) enables multiple agents to learn collaboratively without sharing local data, but it faces key challenges, including multi-agent speedup and high communication costs. This talk focuses on online FRL, where agents collect data online and adapt their policies dynamically. I will present our proposed Federated Q-Learning algorithms with multiple novel designs and rigorous theoretical guarantees. This talk will also explain technical novelty in addressing the technical difficulties unique to policy adaptation and show further improved performance under Markov Decision Processes with a benign structure.

- **Robust Decision Making Without Compromising Learning Efficiency**

Speaker: Laixi Shi (Johns Hopkins University)

Abstract. Decision-making artificial intelligence (AI) has revolutionized human life ranging from healthcare, daily life, to scientific discovery. However, current AI systems often lack reliability and are highly vulnerable to small changes in complex, interactive, and dynamic environments. My research focuses on achieving both reliability and learning efficiency simultaneously when building AI solutions. These two goals seem conflicting, as enhancing robustness against variability often leads to more complex problems that requires more data and computational resources, at the cost of learning efficiency. But does it have to?

In this talk, I overview my work on building reliable decision-making AI without sacrificing learning efficiency, offering insights into effective optimization problem design for reliable AI. To begin, I will focus on reinforcement learning (RL) — a key framework for sequential decision-making, and demonstrate how distributional robustness can be achieved provably without paying statistical premium (additional training data cost) compared to non-robust counterparts. Next, shifting to decision-making in strategic multi-agent systems, I will demonstrate that incorporating realistic risk preferences—a key feature of human decision-making—enables computational tractability, a benefit not present in traditional models. Finally, I will present a vision for building reliable, learning-efficient AI solutions for human-centered applications.

- **Gap-Dependent Analysis for Online Q-Learning**

Speaker: Haochen Zhang (Pennsylvania State University)

Abstract. This talk presents recent advances in gap-dependent analysis for online model-free reinforcement learning in episodic tabular Markov Decision Processes (MDPs). In practice, reinforcement learning algorithms can benefit from benign structures of MDPs, such as positive suboptimality gaps, where the best action in each state outperforms all others by a fixed margin. Although classical Q-learning algorithms achieve minimax regret in the worst case, existing gap-dependent results remain coarse and fail to fully leverage this favorable structure. Our work bridges this gap by providing a refined gap-dependent analysis, advancing the theoretical understanding of model-free reinforcement learning, particularly in terms of regret bounds and policy stability under favorable MDP structures.

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2.26 Experimental sciences and mathematical modeling

MS Abstract. With increasing specialization in the hard sciences, it is becoming rare for applied mathematicians to be actively engaged in physical experiments. This has not always been the case historically; many foundational figures of ‘pure’ mathematics were simultaneously tabulating, tinkering, and measuring their own experiments. We have discovered that there is still a vibrant community of research mathematicians who lead double lives as experimentalists in fields as diverse as physics, chemistry, biological sciences, and materials science. We hope to bring together these researchers under the common theme of ‘mathematician experimentalists,’ to debut their efforts. We encourage researchers from any field to speak at this symposium, as long as their work includes a significant interface with physical experiments.

- **Linear and nonlinear waves in microwave transmission lines**

Speaker: Stephen Sorokanich (Air Force Research Laboratory)

Abstract. In this talk I’ll explain the fundamental principles of dispersion engineering for metamaterial transmission line media, with experimental demonstrations on printed circuit boards. These devices offer novel properties for controlling wave transmission that can be optimized for microwave electronics and superconducting quantum circuits.

- **Two-Dimensional foams and coagulation equations with particle emission**

Speaker: Joe Klobusicky (University of Scranton)

Abstract. In quasi-two-dimensional foams, a coarsening process can be induced by rupturing its edges through applying heat. In contrast to coarsening through gas diffusion, edge rupturing causes massive cells to appear. The generation of such cells can be explained by the similarity of edge rupture processes to sticky particle models studied in the Smoluchowski coagulation equation. The collision of ruptured walls includes a second order topological reaction, with a resulting cell having a number of sides equal to the sum of sides of neighboring cells minus four. The corresponding kinetic equations for cell topology fractions have a collision kernel which is approximately multiplicative. In this talk, we will study generalized kinetic models involving the merging of clusters which have particle emission, or a nonzero number of particle which are ejected from the newly formed cluster. We establish formulas for gelation times using methods from generating functions.

- **Modeling to understand, predict, and control invasive spotted lanternfly populations**

Speaker: Daniel Stroembom (Lafayette College)

Abstract. The invasive spotted lanternfly (SLF) has emerged as a major ecological and agricultural threat. Initial published research focused on empirical studies of stage-specific survival and assessments of potential control measures. These efforts left broader population-level questions unresolved. We developed mathematical models to integrate disparate data to obtain the first estimate of SLF population growth (5.47) and to assess results of empirical control studies under population dynamics and incomplete delivery of control. This work showed that even perfect controls would require treatment of at least 35 percent of individuals across all stages to achieve any decline, challenging expectations based on empirical results alone. Building on this, we explored the potential of social predators as biological control agents and identified conditions, including host tree removal thresholds, under which stable collective biological control could emerge. We also extended our framework to study resource allocation, uncovering robust but sometimes counterintuitive deployment strategies. Finally, we constructed a spread model that links invasion dynamics to human activity and produces forecasts not accessible through observation alone. Together, these examples show how modeling complements empirical research by addressing broader questions, informing management strategies, and generating predictions for targeted experimental testing.

- **Capillary Rise Dynamics Through Fully and Partially Saturated Deformable Porous Material**

Speaker: Javed Siddique (Pennsylvania State University York)

Co-authors: Daniel Anderson (George Mason University)

Abstract. In this study, we plan to develop a mathematical model for fully and partially saturated deformable porous materials. Initially, the liquid front saturates the porous material fully and at a later stage partially saturates the porous material. In these dynamics three moving interfaces are formed i.e. the liquid/fully saturated porous interface, the fully saturated/partially saturated porous material interface and the partially saturated/dry porous material interface. We hope to connect the numerically computed results to experimental data from our previous studies and data available in the existing literature.

- **Using Neural Networks and Persistence Homology to Predict Membrane Filter Throughput**

Speaker: Giovanni Nardone (New Jersey Institute of Technology)

Co-authors: Matthew Illington (New Jersey Institute of Technology), Lou Kondic (New Jersey Institute of Technology), Jonathan Jaquette (New Jersey Institute of Technology), Linda Cummings (New Jersey Institute of Technology)

Abstract. Membrane filters – essentially, sheets of porous material – are widely-used, with applications ranging from medical fields to fluid purification. Therefore, it is desired to be able to make good predictions about how filters with a given internal pore structure will perform. Using standard methods that allow us to idealize a filter’s pore structure as a network of (initially) cylindrical pores connected at pore junctions, we apply techniques from persistence homology, allowing us to convert a filter’s structure into a manipulable mathematical object. Statistical vectorization is then used to summarize this object by recording various topological measures describing the structure. This data is then passed into a neural network package, which has been fine-tuned to predict the total throughput of the filter (the amount of fluid that traverses the filter before the filter ceases to function due to excessive fouling). The results of these neural networks show encouraging accuracy ($r^2 > 0.6$, indicating that over 60% of the variance in throughput is successfully predicted by the neural network), but warrant further refinement. Future research is currently oriented towards determining the limitations of using orientation-agnostic vectorization methods to predict filter throughput.

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2.27 Multiscale Techniques in Scientific Machine Learning

MS Abstract. Deep learning and neural networks have revolutionized fields such as image classification and natural language processing. Recently, machine learning for scientific computing and artificial intelligence for science has gained significant popularity among researchers. Neural networks offer innovative solutions to complex problems, including novel methods for solving partial differential equations, such as physics-informed neural networks, the finite neuron method, and the deep Ritz method. However, alongside these opportunities, significant challenges arise in the interpretability, approximation, and training of neural networks.

This mini-symposium will focus on recent advances in machine learning, deep learning, and scientific computing. Topics of interest include, but are not limited to:

- Approximation theory for neural networks
- Multiscale techniques in scientific computing and machine learning
- Training algorithms for neural network optimization
- Applications of ML techniques in scientific computing, image processing, natural language processing, and more

By bringing together researchers working on multiscale algorithms, theoretical analysis, and practical applications of scientific computing and machine learning, this mini-symposium aims to provide a platform for exchanging ideas and fostering collaborations. It will explore state-of-the-art algorithms and theoretical developments, particularly multiscale techniques in machine learning and scientific computing, showcasing their potential to address real-world challenges across various scientific and engineering disciplines.

- **Hybrid Iterative Solvers with Geometry-Aware Neural Preconditioners for Parametric PDEs**

Speaker: Youngkyu Lee (Brown University)

Co-authors: Francesc Levrero Florencio (ANSYS), Jay Pathak (ANSYS), George Karniadakis (Brown University)

Abstract. The convergence behavior of classical iterative solvers for parametric partial differential equations (PDEs) is often highly sensitive to the domain and specific discretization of PDEs. Previously, we introduced hybrid solvers by combining the classical solvers with neural operators for a specific geometry, but they tend to under-perform in geometries not encountered during training. To address this challenge, we introduce Geo-DeepONet, a geometry-aware deep operator network that incorporates domain information extracted from finite element discretizations. Geo-DeepONet enables

accurate operator learning across arbitrary unstructured meshes without requiring retraining. Building on this, we develop a class of geometry-aware hybrid preconditioned iterative solvers by coupling Geo-DeepONet with traditional methods such as relaxation schemes and Krylov subspace algorithms. Through numerical experiments on parametric PDEs posed over diverse unstructured domains, we demonstrate the enhanced robustness and efficiency of the proposed hybrid solvers for multiple real-world applications.

- **Deep Neural Networks with General Activations: Super-Convergence in Sobolev Norms**

Speaker: Yahong Yang (Georgia Institute of Technology)

Abstract. This paper establishes a comprehensive approximation result for deep fully-connected neural networks with commonly-used and general activation functions in Sobolev spaces $W^{n,\infty}$, with errors measured in the $W^{m,p}$ -norm for $m < n$ and $1 \leq p \leq \infty$. The derived rates surpass those of classical numerical approximation techniques, such as finite element and spectral methods, exhibiting a phenomenon we refer to as *super-convergence*. Our analysis shows that deep networks with general activations can approximate weak solutions of partial differential equations (PDEs) with superior accuracy compared to traditional numerical methods at the approximation level. Furthermore, this work closes a significant gap in the error-estimation theory for neural-network-based approaches to PDEs, offering a unified theoretical foundation for their use in scientific computing.

- **Integral Representations of Sobolev Spaces via ReLU^k Activation Function and Optimal Error Estimates for Linearized Networks**

Speaker: Tong Mao (King Abdullah University of Science and Technology)

Co-authors: Liu Xinliang (King Abdullah University of Science and Technology), Jinchao Xu (King Abdullah University of Science and Technology)

Abstract. We present two main theoretical results concerning shallow neural networks with ReLU^k activation functions. We provide a novel integral representation for Sobolev spaces, showing that every function in $H^{\frac{d+2k+1}{2}}(\Omega)$ can be expressed as an L2-weighted integral of ReLU^k ridge functions over the unit sphere. This result mirrors the known representation of Barron spaces and highlights a fundamental connection between Sobolev regularity and neural network representations. Moreover, we show that linearized shallow networks—constructed by fixed inner parameters and optimizing only the linear coefficients—achieve optimal approximation rates $O(n^{-\frac{1}{2}-\frac{2k+1}{2d}})$ in Sobolev spaces.

- **Dualization: from subspace correction to operator splitting and alternating direction methods of multipliers**

Speaker: Boou Jiang (King Abdullah University of Science and Technology)

Abstract. We show that a broad range of convex optimization algorithms, including alternating projection, operator splitting, and multiplier methods, can be systematically derived from the framework of subspace correction methods via convex duality. To formalize this connection, we introduce the notion of *dualization*, a process that transforms an iterative method for the dual problem into an equivalent method for the primal problem. This concept establishes new connections across these algorithmic classes, encompassing both well-known and new methods. In particular, we show that classical algorithms such as the von Neumann, Dykstra, Peaceman–Rachford, and Douglas–Rachford methods can be interpreted as dualizations of subspace correction methods applied to appropriate dual formulations. Beyond unifying existing methods, our framework enables the systematic development of new algorithms for convex optimization. For instance, we derive parallel variants of alternating projection and operator splitting methods, as dualizations of parallel subspace correction methods, that are well-suited for large-scale problems on modern computing architectures and offer straightforward convergence guarantees. We also propose new alternating direction method of multipliers-type algorithms, derived as dualizations of certain operator splitting methods. These algorithms naturally

ensure convergence even in the multi-block setting, where the conventional method does not guarantee convergence when applied to more than two blocks. This unified perspective not only facilitates algorithm design and the transfer of theoretical results but also opens new avenues for research and innovation in convex optimization.

2.28 Advances in Numerical Linear Algebra and Applications

MS Abstract. This minisymposium aims to forge connections between several distinct frontiers of advanced NLA, with insights from approximation theory, randomized algorithms, data-sparse algorithms, and complex analysis. Experts will speak on a wide range of topics, including factorization-free optimal low-rank approximation of kernel matrices; a unified spectral theory for Volterra kernels and integral operators; the role of deflation in accelerating spectral density estimation; the use of hierarchical rank structure as a regularizing assumption for high-dimensional covariance estimation; and the interplay between Krylov subspaces, rational approximation, and nonlinear model order reduction.

• Kernel Approximation Using the Proxy Point Method via Contour Integration

Speaker: Mikhail Lepilov (Rensselaer Polytechnic Institute)

Co-authors: Andrew Horning (Rensselaer Polytechnic Institute)

Abstract. Large kernel matrices arise frequently in several areas of mathematics, computer science, and related disciplines. Due to their size, in order to effectively perform computations with such matrices, it is often necessary to work with their low-rank approximations instead. Low-rank matrix decompositions to such matrices may be quickly obtained by exploiting the analytic structure of the underlying kernel, for example by using Taylor expansions or an integral representation; such ideas trace back to the fast multipole method. However, there is often a gap between the theoretical epsilon-rank of a given kernel matrix, explicitly obtained using its eigenvalue decomposition, and the existing analytic decompositions of the same rank. In this work, we aim to bridge this gap by exploring the proxy point method, which approximates complex-analytic kernel matrices using a discretized contour integral representation. In particular, we combine this approach with a judicious choice of conformal map applied to the set of points at which the kernel is evaluated in order to obtain close-to-optimal analytic approximations. We apply this new method to some well-studied kernel matrices, such as the Hilbert matrix, in order to compare it with existing analytic methods and with the best available theoretical bounds on approximation accuracy.

• Estimating High-Dimensional Covariance Matrices with Hierarchical Rank Structure

Speaker: Robin Armstrong (Cornell University)

Co-authors: Anil Damle (Cornell University), Samuel Otto (Cornell University)

Abstract. Many algorithms in data assimilation and model order reduction rely on sample-based estimates for a covariance matrix associated with the trajectory of a high-dimensional dynamical system. Due to computational constraints, the number of available samples is often far less than the dimension of the underlying state space. Under these circumstances, extracting meaningful covariance information requires combining the noisy small-sample statistics with a regularizing structural assumption such as spatial localization. This talk will examine the use of hierarchical rank structure as a regularizing assumption for high-dimensional covariance estimation. Whereas spatial localization assumes that long-range correlations are zero, hierarchical rank structure makes a more flexible assumption that correlations vary more smoothly at long distances than at short distances. We will begin the talk by investigating the circumstances under which this type of structure arises. We will then present theory and algorithms which show how to form a regularized, hierarchically rank structured covariance estimate from limited samples. Through numerical experiments with a variety of dynamical systems, we will demonstrate that these techniques are effective at reducing sampling errors in the covariance.

- **A Unified Spectral Approach to Scalar, Linear Volterra Equations**

Speaker: David Darrow (Massachusetts Institute of Technology)

Co-authors: George Stepaniants (California Institute of Technology)

Abstract. Volterra integral, integro-differential, and difference equations have been extensively studied in both pure mathematics and applied science. In one direction, developments in analysis have yielded far-ranging existence, uniqueness, and regularity results for Volterra equations. In the other, scientific applications have inspired a variety of practical techniques for such equations. In particular, the study of strain-stress dynamics in materials science has inspired closed-form solutions to special classes of Volterra equations with exponentially decaying memory, as well as certain Volterra equations involving fractional derivatives and Prony series. Only a limited number of these results have been proven rigorously, however, and their study in materials science has remained largely disjoint from the broader mathematical community.

In this talk, we aim to bridge the gap between pure and applied research on scalar, linear Volterra equations by examining five major classes: integral and integro-differential equations with completely monotone kernels (viscoelastic models); equations with positive definite kernels (partially observed quantum systems); difference equations with discrete, positive definite kernels; a generalized class of delay differential equations; and a generalized class of fractional differential equations. We develop a system of correspondences between these disparate domains, and see how 'interconversion' (operator inversion) arises as a natural, continuous involution within each class. In so doing, we arrive at practical analytical formulas for all five classes, and recover a variety of disparate results in applied science (including the aforementioned results in viscoelasticity) in particular limits. We show how our closed-form solutions can be realized numerically with rational approximation, study the analytical properties of these formulas, and test them on a wide array of problems relating to signal deconvolution, triangular matrix inversion, and interconversion of materials.

- **Modified Lanczos recursions for discrete exterior PDE problems and other large-scale LTI systems with dense spectra**

Speaker: Vladimir Druskin (Worcester Polytechnic Institute, Southern Methodist University)

Co-authors: Jorn Zimmerling (Uppsala University)

Abstract. The optimal properties of the Lanczos algorithm for approximating LTI systems with s.p.d. matrices are well known. However, Lanczos approximations lose their spectral adaptivity for large problems with dense spectra, particularly those arising from the discretization of problems with continuous spectra, such as exterior PDEs. We present Gauss–Radau and Krein–Nudelman extensions of Lanczos recursions that, at negligible additional post-processing cost, significantly accelerate the convergence of MIMO transfer functions for practically important problems, including electromagnetic applications and diffusion on graph Laplacians. We further show that the Krein–Nudelman extension effectively acts as an absorbing boundary condition when applied to non-absorptive discretizations of wave problems. Valeria Simoncini contributed to the early stages of this work.

- **Near-optimal Spectral Density Estimation via Explicit and Implicit Deflation**

Speaker: Rajarshi Bhattacharjee (University of Massachusetts Amherst)

Abstract. We study algorithms for approximating the spectral density of an $n \times n$ symmetric matrix A that is accessed through matrix-vector products. By combining an existing Chebyshev polynomial moment matching method with a deflation step that approximately projects off the largest magnitude eigendirections of A before estimating the spectral density, we give an $\epsilon\sigma_l(A)$ error approximation in the Wasserstein-1 metric using $O(l \log n + 1/\epsilon)$ matrix-vector products, where $\sigma_l(A)$ is the l 'th largest singular value of A . When A exhibits fast singular value decay, this can be much stronger than prior work, which gives error $\epsilon\sigma_1(A)$ using $O(1/\epsilon)$ matrix-vector products. We also show that our bound is nearly tight.

We further show that the popular Stochastic Lanczos Quadrature (SLQ) method matches the above bound, even though SLQ itself is parameter-free and performs no explicit deflation. This explains the strong practical performance of SLQ, and motivates a simple variant that achieves an even tighter error bound. Our error bound for SLQ leverages an analysis that views it as an implicit polynomial moment matching method, along with recent results on low-rank approximation with single-vector Krylov methods. We use these results to show that SLQ can perform implicit deflation as part of moment matching.

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2.29 Collective Behavior for Biologically Inspired and Social Systems

MS Abstract. Collective behavior arises when many agents interact, and this interaction leads to some emergent structure of the group that is not obvious from individual behavior. Examples of such behavior is observed in nature, society, and engineered contexts. From the collective motion of groups of animals in a landscape, to the navigation of groups of vehicles, or the nuanced strategies of multi-agent games, diverse forms of collective behavior emerge from the individuals in these groups interacting with one another while motivated by their own individual goals. These collective behaviors can span spatial domains, where agents attempt to align and move together, adapting their behavior to the landscape, as well as social and strategic contexts, where individuals adapt their behaviors through communication or internal state variables motivating them. The understanding of these systems can help inform us on how certain behaviors of individual agents facilitate the goals of the collective group. In this minisymposium, we will explore mathematical models for collective behavior across biologically inspired systems and observe how individual behaviors affect the collective dynamics of the group.

- **Agent-Based Modeling of Collective Foraging and Movement in Bison Herds**

Speaker: Jacob Woods (Temple University)

Co-authors: Claire Bresnan (Montana State University)

Abstract. Bison are an important species in the habitats they occupy, providing services to the ecosystem through their collective grazing and movement, while having significant cultural importance for Indigenous food sovereignty. In the late 19th century, they were brought to the brink of extinction due to hunting but through significant conservation efforts, bison have been reintroduced to the American grasslands, and efforts have been made to help facilitate the services they provide to the ecosystem. It is unknown what foraging strategies bison use in a landscape and it isn't clear what dictates changes in the bison's behavioral states, such as grazing, resting, and moving. In this talk, I present a model inspired by the bison's behavior that captures how the bison move through a landscape and their social interactions. This model is calibrated with GPS movement data and informed in collaboration with expert ecologists' insights, allowing exploration of scenarios such as enclosure design and herd expansions. This work demonstrates how mathematical models of collective behavior can provide both theoretical insight and practical tools for conservation and ecosystem management.

- **Neuromorphic Decision Making for Resource Constrained Robot Collectives**

Speaker: Himani Sinhar (Princeton University)

Abstract. How can robot collectives make decisions that are fast, reliable, and scalable when every individual robot has only limited sensing, no communication, and minimal onboard compute? In this talk, I will show that the answer lies in a neuromorphic view of collective intelligence. Instead of rules, prediction, or optimization, we design decision-making as continuous dynamics inspired by spiking neurons and nonlinear opinion models. Each robot carries an internal decision variable that evolves in response to local observations and social influence. The saturated nonlinearity in the dynamics allows decisions to emerge quickly, adapt continuously, and switch abruptly when the context changes. At the same time, the dynamics remain analytically tractable and lightweight enough to run on severely

resource-constrained robots. Much like animal groups that resolve conflicts or split across resources without centralized control, these dynamics enable minimal agents to achieve robust coordination. I will illustrate this through two core results. First, in multi robot navigation, I show how dissensus behavior emerges in the decision dynamics, enabling robot teams to negotiate right-of-way and break deadlocks without communication or central coordination. Second, I introduce a multi-option opinion dynamics model for spatial allocation, where agents must distribute across targets that appear, disappear, and vary in value. Here, distributed bifurcations drive scalable target allocation from purely local information. Together, this talk will highlight how neuromorphic principles can yield collective intelligence from individually simple agents, enabling emergent coordination in multi-robot systems operating under limited onboard resources and opening pathways to scalable autonomy in dynamic, unpredictable environments.

- **Structured heterogeneity leads to group-level selective sensitivity and robustness**

Speaker: Ian Xul Belaustegui (Princeton University)

Abstract. A central challenge in collective behavior is navigating the stability-flexibility trade-off: how to be stable against noise while remaining flexible enough to respond to important cues. We investigate how structured individual differences in sensitivity can shape group-level selective sensitivity to distributed inputs, improving the stability-flexibility balance. In our approach, we use a continuous nonlinear opinion dynamics model where agents share opinions through a network and modulate the gain (sensitivity) placed on social information. We also apply this approach to model escape cascades in shoals of fish, which need to optimally use information from neighbors to avoid danger while also rejecting uninformative noise.

- **Emergence of cooperative behavior in multi-agent models of thermal huddles**

Speaker: Nicole Zalewski (Temple University)

Abstract. Multi-agent dynamical systems models are used widely to model the movement of groups of animals. Several species of animal, including penguins and rodent pups, have been observed to huddle for warmth and continuously cycle who is in the center of the huddle. In this talk we present a novel model of individuals that exchange warmth and move based on their own body temperature. We showcase how the movement of individuals leads to emergent macroscopic movement patterns that mimic observed behavior. These dynamics reveal cooperative behavior, in which individuals must yield their advantageous position to allow for movement of the whole group.

- **Adaptive dynamics of reputation, gossip, and moral norms**

Speaker: Taylor Kessinger (University of Pennsylvania)

Co-authors: Joshua Plotkin (University of Pennsylvania)

Abstract. We live in a society. Societies depend on interactions between unrelated individuals with little to no prospect for future interactions—conditions under which one might not expect cooperation to proliferate. And yet, cooperation happens! Why?

Reputations offer a compelling explanation; when I behave well, I may be rewarded with a good reputation and thereby become the recipient of future cooperative acts. But under what conditions is this an effective mechanism for ensuring a cooperative status quo? How can gossip contribute to a high rate of cooperation? And what sorts of rules for assigning reputations are likely to evolve in the first place?

I leverage evolutionary game theory and adaptive dynamics to answer these questions; that is, I model a large population in which traits, such as one’s propensity to cooperate, gossip rate, and even moral rules themselves are continuous traits. As successive “mutants” arise and invade, or fail to invade, a population, its trait composition changes.

Using this toolkit, I demonstrate that cooperative behavior depends on a high rate of gossip, gossip itself is unlikely to evolve in the absence of population structure, and the rule societies are most

likely to follow is “Stern Judging”—which, notably, not only permits but mandates that individuals with bad reputations be punished—which, in turn, creates a problem if disagreement about reputations is widespread. I comment on some implications of these results.

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2.30 Recent Advances in Low-Rank Methods and Their Applications

MS Abstract. From large-scale (multi)linear algebra operations, to computationally expensive scientific simulations, there exists a great need for robust methods that can reduce the storage and complexity requirements. Low-rank methods have gained popularity in recent years as a way to improve algorithm efficiency, reduce storage complexity, and exploit underlying structures. Such frameworks include matrix and tensor decompositions, projection-based techniques, and dimension reduction methods. This mini-symposium will feature presentations showcasing the rich variety of recent algorithmic and theoretical advancements of low-rank methods, as well as their utilization in solving complex physical systems.

- **A Sampling-Based Adaptive Rank Approach to the Wigner-Poisson System**

Speaker: Sining Gong (Michigan State University)

Co-authors: Andrew Christlieb (Michigan State University), Jing-Mei Qiu (University of Delaware), Nanyi Zheng (University of Delaware)

Abstract. We develop a mass-conserving, adaptive-rank solver for the 1D1V Wigner-Poisson system. Our work is motivated by applications to the study of the stopping power of α particles at the National Ignition Facility (NIF). In this regime, electrons are in a warm dense state, requiring more than a standard kinetic model. They are hot enough to neglect Pauli exclusion, yet quantum enough to require accounting for uncertainty. The Wigner-Poisson system captures these effects but presents challenges due to its nonlocal nature. Based on a second-order Strang splitting method, we first design a full-rank solver with a structure-preserving Fourier update that ensures the intermediate solutions remain real-valued (up to machine precision), improving upon previous methods. Simulations demonstrate that the solutions exhibit a low rank structure for moderate to high dimensionless Planck constants ($H \geq 0.1$). This observed low rank structure motivates the development of an adaptive-rank solver, built on a Semi-Lagrangian adaptive-rank (SLAR) scheme for advection and an adaptive-rank, structure-preserving Fourier update for the Wigner integral terms, with a rigorous proof of structure-preserving property provided. Our solver achieves $O(N)$ complexity in both storage and computation time, while preserving mass and maintaining momentum accuracy up to the truncation error. The adaptive rank simulations are visually indistinguishable from the full-rank simulations in capturing solution structures. These results highlight the potential of adaptive rank methods for high-dimensional Wigner-Poisson simulations, paving the way toward fully kinetic studies of stopping power in warm dense plasmas.

- **Discrepancies are Virtue: Weak-to-Strong Generalization through Lens of Intrinsic Dimension**

Speaker: Yijun Dong (Courant Institute of Mathematical Sciences)

Co-authors: Yicheng Li (New York University Shanghai), Yunai Li (Shanghai Jiao Tong University), Jason Lee (University of California, Berkeley), Qi Lei (Courant Institute of Mathematical Sciences)

Abstract. Weak-to-strong (W2S) generalization is a type of finetuning (FT) where a strong student model is trained on pseudo-labels generated by a weak teacher. Surprisingly, W2S FT often outperforms the weak teacher. We seek to understand this phenomenon through the observation that FT often occurs in intrinsically low-dimensional spaces. Leveraging the low intrinsic dimensionality of FT, we analyze W2S in the regression setting from a variance reduction perspective. For a strong student-weak teacher pair with sufficiently expressive low-dimensional feature subspaces $\mathcal{V}_s, \mathcal{V}_w$, we provide an exact

characterization of the variance that dominates the generalization error of W2S. This unveils a virtue of discrepancy between the strong and weak models in W2S: the variance of the weak teacher is inherited by the strong student in $\mathcal{V}_s \cap \mathcal{V}_w$, while reduced by a factor of $\dim(\mathcal{V}_s)/N$ in the subspace of discrepancy $\mathcal{V}_w \setminus \mathcal{V}_s$ with N pseudo-labels for W2S. Our analysis further casts light on the sample complexities and the scaling of performance gap recovery in W2S. The analysis is supported by experiments on synthetic regression problems, as well as real vision and NLP tasks.

- **Why machine learning researchers should care about low-rank structures?**

Speaker: Annan Yu (Cornell University)

Abstract. Nowadays, almost every practitioner in the AI community knows what a low-rank structure is, thanks to the Low-Rank Adaptation (LoRA) method that has been widely used in fine-tuning ML models. But beyond a handy engineering trick, low-rank structure is a deep lens for understanding how neural networks behave. In this talk, I will show two complementary regimes (each illustrated with a concrete example from a broad class of networks) that reveal why low-rank ideas matter. First, we will look at rank-limited regimes: here, the low-rank parameterization actively constrains expressivity, and recognizing this forces us to rethink parameterizations or inductive biases when we need richer representations. Second, I will consider rank-benign regimes: when expressivity isn't the bottleneck, low-rank structure still buys us real benefits in generalization, robustness, and efficiency. We'll wrap up with a high-level takeaway, in addition to the technical details: low-rank structure is not just something to apply; it is a conceptual tool every ML researcher should understand and use to reason about models, trade-offs, and design choices.

- **Efficient oversampled Tensor-Train Cross approximation for large data**

Speaker: Daniel Hayes (University of Delaware)

Co-authors: Jing-Mei Qiu (University of Delaware), Tianyi Shi (Lawrence Berkeley National Laboratory)

Abstract. Recently, there have been many advances in the area of randomized and sampling-based methods for data approximation. This has led to significant progress towards the efficient treatment of large data in both compression and utilization in computation. In this talk, I will discuss a current work that uses random oversampling on a Tensor Train Cross (TT-Cross) approximation in order to reduce the observed error of a tensor approximation. This work includes two separate formulations utilizing projection techniques to construct tensor cores with results demonstrating a reduction in error. Along with the observed reduction in error, we will show that in practice, the oversampling procedure does not substantially increase computation time compared to a standard TT-Cross construction.

3 Contributed Talks

3.1 Session 1

- **A Modified Hermite Radial Basis Function for Accurate Interpolation**

Speaker: Amirhossein Fashamiha (University of Buffalo)

Co-authors: David Salac (University of Buffalo)

Abstract. Interpolating both functions and their derivatives with high precision is fundamental to accurately solve partial differential equations (PDEs). The Radial Basis Function (RBF) method has proven to be a robust technique for interpolating scattered datasets. The Hermite RBF (HRBF) method extends traditional RBFs by incorporating derivative information, resulting in improved approximation accuracy. Infinitely smooth kernels, such as the Gaussian, are often preferred for their ability to capture

fine-scale features, with their behavior controlled by a shape parameter. However, at low to moderate shape parameter values, these kernels can become ill-conditioned, reducing their effectiveness. In our proposed work, we introduce a Modified Hermite RBF (MHRBF) approach that enhances the interpolation by including an additional polynomial term, improving kernel behavior and boosting accuracy. Using standard double-precision mathematics, the results demonstrate that the MHRBF method consistently achieves lower interpolation errors and reduced computational cost compared to the standard HRBF approach. These advantages are further validated through applications in level-set reinitialization and closest-point computation.

- **Cryo-EM images are intrinsically low-dimensional**

Speaker: Luke Evans (Flatiron Institute)

Co-authors: Octavian-Vlad Murad (University of Washington), Lars Dingeldein (Frankfurt Institute for Advanced Study), Pilar Cossio (Flatiron Institute), Roberto Covino (Frankfurt Institute for Advanced Study, Goethe University Frankfurt), Marina Meila (University of Washington, University of Waterloo)

Abstract. Simulation-based inference provides a powerful framework for cryo-electron microscopy, employing neural networks in methods like CryoSBI (Dingledein et al. 2025) to infer biomolecular conformations via learned latent representations. This latent space represents a rich opportunity, encoding valuable information about the physical system and the inference process. Harnessing this potential hinges on understanding the underlying geometric structure of these representations. We investigate this structure by applying manifold learning techniques to CryoSBI representations of a simulated benchmark dataset, and both simulated and experimental images of hemagglutinin. We reveal that these high-dimensional data inherently populate low-dimensional, smooth manifolds, with simulated data effectively covering the experimental counterpart. By characterizing the manifold’s geometry using Diffusion Maps and identifying its principal axes of variation via coordinate interpretation methods, we establish a direct link between the latent structure and key physical parameters. Discovering this intrinsic low-dimensionality and interpretable geometric organization not only validates the CryoSBI approach but enables us to learn more from the data structure and provides opportunities for improving future inference strategies by exploiting this revealed manifold geometry.

- **Dense binary images have large connected components**

Speaker: Kyle Fridberg (Cornell University)

Abstract. Suppose an $n \times m$ pixel image—equivalently, an $n \times m$ grid of colored squares—contains at least dnm “white” pixels. If d is close to 1, must the image contain a large four-connected component of white pixels? We define the function (d, n, m) as the minimum size of the maximum white four-connected component in any $n \times m$ image with at least dnm white pixels. By converting the computation of (d, n, m) into a connected component tiling problem on the infinite grid, we leverage Pick’s theorem, connected component isoperimetry results, and explicit tiling constructions to obtain tight lower and upper bounds on (d, n, m) . This quantity represents a new statistic on the size distribution of connected components in images.

- **HV Metric For Time-Domain Full Waveform Inversion**

Speaker: Matej Neumann (Cornell University)

Abstract. Full-waveform inversion (FWI) is a powerful technique for reconstructing high-resolution material parameters from seismic or ultrasound data. The conventional least-squares (L^2) misfit suffers from pronounced non-convexity that leads to cycle skipping. Optimal-transport misfits, such as the Wasserstein distance, alleviate this issue; however, their use requires artificially converting the wavefields into probability measures, a preprocessing step that can modify critical amplitude and phase information of time-dependent wave data. We propose the HV metric, a transport-based distance that acts naturally on signed signals, as an alternative metric for the L^2 and Wasserstein objectives

in time-domain FWI. After reviewing the metric’s definition and its relationship to optimal transport, we derive closed-form expressions for the Fréchet derivative and Hessian of the map $f \mapsto d_{HV}^2(f, g)$, enabling efficient adjoint-state implementations. A spectral analysis of the Hessian shows that, by tuning the hyperparameters $(\kappa, \lambda, \epsilon)$, the HV misfit seamlessly interpolates between L^2 , H^{-1} , and H^{-2} norms, offering a tunable trade-off between the local point-wise matching and the global transport-based matching. Synthetic experiments on the Marmousi and BP benchmark models demonstrate that the HV metric-based objective function yields faster convergence and superior tolerance to poor initial models compared to both L^2 and Wasserstein misfits. These results demonstrate the HV metric as a robust, geometry-preserving alternative for large-scale waveform inversion.

- **Image Registration and Direct Inversion in the Ultrasound Elasticity Imaging Field**

Speaker: Rebecca Rodrigues (Rochester Institute of Technology)

Co-authors: Olalekan Babaniyi (Rochester Institute of Technology)

Abstract. Ultrasound elasticity imaging (UEI) is a technique used to visualize the mechanical properties of soft tissue, which can be used for noninvasive diagnosis of diseases. An important step in UEI is to measure the deformation of tissue induced by an applied load. Displacements measured with ultrasound are typically more precise in the axial direction (i.e. the direction of sound propagation) than in the lateral direction (the direction orthogonal to the axial direction). If precise estimates of the full displacement field are available, then efficient direct methods can be used to solve the inverse problem instead of computationally expensive iterative techniques. In the first part of this project, we develop four different optimization formulations with regularization for the image registration problem: two formulations are implementations of existing methods proposed in literature, and the last two add a regularization term that constrains the displacements to satisfy the conservation of momentum equations. We use several computational experiments to demonstrate that all image registration methods are able to reconstruct precise estimates of the full displacement field, and the methods with a momentum-based regularization term produce displacement and strain estimates that are qualitatively and quantitatively better than those produced by existing approaches. In the second half of this project, we develop a direct error in the constitutive equations (DECE) formulation to solve the inverse problem for the mechanical properties. We show that the DECE formulation is capable of reconstructing continuous and discontinuous displacement fields, and the reconstructions converge to the true solution with mesh refinement.

3.2 Session 2

- **An Explicit Description of Implementation of 4D, H(div)-conforming Simplicial Finite Elements in MFEM**

Speaker: Saber Patrick (Pennsylvania State University)

Abstract. In this talk, we will provide an explicit description of our implementation of 4D, H(div)-conforming simplicial finite elements in MFEM. We choose to develop finite elements in 4D because of their usefulness in space-time applications. Furthermore, we are interested in simplicial elements due to their potential for anisotropic mesh adaptivity. Our work modifies and updates a previously generated MFEM branch developed by Andreas Schafelner and Martin Neumüller. Our implementation consists of the following stages: 1) defining degrees of freedom on a reference element, 2) constructing a Vandermonde matrix to transform modal functions to nodal functions, 3) methods for computing both the value of H(div)-conforming basis functions and their derivatives, and 4) orientation mappings for interfaces between neighboring elements. We then show the performance of our newly-developed basis functions with an order of accuracy study on a simple grad-div problem

- **Complete and Final Solution to the Problem of Rounding Errors and Their Accumulation in Python**

Speaker: Isom Jurayev (Retired, USA)

Abstract. A new efficient PDA (Python Decimal Arithmetic) module has been developed for Python. It has five main functions: Addition, Subtraction, Multiplication, Division, and Rounding. For arbitrary real numbers with whole and fractional parts of any finite length:

- Addition, Subtraction, and Multiplication give accurate results.
- Division gives an exact result if an actual result is expected. Otherwise, it returns an approximate result with any predetermined accuracy.
- Division is performed using only $8 \cdot n$ Multiplications and a maximum of $(m + k - n) \cdot n$ comparisons, where m is the length of the dividend, n is the length of the divisor, and k is a predefined precision parameter. If the result of the Division is an integer or an exact real number, then $k = 0$. This is a fundamentally new approach and a significant breakthrough. This method is similarly applicable to Multiplication.
- Rounding is associated only with Division.

PDA naturally and conclusively resolves the issues of rounding errors and their accumulation in Python. During computational experiments, two major shortcomings were found in the well-known Decimal and mpmath modules—the input of new data and the variability of precision estimates. These modules are unnatural, ineffective, and create some difficulties (see, for example, their documentation). PDA is free from these drawbacks. Numerous and diverse examples confirm this.

• Polynomial Extrapolation for Error Mitigation in Quantum Simulation

Speaker: Pegah Mohammadipour (Pennsylvania State University)

Co-authors: Xiantao Li (Pennsylvania State University)

Abstract. Simulating open quantum systems, governed by the Lindblad equation, is critical for realistic modeling but is hampered by two error sources on near-term devices:

- **Algorithmic Error:** Discretization of the time evolution $e^{t\mathcal{L}}$ into steps of size τ introduces errors that scale with τ^p .
- **Physical Noise:** Decoherence and gate errors from device imperfections, often modeled by a noise parameter λ .

We address and combine both: (i) zero-noise extrapolation to mitigate hardware bias, (ii) step-size extrapolation to suppress algorithmic error, and (iii) a joint strategy with $\lambda = O(\tau^2)$ to handle both. Moreover, we justify the use of extrapolation-based algorithmic error mitigation for Lindblad evolution.

• The many faces of stiffness: How a Runge-Kutta method can exhibit multiple convergence orders at the same time

Speaker: Benjamin Seibold (Temple University)

Abstract. While the study of stiff problems is a cornerstone of numerical analysis, a precise definition and characterization of stiffness is a challenging endeavor. This talk highlights how Runge-Kutta time stepping methods can exhibit multiple different types of convergence orders, when applied to families of stiff equations. In particular, it is shown how classical convergence, stiff convergence, and B-convergence can exhibit reduced convergence orders—and which conditions on the Runge-Kutta method mitigate order reduction.

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3.3 Session 3

- **Modeling Regulatory Crosstalk among Cellular Pathways in Colorectal Cancer**

Speaker: Pascal Kingsley Kataboh

Abstract. Regulatory interactions among cellular signaling and transcriptional pathways play a critical role in colorectal cancer progression, yet their dynamic coordination is not fully understood. We develop and analyze a nonlinear system of coupled differential equations that captures key feedback mechanisms among these pathways. The model provides a quantitative framework for analyzing how transcriptional regulation influences signaling activity, cellular differentiation, and tumorigenic behavior. Using numerical simulations and dynamical systems analysis, we investigate how parameter perturbations affect pathway activation and transitions between signaling states associated with stem cell-like characteristics. This framework integrates biological insight with mathematical modeling to elucidate the mechanistic principles underlying regulatory crosstalk in colorectal cancer.

- **Persistence of Lotka-Volterra Food Chains Using an Averaged Rate Model**

Speaker: Sepideh Vafaie (Montclair State University)

Co-authors: Deepak Bal (Montclair State University), Eric Forgoston (Montclair State University), Michael Thorne (British Antarctic Survey)

Abstract. Food webs represent complex ecological systems where species interact through predator-prey relationships. In this work, we consider a food chain with Lotka-Volterra dynamics, where each species preys exclusively on the species below it and is preyed upon by the species above. While traditional analytical techniques can be applied for small systems, high-dimensional chains require simplifying assumptions, i.e., neglecting the self-regulation terms, due to analytical intractability. Building on our prior machine learning work which identified key rate sums as predictors of extinction, we propose a simplified Lotka-Volterra model in which self-regulation, predator-prey interaction, birth, and death rates are averaged across their respective groups. This leads to an analytically solvable system that retains essential food chain dynamics, including persistence. Our theoretical and numerical results demonstrate that the simplified model maintains predictive accuracy while offering clearer analytical insight into species survival and extinction.

- **Quantification of the Economic and Environmental Value of a Green Hydrogen Energy Market in the United States**

Speaker: Ashira Mawji (Cornell University)

Co-authors: Lindsay Anderson (Cornell University), Michael Charles (Cornell University)

Abstract. Green hydrogen is a clean energy carrier produced by electrolyzing water with renewable electricity. It has the power to bridge the gap between renewable energy's limitations and global decarbonization. However, its high cost makes it intractable for large-scale use. Green hydrogen plants in the United States currently operate independently of each other; this creates cost inefficiencies, particularly due to green hydrogen's dependence on renewable energy generation.

This research proposes a green hydrogen energy market in the United States and quantifies its economic and environmental value, compared to plants operating independently of each other as is common today. Green hydrogen infrastructure is modeled as a graph, simulated over one year, and a mixed-integer linear program spatio-temporally optimizes energy decision-making across its energy pathway considering alternative energy options. We find that a green hydrogen energy market would decrease the total cost and carbon dioxide equivalent emissions of meeting the system's energy demand, while it would increase water usage.

- **Estimation of Degradation rate in Biological cells**

Speaker: Lan Trinh (Tulane University)

Abstract. In the biological cells of interest, particles are born at a source location and diffused as in Brownian motion. Over time, they may exit the domain, degrade, or remain alive at specific time points. Assuming the time is long enough for the system to be steady at the observed time, the number of alive particles is shown to follow a Poisson process with an intensity function governed by a Boundary Value Problem. Using spatial snapshots of these particles, we study the estimation of the degradation rate and its statistical properties. We present numerical results showing that heterogeneous spatial data can improve estimator efficiency, and demonstrate consistency and asymptotic behavior of the estimator in simplified settings.

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3.4 Session 4

- **Asymptotic Expansion of the Iterated Solution in the Case of Multiple Scattering Configurations**

Speaker: Souaad Lazergui (New Jersey Institute of Technology)

Abstract. We analyze an asymptotic method for solving electromagnetic and acoustic scattering problems using boundary integral equations, which remain computationally efficient in the high-frequency regime, and it avoids the typical increase in numerical cost. For a single convex obstacle, we employ an integral representation where the unknown surface densities are obtained in a way that allows the application of the stationary phase method, which effectively captures the dominant contributions of the scattered wave field.

For multiple scattering configurations that involve several well-separated convex obstacles, we develop an iterative framework that leads to find a successive wave reflection between the objects. In this setting, the scattered field is represented as a series where each term corresponds to a specific sequence of reflections, allowing us to capture the complex interactions among obstacles while maintaining high accuracy and efficiency. To illustrate this, we focus more on the two-dimensional convex obstacles. We demonstrate that the iterated solution can be expressed as a sum over periodic ray paths—trajectories in which waves reflect repeatedly in a fixed pattern among the obstacles. This decomposition does not only provide a physically intuitive picture of the wave interaction but also offers a rigorous understanding of the structure of the scattered field in complex geometric settings. The framework highlights how geometric optics and wave phenomena interplay in high-frequency regimes, making it especially valuable for applications in radar, sonar, and other wave-based imaging or detection technologies.

- **Modeling and Simulation of the Cholesteric Landau–de Gennes model**

Speaker: Andrew Hicks (Carnegie Mellon University)

Co-authors: Shawn Walker (Louisiana State University)

Abstract. Liquid Crystals (LCs) are a key component of our life in the modern world, appearing in various technologies, such as LC displays and temperature sensors. A classic, yet sophisticated, model is the Landau-de Gennes (LdG) model, which utilizes a 3×3 tensor as the order parameter (the so-called “Q-tensor”). We show how the standard LdG model can be extended to model cholesteric shells, which have applications as droplet lasers, novel bio-sensors, and anti-counterfeiting markers. In particular, we describe the various energetic terms in the Landau-de Gennes free energy, and discuss its variational formulation.

Furthermore, we give a numerical discretization of LdG using a finite element method. Since the LdG energy is non-convex, we use an L^2 gradient flow to compute equilibrium points (minimizers). We also discuss various time step and mesh size conditions to ensure stability, some of which are not well-known in the LC literature, particularly when simulating cholesteric LCs that exhibit “twist”. We present various numerical simulations in 3-D, on both slab geometries and spherical shells, and connect these results with experiments. Finally, we discuss new ongoing work to model so-called “defects” in cholesteric shells.

- **On generalizing the induced surface charge method to heterogeneous Poisson-Boltzmann models for electrostatic free energy calculation**

Speaker: Idowu Ijaodoro (University of Alabama)

Abstract. The induced surface charges (ISC) method, which computes the induced charges on the molecular surface of macromolecules and uses them via Coulomb’s law to calculate the polar solvation energy, was shown to be a robust and almost grid independent approach for electrostatic analysis based on the sharp-interface Poisson-Boltzmann (PB) model. Besides being physically intuitive, the ISC method avoids using the potential near the point charges, which is singular at each atom center. However, the ISC method cannot be physically generalized to heterogeneous dielectric PB models, due to the non-existence of a dielectric boundary. In this work, a novel far-field (FF) method is proposed to calculate the polar solvation free energy, which is derived through reformulating the energy functionals of nonlinear PB potential in solvent and vacuum states. Built upon a rigorous mathematical analysis, the FF method reconstructs the free energies by using far-field solutions outside the solute so that the self-energy terms generated by the singular charges are avoided, just as in the ISC method. Being valid for both sharp-interface and heterogeneous PB models, the performance of the proposed FF method has been validated by considering diffuse interface, Gaussian and super-Gaussian PB models for Kirkwood spheres and various protein systems. Comparison with grid-energy cancellation and regularization methods is also considered. The robustness of the FF method in treating a non-rigid biomolecule with different molecular structures in solvent and vacuum states has been explored, taking advantage of the fact that the far-field potential is insensitive to perturbations of singular charge locations.

- **The Phase Space of the Three-Vortex Problem and Its Application to Vortex-Dipole Scattering**

Speaker: Roy Goodman (New Jersey Institute of Technology)

Abstract. The three-vortex problem was shown to be integrable by Gröbli in 1877. His reduced dynamics, describing a system of three equations for the pairwise distance between vortices, has been rediscovered several times since. This system is singular whenever the three vortices are collinear, which makes applying standard phase-plane reasoning difficult. We derive a new system of equations using Jacobi coordinates followed by Lie-Poisson reduction. This leads to an effectively one-degree-of-freedom integrable system with no such coordinate singularities. We apply this system to several problems: vortex-dipole scattering, the complete classification of the dynamics, a related integrable four-vortex problem, and dipole-dipole scattering.

3.5 Session 5

- **A generalized reduction scheme for the Stochastic Weighted Particle Method**

Speaker: John Zweck (New York Institute of Technology)

Co-authors: Donovan Harcey (University of Texas at Dallas), Matthew Goeckner (University of Texas at Dallas)

Abstract. The Stochastic Weighted Particle Method (SWPM) of Rjasanow and Wagner is a generalization of the Direct Simulation Monte Carlo method for computing the probability density function of the velocities of a system of interacting particles for applications that include rarefied gas dynamics and plasma processing systems. Key components of a SWPM simulation are a particle grouping technique and particle reduction scheme. These are periodically applied to reduce the computational cost of simulations due to the gradual increase in the number of stochastic particles. A general framework for designing particle reduction schemes is introduced that enforces the preservation of a prescribed set of moments of the distribution through the construction and explicit solution of a system of linear equations for particle weights in terms of particle velocities and the moments to be preserved.

This framework is applied to preserve all moments of the distribution up to order three. Numerical simulations are performed to verify the scheme and quantify the degree to which even higher-order moments and tail functionals are preserved. These results reveal an unexpected trade off between the preservation of these higher-order moments and tail functionals.

- **Convergence of Markov Chains for Stochastic Gradient Descent with Separable Functions**

Speaker: Zaleski Philip (New Jersey Institute of Technology)

Co-authors: David Shirokoff (New Jersey Institute of Technology)

Abstract. Stochastic gradient descent (SGD) is a popular algorithm for minimizing objective functions that arise in machine learning. For constant step-sized SGD, the iterates form a Markov chain on a general state space. Focusing on a class of separable (nonconvex) objective functions, we establish a “Doebelin-type decomposition,” in that the state space decomposes into a uniformly transient set and a disjoint union of absorbing sets. Each of the absorbing sets contains a unique invariant measure, with the set of all invariant measures being the convex hull. Moreover, the set of invariant measures are shown to be global attractors to the Markov chain with a geometric convergence rate. The theory is highlighted with examples that show (1) the failure of the diffusion approximation to characterize the long-time dynamics of SGD; (2) the global minimum of an objective function may lie outside the support of the invariant measures (i.e., even if initialized at the global minimum, SGD iterates will leave); and (3) bifurcations may enable the SGD iterates to transition between two local minima.

- **Polynomial complexity sampling from multimodal distributions using Sequential Monte Carlo**

Speaker: Ruiyu Han (Carnegie Mellon University)

Co-authors: Gautam Iyer (Carnegie Mellon University), Dejan Slepčev (Carnegie Mellon University)

Abstract. We study a sequential Monte Carlo algorithm to sample from the Gibbs measure with a non-convex energy function at a low temperature. We use the practical and popular geometric annealing schedule, and use a Langevin diffusion at each temperature level. The Langevin diffusion only needs to run for a time that is long enough to ensure local mixing within energy valleys, which is much shorter than the time required for global mixing. Our main result shows convergence of Monte Carlo estimators with time complexity that, approximately, scales like the forth power of the inverse temperature, and the square of the inverse allowed error. We also study this algorithm in an illustrative model scenario where more explicit estimates can be given.

- **Rescuing double robustness: safe estimation under complete misspecification**

Speaker: Lorenzo Testa (Carnegie Mellon University)

Co-authors: Francesca Chiaromonte (Pennsylvania State University), Kathryn Roeder (Carnegie Mellon University)

Abstract. Double robustness is a major selling point of semiparametric and missing data methodology. Its virtues lie in protection against partial nuisance misspecification and asymptotic semiparametric efficiency under correct nuisance specification. However, in applications, complete nuisance misspecification should be regarded as the norm (or at the very least the expected default), and thus doubly robust estimators may behave fragily. In fact, it has been amply verified empirically that these estimators can perform poorly when all nuisance functions are misspecified. Here, we first characterize this phenomenon of double fragility, and then propose a solution based on adaptive correction clipping (ACC). We argue that our ACC proposal is safe, in that it inherits the favorable properties of doubly robust estimators under correct nuisance specification, but its error is guaranteed to be bounded by a convex combination of the individual nuisance model errors, which prevents the instability caused by the compounding product of errors of doubly robust estimators. We also show that our proposal provides valid inference through the parametric bootstrap when nuisances are well-specified. We showcase the efficacy of our ACC estimator both through extensive simulations and by applying it to the analysis of Alzheimer’s disease proteomics data.

3.6 Session 6

- **Exact analysis of basis pursuit denoising via differential inclusions and a selection principle**

Speaker: Gabriel Provencher Langlois (New York University)

Co-authors: Jérôme Darbon (Brown University)

Abstract. Basis pursuit denoising (BPDN), also known as the lasso problem or 1-regularized least-squares, is a cornerstone of compressive sensing, statistics and machine learning. While various algorithms for BPDN have been proposed, they invariably suffer from drawbacks and must either favor efficiency at the expense of accuracy or vice versa. As such, state-of-the-art algorithms remain ineffective for high-dimensional applications requiring accurate solutions within a reasonable amount of computational time. In this talk, I will present an exact and efficient algorithm for BPDN based on differential inclusions that overcome these drawbacks. Specifically, I will prove that a selection principle from the theory of differential inclusions turns the dual problem of BPDN into calculating the trajectory of an integrable projected dynamical system, that is, whose trajectory and asymptotic limit can be computed exactly. The analysis naturally yields an exact algorithm, numerically up to machine precision, that is also very fast. Numerical experiments confirm that the algorithm outperforms the state-of-the-art algorithms in both accuracy and efficiency. Finally, I will briefly discuss how I expect that the results and analysis can be adapted to compute exact or approximate solutions to a broader class of polyhedral-constrained optimization problems.

- **Lattice Annotated Temporal (LAT) Logic for Non-Markovian Reasoning**

Speaker: Kaustuv Mukherji (Syracuse University)

Co-authors: Jaikrishna Manojkumar Patil (Syracuse University), Dyuman Aditya (Syracuse University), Paulo Shakarian (Syracuse University), Devendra Parkar (Arizona State University), Lahari Pokala (Arizona State University), Clark Dorman (Scientific Systems Company, Inc.), Gerardo I. Simari (Universidad Nacional del Sur, Institute for Computer Science and Engineering)

Abstract. In this talk, I will introduce Lattice Annotated Temporal (LAT) Logic, a new framework that extends generalized annotated logic programs with temporal reasoning and an open-world perspective. The key idea is to replace the usual upper-lattice annotations with a lower-lattice structure, which naturally supports open-world semantics while still enabling efficient grounding—even in settings with infinitely many or heterogeneous constants. This allows us to bring together temporal logic programming and reasoning under uncertainty in a way that handles non-Markovian dynamics directly. I will present the theoretical foundations of the framework, including complexity bounds for grounding and connections to existing results on annotated logics. I will then describe our open-source implementation, PyReason, which is optimized for practical use and integrates with reinforcement learning environments. Finally, I will share empirical results: across multi-agent simulations and knowledge graph tasks, PyReason achieves dramatic speed and memory improvements (sometimes several orders of magnitude) while maintaining or improving performance. In reinforcement learning settings, LAT Logic enables faster non-Markovian simulation and improves agent outcomes by capturing richer temporal dependencies.

Altogether, this work illustrates how combining lattice-based annotations with temporal logic opens new opportunities for reasoning in dynamic, uncertain, and open-world domains including those with non-Markovian dynamics.

- **On Healthy, Sick, and Dead Equations of Systems of Linear Algebraic Equations**

Speaker: Isom Jurayev (Retired, USA)

Co-author: Islom Juraev (Georgia Institute of Technology)

Abstract. This work proposes a natural and straightforward method for determining whether an arbitrary SLAE is well-posed or ill-posed. The system is represented in terms of Healthy, Sick, and Dead equations. Using several illustrative examples, we demonstrate the results of a simple algorithm designed to identify these types of equations directly from the input data. Healthy, Sick, and Dead equations provide clear and practical insights into the well-posedness of SLAEs. The algorithm has been implemented and tested in Python, and a separate paper will be devoted to its description.

- **Orthogonality Spaces over Finite Fields**

Speaker: Thang Nguyen (New Mexico State University)

Abstract. We give fast, implementation-ready rules for detecting and generating “centers”—balanced points tied to orthogonality—in 3-dimensional finite-field models. Using a projective operator $[x, y]$, we show: (i) in the orthogonal model $(3, q)$ with q odd, *no* block has a center; (ii) in the unitary model $(3, q)$, a point $c = \langle (x, y, z) \rangle$ with $xyz \neq 0$ is a center *iff* $\text{char}_q = 2$ and $(x) = (y) = (z)$. This yields a simple parametrization $= \langle (1, u, v) \rangle : u, v \in S, (u) = (v) = 1 \cong S \times S$, and a clear graph structure on centers: edgeless if $3 \nmid (q + 1)$; disjoint triangles if $3 \mid (q + 1)$. The criteria support constant-time membership checks and explicit triples, with applications to small orthogonal packings in coding, network coding, and combinatorial design.

- **Synchronization of coupled oscillators on self-similar sets**

Speaker: Matthew Mizuhara (The College of New Jersey)

Abstract. Coupled phase oscillators on networks are ubiquitous in the study of spontaneous synchronization and pattern formation. Many real-world networks (e.g., neural systems and the Internet) exhibit fractal-like self-similarity across multiple scales. However, existing techniques for analyzing synchronization do not apply in these settings.

In this work, we develop new analytical tools and numerical simulations for Kuramoto oscillators on self-similar networks approximating fractals. We show that the complex topology of fractals gives rise to a rich diversity of equilibria, generalizing classical twisted states on simpler networks.

Our approach combines ideas from fractal geometry, topology, and analysis to construct and classify these states. In particular, our method relies on harmonic extensions, which algorithmically provide exact solutions to the Laplace equation on fractals. Finally, we use Γ -convergence to establish convergence results for the nonlinear problems.

This work is joint with Georgi Medvedev (Drexel University) and is supported by the NSF.

3.7 Session 7

- **Inertial Particle Dynamics of Different Shapes in Fluid Flows**

Speaker: Takashi Yashiro (Montclair State University)

Abstract. We investigate the dynamics of inertial particles of various shapes advected in a fluid flow. The Maxey-Riley (MR) equation is used to model the motion of small spherical particles. To account for non-spherical shapes such as cubes, tetrahedrons, ellipsoids, and a barrel-like shape inspired by a type of origami robot, the MR equation is modified using a shape-dependent corrective factor. Particle trajectories are analyzed within the Double-Gyre (DG) flow, which is rescaled to ensure that particle behavior remains consistent across domains of different sizes. This scaling allows the MR equation to accurately model the dynamics of larger particles, as long as their size remains small relative to the flow length scale. A comprehensive study is performed for varying Stokes numbers, mass ratios, and shapes, highlighting changes to the particle dynamics.

- **The Rayleigh Collapse of Two Spherical Bubbles**

Speaker: Daniel Hobbs (Rochester Institute of Technology)

Co-authors: Anthony Harkin (Rochester Institute of Technology), Nathaniel S. Barlow (Rochester Institute of Technology), Steven J. Weinstein (Rochester Institute of Technology)

Abstract. The inertial collapse of two interacting and non-translating spherical vacuum bubbles of equal size is considered. The exact analytic solution to the nonlinear ordinary differential equation that governs the bubble radii during collapse is first obtained via a slowly converging power series. An asymptotic approximant is then constructed that accelerates convergence of the series and imposes the asymptotic collapse behavior when the radii are small. Finally, an exact analytic series solution as a function of a gauge variable that removes the singular behavior is found as well, and a comparison of the estimated numerical errors of the different solution methods is considered. The solution generalizes the classical 1917 Rayleigh problem of single bubble collapse, as this configuration is recovered when the distance between the bubble centers far exceeds that of their radii.

- **Optimizing Peristaltic Pump Shapes for Particle Transport in Stokes Flow**

Speaker: Ruowen Liu (Rider University)

Abstract. This talk presents a computational method for optimizing the shapes of peristaltic pumps that transport rigid particles in Stokes flow. The goal is to design pump shapes that minimize energy dissipation while achieving desired fluid and particle transport. The method builds on a fast, accurate boundary integral solver for multiphase flows in periodic geometries. Analytic shape sensitivities are derived solely from the physical variables on fluid boundary and can be computed with only one forward and one adjoint problems. This approach significantly outperforms finite-difference gradients. I will also present several numerical examples of optimal pump shapes under specific physical constraints.

- **Dynamics of Ocean Kinematic Properties**

Speaker: Denny Kirwan (University of Delaware)

Co-authors: Helga Huntley (Rowan University), James Turbett (Rowan University)

Abstract. Near-surface ocean velocity gradients play critical roles in the distribution of pollutants, flotsam, and carbon exchange with the atmosphere. To link observed time series of such gradients to the fluid dynamics driving their evolution, we study solutions to a dynamical system obtained from the gradient of the horizontal equations of motion on a rotating Earth. In the Lagrangian frame this reduces to 4 nonlinearly coupled equations with forcing terms arising from the gradients of applied forces in the equations of motion. Although nonlinear, there are analytic steady state solutions. We report on studies of solutions when these equilibrium states are perturbed. Here the focus is on just time-independent forcing, which already gives rise to an 8-dimensional solution space. With no forcing, perturbed initial states result in exactly inertial oscillations, but with nonlinear amplitudes. With finite forcing, the solutions are either unstable, quickly relax back to the equilibrium states, or are oscillatory with frequencies ranging from super to sub-inertial.

- **The Complexities of Discontinuous Attractor Trajectories: Explorations of Periodic Forcing of the Ocean Vorticity Equation**

Speaker: Helga Huntley (Rowan University)

Co-authors: Denny Kirwan (University of Delaware)

Abstract. The time evolution of vorticity, divergence, and strain rate following a buoyant particle in the ocean is captured by a set of nonlinearly coupled ordinary differential equations. Under steady forcing, the solutions can be periodic, convergent, and unstable. Introducing time-dependence in the forcing gives rise to new levels of complexity. Here we focus on forcing of the vorticity equation alone. Starting with a convergent scenario under steady forcing, periodic perturbations to the forcing are introduced. This can result in a chronotaxic system with a classic limit cycle. However, in other situations, the point attractor follows a discontinuous path, leading to a highly complex solution that neither converges nor becomes periodic.

4 Poster Presentations

- **1D/2D Modeling of Parabolic PDEs in Shallow Ice Sheets Approximation (SIA)**

Speaker: Ricardo Kabila (University of Massachusetts Dartmouth)

Abstract. This poster presents on research in numerical modeling and analysis of shallow ice sheets approximation (SIA) models using Mathematica language. The flow of ice sheets can be described by nonlinear partial differential equations (PDEs), and these models arise from convection-diffusion continuous processes. In this, we're interested in the ice thickness evolution equation assuming an isothermal non-sliding flat ice (base). Kinematically/dynamically, ice has very high viscosity with slow diffusivity, and often is modeled under Glen's flow constitutive law with mass continuity/stokes equations. Giving fit-for-purpose, solved simple PDE model with a smooth halfar/dome-like exponential function, using Mathematica as modeling software for seamless implementation and visualization.

- **A Coupled Hodgkin-Huxley-Lotka-Volterra Model of Functional-Structural Interactions of Neurons**

Speaker: Audrey Moore (Pennsylvania State University)

Co-authors: Corina Drapaca (Pennsylvania State University)

Abstract. Neuronal synchronization is essential to memory processes, motion control, and some brain disorders like epilepsy. Action potentials and chemical neurotransmitters facilitate numerous communications among neurons and their synchronization. The propagation of action potentials can be described mathematically by the Hodgkin-Huxley model, and the synchronization of two neurons may be attained using two Hodgkin-Huxley models coupled by a controller-based synchronizer.

Neurons in the brain are immersed in cerebrospinal fluid and thus share a common environment containing the resources needed for survival. Two adjacent neurons share access to the same pool of resources, and thus may either work together or compete to attain nutrients.

The Lotka-Volterra model describes interactions between two species sharing common resources. In this poster, a coupled Hodgkin-Huxley-Lotka-Volterra model of the functional-structural interactions between two nearby synchronized neurons and corresponding numerical simulations will be presented.

- **A Data-Driven Framework for Non-Destructive Age Estimation of Abalone Using Enhanced Regression Modeling**

Speaker: Sharindi Amasha Samaraweera (Texas Tech University)

Abstract. Determining the age of abalone is traditionally performed by cutting the shell and counting growth rings, a precise but labor-intensive method. This study proposes and validates a predictive framework that uses measurable physical and biological characteristics to estimate abalone age more efficiently. Using a dataset of 4,177 observations from the UCI Machine Learning Repository, eight predictors, including shell dimensions, weights, and sex, were analyzed with multiple linear regression. Model assumptions were examined, and violations of heteroscedasticity and non-normality were mitigated through a Box-Cox transformation ($\lambda = -0.22$). Variable and model selection techniques, including forward, backward, and best-subset procedures, identified an optimal regression model with 12 variables, incorporating key interaction terms such as Length $\times$ Diameter and Sex $\times$ Height. The final model achieved a moderate adjusted R^2 with low residual error (≈ 0.0255), validated through 10-fold cross-validation (RMSE ≈ 0.025). These results demonstrate that regression-based methods provide reliable, non-destructive alternatives for age estimation, offering valuable insights for ecological research and fisheries management. Future directions include integrating environmental and genetic variables or applying machine learning approaches to capture potential nonlinear effects.

- **A Generalized Rosanov Bound: An upper bound on absorption for active materials**

Speaker: Kyle Stephens (New York Institute of Technology)

Abstract. Finding an ideal lightweight electromagnetic absorber is of great interest in current engineering applications including the development of stealth technologies and metamaterials. There exist fundamental physical limitations on how much incident radiation a material can absorb over a given bandwidth. Indeed, the Rosanov bound establishes this limit in terms of the reflection coefficient for a thin material coating a perfect mirror with a simple planar geometry at normal incidence. Using techniques from complex analysis, we derive a generalization of the Rosanov bound for the case of an active material, where the wavelength-dependent reflection coefficient can be extended to a meromorphic function in the upper-half complex plane. The derived bound implies that there exists a trade-off between the amount of radiation absorbed and the absorption bandwidth.

- **A level-set based finite difference method for the ground state Bose-Einstein condensates**

Speaker: Hwi Lee (New York Institute of Technology)

Co-authors: Yingjie Liu (Georgia Institute of Technology)

Abstract. We present a novel third-order finite difference method for computing the ground states of Bose-Einstein condensates (BECs) in domains with arbitrary boundaries defined by arcs and angles. Our approach is based on a new PDE-driven extension of the level set method, which enables automatic handling of complex geometries on rectangular grids. Our work pioneers the intersection of the highly influential level set method, and the imaginary time method which is the most popular method in physics literature for computing the ground states of BECs.

- **A Mathematical Model of a Multi-Variant Pathogen Emerging Infectious Disease**

Speaker: Borkor Gifty Tracy (Rochester Institute of Technology)

Abstract. The COVID-19 pandemic showed how tough it is to deal with emerging diseases that keep producing new variants. SARS-CoV-2 mutates quickly, which makes it important to have models that can track how different variants change the course of an outbreak. In this work, we extend a basic SEIRV model by adding compartments for both the original strain and a new variant, while also including vaccination and reinfection. The model is written as a system of nonlinear differential equations, and we show it is well-posed so the solutions stay biologically meaningful. To capture the timing of new variants, we use a Hill function that lets the variant emerge smoothly at random times. We also compute the basic reproduction number, R_0 , using the next-generation matrix approach, and explore how parameters like contact rate, shedding rate, and vaccine efficacy affect transmission. This model sets the stage for analyzing real COVID-19 data from Cameroon and Nigeria and gives insight into how new variants and imperfect vaccination shape the spread of the disease.

- **A Structure-Preserving Low-Rank Implicit-Explicit Integrator for a 1D2V Vlasov-Fokker-Planck Model in Cylindrical Coordinates**

Speaker: Dylan Jacobs (Swarthmore College)

Co-authors: William Taitano (Los Alamos National Laboratory), Joseph Nakao (Swarthmore College)

Abstract. Many traditional methods for solving partial differential equations (PDEs) suffer from exponentially increasing computational storage complexity as the number of dimensions increases. Low-rank matrix (or tensor) decompositions can be used to exploit low-rank structure in the solution, helping mitigate this curse of dimensionality. However, many PDEs that model physical phenomena include stiff operators that must be evolved implicitly, and combining low-rank and implicit methods while preserving structures such as mass, momentum, and energy remains a challenge. In this poster, we present a low-rank, implicit-explicit integrator that utilizes structure-preserving discretizations for the stiff Fokker-Planck collision operator to solve a Vlasov-Fokker-Planck model in 1d2v phase space.

- **A study of a generalized subset of centrally symmetric Riordan arrays**

Speaker: Ifeyinwa Madu (Morgan State University)

Co-authors: Nkwanta Asamoah (Morgan State University)

Abstract. In this poster, we study a certain generalized subset of centrally symmetric Riordan arrays. Riordan arrays are a class of infinite lower-triangular matrices, where the array entries are determined by the coefficients of two specific generating functions. A centrally symmetric Riordan array is one in which the entries are symmetric with respect to the center of the array. For example, Pascal's triangle is a well-known instance of such symmetry and serves as a classical example of a centrally symmetric Riordan array. Because of the resemblance between these structures and the familiar Pascal triangle, centrally symmetric arrays are often referred to as Pascal-like matrices. This terminology reflects their symmetric properties and recurrence relationships. The intersection of Pascal-like matrices, centrally symmetric matrices, and Riordan arrays opens a rich avenue of investigation in combinatorics, matrix groups, and linear algebra. These connections are particularly valuable for deriving new combinatorial identities, solving recurrence relations, discovering structural properties of matrix transformations, and exploring applications across various areas of the mathematical sciences. Preliminary results from our study reveal interesting links between this class of arrays and well known combinatorial sequences and polynomials, such as the Fibonacci numbers and Chebyshev polynomials. These findings suggest potential for further exploration in algebraic combinatorics, discrete mathematics, and symbolic computation.

- **A Study of a Generalized Subset of Centrally Symmetric Riordan Arrays**

Speaker: Name (Institution)

Co-authors: Name ()

Abstract. text

- **Adaptations to Dynamic Modeling of LH and Endogenous Testosterone for Applications to Transgender Men**

Speaker: Parker Potter (Rochester Institute of Technology)

Co-authors: Kara Maki (Rochester Institute of Technology), Nathaniel Barlow (Rochester Institute of Technology), Steven Weinstein (Rochester Institute of Technology)

Abstract. Hormone replacement therapy (HRT) consists of exogenous delivery methods to suppress endogenous hormone production and control testosterone and/or estrogen within a safe, effective biological range. In this work, we utilize a pharmacokinetic-pharmacodynamic approach to model testosterone and luteinizing hormone (LH) in transgender men taking testosterone injections. Presently, the literature primarily consists of clinical studies focused on hypogonadal cisgender males and HRT models that fail to account for the complexities of endogenous hormone release. As a basis for our modeling efforts, we turn to the non-autonomous system of ODEs presented by Fattinger et al. to track LH and testosterone in the bloodstream in response to GnRH antagonist injections. Our modified model first concentrates on reaching pseudo-homeostasis without HRT pharmacokinetics. By applying biological intuition of the application field and examining parameter elasticity within the linearized system, we revised four parameters to predict an unforced steady-state inside the expected ranges of hormonal variation. Further, we found that testosterone concentrations can be approximated with an analytic solution that does not exhibit pronounced deviations from numerical simulations for long-time. With a precursory explanation of hormonal behavior in pre-HRT transgender men, we plan to further develop the control problem through addition of exogenous testosterone dynamics.

- **An Exact SIR Series Solution and An Exploration of the Related Parameter Space**

Speaker: Daniel Hobbs (Rochester Institute of Technology)

Abstract. A convergent power series solution is obtained for the SIR epidemiology model, using an asymptotically motivated gauge function. For certain choices of model parameter values, the series converges over the full physical domain (i.e., for all positive time).

- **Analysis of Polygonal Tessellations**

Speaker: Riley Clarke (University of Scranton)

Co-authors: Joseph Klobusicky (University of Scranton)

Abstract. This poster consists of computational geometry work, related to finding data about polygonal tessellations in a closed space. We analyzed network data including area, average number of vertices, and how both cut and break operations evolve network statistics. We also looked at frequencies of regular (Y junction) and irregular (T junction) vertices and their trajectories in time. We implemented a NODE (Neural ODE) to model network statistics.

- **Anchored PnP-Flow for Cytoskeletal Timelapse**

Speaker: My Nguyen (University of New Mexico)

Co-authors: T. Hang Nguyen (University of New Mexico)

Abstract. Traditional bottom-up physical models and modern data-driven methods each illuminate different facets of cytoskeletal dynamics. We combine the two by adopting a time-aware Plug-and-Play solver whose structure is motivated by the mathematics of Optimal Transport. The method is paired with an anchored geometric readout that tracks spindle-pole separation over time in HeLa timelapse microscopy. Our results show improved structural similarity while preserving biologically meaningful trends in spindle geometry.

- **Constructing a Low-rank Implicit Algorithm for Solving High Dimensional Equations in the Hierarchical Tucker Tensor Format**

Speaker: Paolo Bosques-Paulet (Swarthmore College)

Co-authors: Joseph Nakao (Swarthmore College), Gianluca Ceruti (University of Innsbruck)

Abstract. High-dimensional partial differential equations (PDEs) show up in many applications across physics, biology, and finance. Standard integrators for PDE solutions quickly exhaust the storage capacity of most computers, thus necessitating efficient and highly accurate numerical schemes. To address this problem, PDE solutions can be decomposed using low-rank tensor decompositions, e.g., the hierarchical Tucker decomposition (HTD). However, there are limited low-rank methods that are high-order implicit and can accommodate high-dimensional solutions. In this project, we develop a novel algorithm using the HTD to implicitly compute the solutions to high-dimensional diffusion equations. A working algorithm is developed for 3D solutions before extending to higher dimensions. We hope to extend the proposed method to advection-diffusion-reaction problems.

- **Denoising diffusion models for inverse design of inflatable structures with programmable deformations**

Speaker: Sara Karimi (Rutgers University)

Co-authors: Nikolaos Vlassis (Rutgers University)

Abstract. Programmable structures are systems whose undeformed geometries and material property distributions are deliberately designed to achieve prescribed deformed configurations under specific loading conditions. Inflatable structures are a prominent example, using internal pressurization to realize large, nonlinear deformations in applications ranging from soft robotics and deployable aerospace systems to biomedical devices and adaptive architecture. We present a generative design framework based on denoising diffusion probabilistic models (DDPMs) for the inverse design of elastic structures undergoing large, nonlinear deformations under pressure-driven actuation. The method formulates the inverse design as a conditional generation task, using geometric descriptors of target deformed states as inputs and outputting image-based representations of the undeformed configuration. Representing these configurations as simple images is achieved by establishing a pre- and postprocessing pipeline

that involves a fixed image processing, simulation setup, and descriptor extraction methods. Numerical experiments with scalar and higher-dimensional descriptors show that the framework can quickly produce diverse undeformed configurations that achieve the desired deformations when inflated, enabling parallel exploration of viable design candidates while accommodating complex constraints.

- **Distinguishing Stochastic Fluctuations from Deterministic Population Dynamics**

Speaker: Zoe Tang (Swarthmore College)

Co-authors: James Flagg (University of Idaho), Paris Lewis (North Carolina State University), Mason Mannin (Arizona State University), John Nagy (Arizona State University)

Abstract. Long-term prediction and conservation planning of ecological systems is challenging as a result of chaos, in which small differences in initial conditions can lead to drastically different outcomes over time. Traditional methods for detecting chaos, such as those based on Lyapunov exponents (LEs), seem unreliable when high levels of noise are present in field data. In this study, we address a critical gap in the literature: quantifying the extent to which prediction error is due to deterministic variance versus stochastic noise. In our work, the reliability of the LE is assessed by quantifying the proportion of forecast error due to noise. We introduce an ensemble-based framework that perturbs observed initial conditions and propagates forecasts through a local surrogate model to estimate the contribution of deterministic divergence, intrinsic stochasticity, and measurement error to total forecast variance. Additionally, we explore applications of this framework within ecological data. Preliminary results suggest that increasing levels of noise require greater measurement uncertainty to account for the observed dynamics through deterministic models. Our approach potentially enables the more accurate detection of chaos and yields insight into the forecasting of complex ecological systems.

- **Enabling the Macroscopic Validation of Hyperbolic Traffic Flow Models Using I-24 MOTION Data**

Speaker: Blessing Nwonu (Temple University)

Abstract. Macroscopic models play an important role in traffic simulation, forecasting, and control. At the same time, the validity of macroscopic model remains hard to establish, in part due to limitations on high-quality existing data sets. We present a systematic framework for the evaluation of scalar hyperbolic traffic flow models against high-resolution vehicle trajectory, with a particular focus on data from the I-24 MOTION testbed. Properly reconstructed space–time fields of traffic density, flux, and velocity from the microscopic trajectories are combined with appropriate numerical approximations of the underlying Lighthill–Whitham–Richards–type conservation laws to be tested. This work both demonstrates the utility of high-resolution trajectory data for macroscopic model validation, and it highlights some key challenges incurred with first-order traffic models.

- **Fast Laplacian-Free Clustering Algorithm with Fairness Constraints**

Speakers: Malcolm Dickens (University of Maryland, Baltimore County), Leonardo Cambisaca (Colgate University)

Co-authors: Iván Ojeda-Ruiz (Lamar University), Young-Ju Lee (Texas State University)

Abstract. Recent research has focused on mitigating algorithmic bias in clustering by incorporating fairness constraints into algorithmic design. Notions such as disparate impact, community cohesion, and cost per population have been implemented to enforce equitable outcomes. Among these, group fairness (balance) ensures that each protected group is proportionally represented within every cluster. However, incorporating balance as a metric of fairness into spectral clustering algorithms has led to computational times that can be improved. This study aims to enhance the efficiency of spectral clustering algorithms by reformulating the constrained optimization problem using a new formulation derived from the Lagrangian method and the Sherman-Morrison-Woodbury (SMW) identity, resulting in the Fair-SMW algorithm. Fair-SMW employs three bilateral operators with different spectral gaps

to generate multiple variations of Fair-SMW, achieving clustering solutions with comparable balance to existing algorithms while offering improved runtime performance. We present the results of Fair-SMW, evaluated using the Stochastic Block Model (SBM) to measure both runtime efficiency and balance across real-world network datasets, including LastFM, FacebookNet, Deezer, and German.

- **Identifying Particle Features That Drive Clustering in Shear-Driven Dense Suspensions**

Speaker: Kinjal Gadgil (New Jersey Institute of Technology)

Co-authors: Ismaeel Malek (New Jersey Institute of Technology), Zhaoshu Cao (New Jersey Institute of Technology), Jonathan Jaquette (New Jersey Institute of Technology), Linda Cummings (New Jersey Institute of Technology), Lou Kondic (New Jersey Institute of Technology)

Abstract. Clustering of rigid particles in shear-driven dense suspensions strongly affects how these materials flow, but the processes that lead to cluster formation are not yet well understood. This project examines the properties of individual particles and their contact patterns to identify features that distinguish clustered from non-clustered particles. Simulation data provided by our collaborators at the City College of New York are analyzed using a combination of visual, numerical, and machine-learning methods to reveal correlations between local structure and clustering behavior. Local interaction networks are built with a “swatch and cloth” approach: the “cloth” represents the full interaction network of the suspension, while a “swatch” captures the small neighborhood surrounding a single particle. Each swatch includes particles in direct frictional contact with the chosen particle and extends up to four neighboring layers. Total persistence and feature lifetime are being explored as ways to distinguish clustered and non-clustered particles. Although the present study focuses on two-dimensional simulations, the methods are designed to extend to fully three-dimensional systems.

- **Implementation of Worsey-Farin Splines for Solution Transfer**

Speaker: Logan Larose (Pennsylvania State University)

Co-authors: David M. Williams (Pennsylvania State University)

Abstract. This poster will demonstrate the effectiveness of the Worsey-Farin spline space for interpolation, i.e. solution transfer, between 3-dimensional tetrahedral meshes. The proposed transfer process is especially relevant for slab-based space-time finite element methods. The poster presents results of numerical experiments which highlight the conservative nature and order of accuracy of the transfer process, and presents a qualitative evaluation of the visualization properties of the smoothed solution. Additionally, the poster will provide explicit and comprehensive implementation details for this spline space—which have been lacking since its inception.

- **Machine-Learning Interatomic Potentials for Long-Range Systems**

Speaker: Jiuyang Liang (Flatiron Institute)

Abstract. Machine-learning interatomic potentials have emerged as a revolutionary class of force-field models in molecular simulations, delivering quantum-mechanical accuracy at a fraction of the computational cost and enabling the simulation of large-scale systems over extended timescales. However, they often focus on modeling local environments, neglecting crucial long-range interactions. We propose a Sum-of-Gaussians Neural Network (SOG-Net), a lightweight and versatile framework for integrating long-range interactions into machine learning force field. The SOG-Net employs a latent-variable learning network that seamlessly bridges short-range and long-range components, coupled with an efficient Fourier convolution layer that incorporates long-range effects. By learning sum-of-Gaussians multipliers across different convolution layers, the SOG-Net adaptively captures diverse long-range decay behaviors while maintaining close-to-linear computational complexity during training and simulation via non-uniform fast Fourier transforms. The method is demonstrated effective for a broad range of long-range systems.

- **Mathematical Assessment of the Role of Vaccination on Chlamydia Control**

Speaker: Jane Odeh (Morgan State University)

Co-authors: Jemal Mohammed-Awel (Morgan State University)

Abstract. PURPOSE. Chlamydia is a bacterial infection and the most commonly reported sexually transmitted infection (STI) in the United States that can infect both men and women. In 2023, 1.6 million new chlamydia cases were reported in the United States. If not treated, chlamydia can cause pelvic inflammatory disease, increase the risk of infertility, be transmitted to the babies during childbirth, potentially causing neonatal conjunctivitis or pneumonia in babies, and facilitate the transmission of other STIs such as HIV. The goal of the study is to develop and analyze mathematical models (parameterized with data from Maryland) to investigate the impact of chlamydia treatment combined with chlamydia vaccination on chlamydia transmission dynamics and control (if the vaccine under development becomes available).

METHODS. This study presents a mathematical model (nonlinear differential equations) that incorporates chlamydia, HIV, and chlamydia-HIV infection/co-infection in humans. The model incorporates treatment for chlamydia and HIV-infected individuals and chlamydia vaccination, which is under development. The model is rigorously analyzed, the basic reproduction number is calculated, and the asymptotic stability property of the disease-free equilibrium is established.

RESULTS. The theoretical analyses revealed that the disease-free equilibrium is locally asymptotically stable if the basic reproduction number of the model is less than unity; the parameters related to the treatment, vaccination rate, and vaccination efficacy play a major role in bringing and maintaining the value of the basic reproduction numbers below one (the epidemiological significance is that the disease can be eliminated if the basic reproduction number of the model is less than one). The model is parameterized with data from Maryland. Numerical simulation results show the importance of chlamydia screening, access to treatment, vaccination coverage, and efficacy.

CONCLUSION. The research results showed that the prospects of effectively controlling chlamydia transmission is promising with optimal vaccine coverage and vaccine efficacy, screening, and access to treatment.

- **Mathematics of Computed Tomography scans**

Speaker: Anna Dykhno (New York Institute of Technology)

Abstract. Computed Tomography (CT) scanning is a power tool in modern medical imaging, enabling the analysis and reconstruction of internal structures from X-ray data. During a CT scan, X-ray beams are emitted from multiple angles and pass through the body, undergoing attenuation based on the density of the tissues encountered. The mathematical model, that is used to numerically simulate the data collected during a CT scan, is known as the Radon Transform. It integrates a function over straight lines corresponding to the X-ray paths. The inverse Radon Transform can be used to reconstruct the original image from the projection data.

This poster demonstrates the application of the Radon Transform to simulate X-ray projection data from multiple angles, along with image reconstruction using Unfiltered Back Projection (UBP). The limitations of UBP are examined, highlighting the importance of the Filtered Back Projection (FBP) method, which entails Fourier-filtering.

Examples generated in MATLAB demonstrate the Radon Transforms of various functions and images and show the process of reconstructing the original image via both Unfiltered and Filtered back projections approaches. The poster aims to reveal the mathematical foundations of Computed Tomography imaging and bridge the gap between the theoretical and practical aspects of mathematical tomography.

- **Mechanics of Entangled Networks**

Speaker: Juntao Huang (University of Delaware)

Abstract. Entangled networks are ubiquitous in biological and physical systems, spanning from tissues and gels to cotton and fabrics across multiple length scales. In contrast to classical spring networks, entangled networks are made of chains interconnected by entanglements as topological constraints that can slide along chains while maintaining intersections between adjacent chains. Recent experimental

observations highlight the crucial role of entanglements in enabling extreme mechanical properties of materials. However, their mechanics remain poorly understood theoretically due to the complexity of the topological constraints of entanglements.

In this talk, we present a mathematical framework that models entangled networks as graphs, capturing both network topology and entangled interactions. For entangled networks of arbitrary size and topology, we prove that the entanglements reduce system energy by enabling stress redistribution through sliding. In addition, we prove that the energy landscape is convex. Using this framework, we study elasticity and fracture, validated by experiments on entangled fabrics and hydrogels. This framework establishes fundamental principles of entangled mechanics and offers a theoretical foundation for designing reconfigurable materials. This is a joint work with Jiabin Liu and Shaoting Lin from Michigan State University.

- **Mitigating Topological Noise in 3D Images of Porous Media**

Speaker: Aakash Karlekar (New Jersey Institute of Technology)

Co-authors: Ebru Dagdelen (New Jersey Institute of Technology), Manav Arora (New Jersey Institute of Technology), Matthew Illingworth (New Jersey Institute of Technology), Zhaoshu Cao (New Jersey Institute of Technology), Linda Cummings (New Jersey Institute of Technology), Lou Kondic (New Jersey Institute of Technology), Jonathan Jaquette (New Jersey Institute of Technology)

Abstract. Porous media flow is essential to many natural and industrial processes, including environmental cleanup, oil recovery, and CO₂ storage. Understanding and optimizing these processes requires characterizing the complex internal structure of these materials. Techniques from Topological Data Analysis, especially persistent homology, are very helpful for this task. However, when working with real-world data—specifically 3D images of porous media—we face significant computational challenges because of the complexity of the datasets and the presence of experimental noise, which can hide key topological features and increase computational costs. We propose a denoising method using Gaussian convolution to smooth the data and reduce noise. We demonstrate the effectiveness of our method using simulated image datasets, where we add noise to simulate real experimental data and then apply our smoothing technique for denoising. To assess the effectiveness of our method, we use several topological measures to compare the original and denoised datasets. Finally, we discuss the optimal denoising approach that makes these measures closest to the original, noise-free data.

- **Modeling the Transmission Dynamics of the Monkeypox Virus Infection with Intervention Measures**

Speaker: Emiliano Morales-Lopez (Swarthmore College)

Co-authors: Nyvisalsnuk Rith (Swarthmore College), Nsoki Mavinga (Swarthmore College), Tendai Mugwagwa (Pfizer UK)

Abstract. Mpox is an infectious disease caused by the monkeypox virus that can be spread between humans and animals, and is endemic to western and central Africa particularly in the Democratic Republic of the Congo (DRC). We develop a deterministic model to analyze the effectiveness of vaccination and other intervention measures for Mpox, while also demonstrating the transmission dynamics including the potential transmission event from a human to an animal. Through mathematical analysis, we show the positivity and boundedness properties of the solutions within the model. Furthermore, we derive the basic reproduction number R_0 using the next generation method, and provide the necessary conditions for disease-free equilibrium to be locally stable through a combination of the linearization method and the Routh-Hurwitz criterion. Additionally, we give sufficient conditions for global stability of the disease-free equilibrium. The model is fitted using the nonlinear least square method to describe the dynamics of the disease based on reported cases of Mpox from DRC between 2023 and May 2025. Sensitivity analysis is performed to show the responsiveness of R_0 with respect to the model parameters.

- **Modified Mapper: Estimating ReebGraphs through Topological Change point Detection with applications to fMRI data**

Speakers: Padma Ragaleena Tanikella (Pennsylvania State University), Nicole Lazar (Pennsylvania State University)

Abstract. Topological Data Analysis (TDA) utilizes tools from algebraic topology to model the shape of data. The mapper algorithm, introduced by Singh et al. (2007), provides a graphical summary of the data's topology. The authors introduced mapper as a statistical counterpart of a mathematical concept called the Reeb graph. In other words, mapper output is an estimate of the Reeb graph. However, we noticed that the approach proposed by Singh et al.(2007) can be modified to estimate the Reeb graph better using ideas from discrete Morse theory, extended persistence, and changepoint analysis. We address the problem of estimating the Reeb graph by transforming it into a problem of identifying topological changepoints. To the best of our knowledge, no prior work has viewed Reeb graph estimation through the lens of changepoint detection. We have preliminary results to show that our proposed modified mapper algorithm accurately identifies topological changepoints which allows for better Reeb graph estimation. Currently, we are working on using a topological changepoint approach to analyze "raw" fMRI data in order to better understand the pain network and theory of mind regions of adults and children. Future work will explore how the proposed modified mapper can be used to better understand brain activation patterns in response to specific stimuli.

- **Multi-frequency Electromagnetic Inversion for Soil Characterization**

Speaker: Tyler Casas (Rowan University)

Co-authors: Thanh Nguyen (Rowan University), Jie Li (Rowan University), Cheng Zhu (Rowan University)

Abstract. In cold regions, permafrost degradation poses a significant challenge to maintain transportation systems and facilities. In recent years, geophysical hazard detection was instrumental in identifying permafrost to minimize the potential for ground subsidence, which enabled the construction of more infrastructure in cold regions. As a common choice for geophysical applications, electromagnetic induction (EMI) based methods can be used to (i) detect subsurface layers in the ground and (ii) characterize soil types by electrical conductivities. However, EMI technology struggles with low resolution at lower frequencies and shallower depth of penetration at higher frequencies. Employing multi-frequency EMI (MFEMI) sensors is one such way to minimize the impact of both issues. This poster addresses the reconstruction of the 1-D conductivity profile of layered earth from data measured by an MFEMI sensor. To solve this inverse problem to obtain the reconstructed conductivity profile, a least-squares minimization was utilized. The inversion results for both simulated and experimental data showcased the proposed inversion algorithm was able to accurately reconstruct the conductivity profile of layered soil.

This study is supported by the Broad Agency Announcement Program and the U.S. Army Engineer Research and Development Center (ERDC) under Contract No. W913E523C0007. The opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Broad Agency Announcement Program and the U.S. Army Engineer Research and Development Center (ERDC).

- **Multivariate Characterization of Wine Quality via PCA and Hypothesis Testing**

Speaker: Kalana Kushan Munasinghe Arachchige (Texas Tech University)

Abstract. Wine quality is a critical determinant for consumer acceptance and industry success, influenced by complex interactions among chemical and physical properties. This study investigated the physicochemical composition of Portuguese "Vinho Verde" wines, comparing a total of 6,463 observations after data cleaning. Eleven quantitative variables, including acidity measures, residual sugar, sulfur dioxide levels, density, pH, sulfates, and alcohol content, along with categorical variables for wine type and expert-rated quality (0–10 scale) were analyzed. Using stratified sampling, the dataset was divided into exploratory and confirmatory subsets. Principal Component Analysis (PCA) revealed that the first six principal components explained 85.45% of the overall variation, with clear clustering

patterns between red and white wines. Confirmatory analyses employed Hotelling's T^2 tests and simultaneous confidence intervals to compare mean vectors across wine types and quality levels. Results confirmed statistically significant differences between red and white wines, as well as between quality categories, particularly for variables such as volatile acidity, total SO, density, sulfates, and alcohol content. These findings highlight the distinct compositional profiles underlying wine quality and provide a framework for winemakers to optimize production strategies in response to consumer preferences.

- **Nonlinear Dynamics of Vibrating Fluid Drops**

Speaker: Joseph D'addesa (New Jersey Institute of Technology)

Abstract. We investigate experimentally and theoretically the spreading and deformation of fluid puddles on bounded substrates under vertical surface vibrations. For a fluid volume with a characteristic height on the order of the capillary length, a finite-radius puddle remains stable in the absence of forcing. Upon applying vibrations, the puddle front expands progressively, with the extent of spreading increasing with vibration strength. We find that the equilibrium puddle radius increases with both liquid volume and excitation amplitude. This behavior is captured by an effective capillary length framework, where vibrational forcing reduces the apparent surface tension. These findings offer new insight into how dynamic surface forces influence the shape and stability of vibrated fluid volumes.

- **Numerical Study of a Traffic Flow Inspired by DNA Transcription Modeling**

Speakers: Kevin Courtney (Pennsylvania State University), Kyle Courtney (Pennsylvania State University), Andrew Hertzberg (Pennsylvania State University), Tanisha Shah (Penn State Abington)

Co-authors: Faranak Courtney-Pahlevani (Penn State Abington), Lisa Davis (Montana State University)

Abstract. The research presented in this poster is motivated by a biology application that aims to study the mechanism of RNA polymerases transcribing the DNA strand in the protein production process. Transcription and translation are two key stages of protein synthesis, and they are crucial components in the transfer of genetic information from DNA to protein.

The study in [1] uses the first order traffic flow model known as Lighthill-Whitham-Richards (LWR) to describe this bio-polymerization phenomena. The research work considers the model analysis and computations in three cases of constant, piecewise-defined constant, and a variable traffic flow velocity. The LWR model is a non-linear hyperbolic partial differential equation, and for a portion of this work, the model is reduced to a linear hyperbolic equation in the case of a constant flow velocity. A new time filtering technique introduced in [2, 3] is applied to different schemes, such as upwind and fully implicit, for numerically solving the linear model. The filtering technique is also combined with fully explicit and semi-implicit schemes for numerically solving the original nonlinear LWR model. In both cases, the filtering technique is shown to achieve high accuracy in the estimation of key biological measures with very little extra computational cost. The computational results test the accuracy of implementing the numerical schemes to determine parameters and factors affecting the transcription time and the concentration of RNAP along the DNA strand.

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(2) K. Boatman, L. Davis, F. Pahlevani and T. Susai Rajan, Numerical Analysis of a Time Filtered Scheme for a Linear Hyperbolic Equation Inspired by DNA Transcription Modeling, *Journal of Computational and Applied Mathematics*, Vol. 429 (2023), pp. 1-14.

(3) K. Boatman, L. Davis, C. Drapaca, F. Pahlevani and T. Susai Rajan, Time Filtered Finite Difference Schemes for Linear Hyperbolic Problems, *AMMCS 2023 Proceedings*.

- **On the Application of Fractional Order Viscoelasticity for Characterizing Brain White Matter**

Speaker: Parameshwaran Pasupathy (Rutgers University)

Abstract. Predicting the mechanical response of brain white matter (BWM), even in the limit of small strains is challenging owing to the inherent anisotropy of the three-dimensional microstructure and the various interactions between the heterogeneous structural components of brain tissue. Conventional viscoelastic characterization of BWM, typically carried out within the classical framework of springs and dashpots expressed as a Prony series, remains a purely empirical representation that is difficult to physically interpret.

MRE measurements increasingly suggest that the mechanical response of BWM exhibits power-law behavior. A power-law model in the frequency domain, under the assumptions of linear viscoelasticity and causality, yields a fractional viscoelastic model in the time domain. Here, we develop a fractional viscoelastic model of the axon and extracellular matrix (ECM). which is implemented in a Fortran VUMAT subroutine. A biphasic finite element model of hexagonally packed representative volume elements (RVEs) of axons in ECM, subjected to periodic and quasi-static displacement-controlled boundary conditions, is built in Abaqus. An optimization algorithm is then applied to solve the inverse problem and extract the homogenized properties of the biphasic model.

This framework provides a succinct, physically meaningful description of BWM’s mechanical response, which is difficult to capture with Prony series models. The results reveal the nonlinear variation of material parameters with axon volume fraction, the directional dependence of BWM mechanics, and the complex interplay among microstructural elements—all of which are crucial for understanding neuropathological changes associated with disease and aging.

- **On the study of exponential mixing properties of the stochastically forced Boussinesq system for Rayleigh-Bénard convection**

Speaker: Juliane Baiochi Dalben (Drexel University)

Co-authors: Cecilia Freire Mondaini (Drexel University), Nathan Glatt-Holtz (Indiana University Bloomington)

Abstract. The ergodicity for stochastic partial differential equations has been studied by several mathematicians recently, and Harris’ theorem provides a result concerning the question of stability of long-time statistical properties for dynamical systems. In [Glatt-Holtz and Mondaini, Long-term accuracy of numerical approximations of SPDEs with the stochastic Navier-Stokes equations as a paradigm, ’24], the authors obtained a weak form of Harris’ theorem, showing that the Markov semigroup is a contraction in a suitable Wasserstein distance, which implies existence uniqueness and exponential rates of convergence towards the invariant measure.

In this poster, we apply this result to the Boussinesq approximation for Rayleigh-Bénard convection, a model for the evolution of a fluid flow’s velocity field, temperature field, and pressure under buoyancy-driven flow caused by thermal gradients. Our main result concerns the stability of the long-time statistics with respect to the Prandtl and Rayleigh numbers. We show that the invariant measure of the Markov semigroup associated to the dynamics of the system depends continuously on these parameters. Our proof consists of two crucial steps: firstly, we show that the underlying Markov semigroup satisfies a contraction estimate, in a suitable Wasserstein distance; and secondly, we obtain a finite-time pointwise continuity estimate.

- **Optimizing the Magic Constant in Fast Inverse Square Root Using Differential Evolution**

Speaker: Xuanlin Zhu (College of William and Mary)

Abstract. The fast inverse square root algorithm, popularized by the Quake III Arena game engine, is a computational method that approximates $\frac{1}{\sqrt{x}}$ using bit manipulation and Newton’s method. Central to this algorithm is the “magic number” constant that initializes the approximation. Traditional approaches to finding this constant have relied on analytical derivations based on assumptions on input distributions. This paper introduces a machine learning approach using Differential Evolution (DE) to optimize the magic number for 32-bit floating-point arithmetic. Our method eliminates the need for complex mathematical derivations while producing a highly accurate constant optimized for a specified range of inputs. We demonstrate that the DE-optimized magic number achieves a worst-case

relative error of approximately 4.73×10^{-6} after two Newton iterations. This computational approach offers a generalizable framework for optimizing similar bit-manipulation algorithms, particularly when analytical solutions are unwieldy or when optimizing for specific input distributions.

- **Point-Cloud vs Distance Filtration TDA for Permeability Estimation**

Speaker: Manav Arora (New Jersey Institute of Technology)

Co-authors: Ebru Dagdelen (New Jersey Institute of Technology), Aakash Karlekar (New Jersey Institute of Technology), Matthew Illingworth (New Jersey Institute of Technology), Zhaoshu Cao (New Jersey Institute of Technology), Jonathan Jaquette (New Jersey Institute of Technology), Linda Cummings (New Jersey Institute of Technology), Lou Kondic (New Jersey Institute of Technology)

Abstract. The overall goal of this work is to determine whether, in controlled settings, the fluid transport parameters of synthetic 3D porous microstructures can be predicted using topological descriptors. We use PuMA (Porous Microstructure Analysis) open source software to generate porous structures of specified porosity comprising overlapping spheres, and to calculate the permeability. We extract topological measures in parallel using two complementary Topological Data Analysis (TDA) pipelines: (i) distance-transform filtrations (a process that gradually reveals structure at different scales) using HomCloud software applied to both pore and solid phases, and (ii) alpha complexes (geometric structures built from point sets) using GUDHI software based on voxel-center point clouds. We created size-sensitive summaries of each persistence diagram (a visual representation of topological features across scales), including the overall (net) persistence in $H_0/H_1/H_2$ and the corresponding Betti counts (numbers quantifying holes and connected components). The permeability and these topological summaries show strong, monotonic connections over hundreds of synthetic samples with a given porosity. We measure the effects of point-budget limits on correlation strength and stability, the subsampling approach for alpha complexes, and phase choice (pore vs. solid).

- **Quantum DeepONet: Neural operators accelerated by quantum computing**

Speaker: Pengpeng Xiao (Yale University)

Abstract. In the realm of computational science and engineering, constructing models that reflect real-world phenomena requires solving partial differential equations (PDEs) with different conditions. Recent advancements in neural operators, such as deep operator network (DeepONet), which learn mappings between infinite-dimensional function spaces, promise efficient computation of PDE solutions for a new condition in a single forward pass. However, classical DeepONet entails quadratic complexity concerning input dimensions during evaluation. Given the progress in quantum algorithms and hardware, here we propose to utilize quantum computing to accelerate DeepONet evaluations, yielding complexity that is linear in input dimensions. Our proposed quantum DeepONet integrates unary encoding and orthogonal quantum layers. We benchmark our quantum DeepONet using a variety of PDEs, including the antiderivative operator, advection equation, and Burgers' equation. We demonstrate the method's efficacy in both ideal and noisy conditions. Furthermore, we show that our quantum DeepONet can also be informed by physics, minimizing its reliance on extensive data collection. Quantum DeepONet will be particularly advantageous in applications in outer loop problems which require exploring parameter space and solving the corresponding PDEs, such as uncertainty quantification and optimal experimental design.

- **Stability and Bifurcation Analysis on Fishery Models with Strong Allee Effect and Holling's Type III Functional Response**

Speaker: Nyvisalsnuk Rith (Swarthmore College)

Co-authors: Nsoki Mavinga (Swarthmore College)

Abstract. Fish harvesting is an important economic sector worldwide. They also play an important role in the aquatic ecosystem and over-exploitation could have a devastating consequence in the environment. Therefore, harvesting models has gathered much interest in mathematical bio-economics.

In this research, we present differential equation models that describe the dynamics of the fish population under harvesting activity. We assume that the growth of the fish population follows the logistic growth and the strong Allee effect which is the correlation between the population size to its individual fitness. The harvesting rate is given by the Holling’s type III (Sigmoid) functional response where the maximum effort exerted by the predator-human is constant. We provide the conditions for the existence of nonnegative equilibrium solutions and prove the stability of each equilibrium solution. Through bifurcation analysis, we formulate a family of parameter values that guarantees the occurrence of a saddle-node bifurcation within the model. Our results show that the strong Allee effect has a significant impact on the dynamics of the fish population, especially in the extinction and the population threshold within the fishery. Numerical simulations are performed to further comprehend the theoretical result.

- **Tensor density estimation in cryo-EM**

Speaker: Matias Andia (Princeton University)

Co-authors: Marc Aurèle Gilles (Princeton University)

Abstract. In the last decade, low-rank tensor methods have received a lot of attention for density estimation due to their ability to overcome the curse of dimensionality in high dimensions. In this poster, we investigate how the “tensor-train density estimator” (TT-DE), can be applied to recover the conformational density in cryo-EM datasets. TT-DE significantly outperforms kernel density estimation (KDE) on synthetic datasets and slightly outperforms it on cryo-EM datasets in initial experiments, with much room for further improvements.

- **Training AI Models to Predict Permeability on Porous Media**

Speaker: Ebru Dagdelen (New Jersey Institute of Technology)

Co-authors: Aakash Karlekar (New Jersey Institute of Technology), Manav Arora (New Jersey Institute of Technology), Matthew Illingworth (New Jersey Institute of Technology), Zhaoshu Cao (New Jersey Institute of Technology), Jonathan Jaquette (New Jersey Institute of Technology), Linda Cummings (New Jersey Institute of Technology), Lou Kondic (New Jersey Institute of Technology)

Abstract. This work presents a multi-stage investigation into the relationship between porous structures and permeability through computational modeling and topological analysis. It focuses on generating synthetic porous structures, extracting their geometric and statistical descriptors, and computing permeability using numerical simulations. Then, we assess the applicability of network representations by comparing permeability results derived from simplified graph-based models against those obtained from the original data. Finally, we explore the use of computational topology, particularly persistent homology, to characterize the structural complexity of simulated media and predict permeability. By integrating structural descriptors, network theory, and topological data analysis, this study aims to enhance our understanding of how microstructural features govern macroscopic transport properties. The described project was carried out as a part of the Math 451H class in the Department of Mathematical Sciences at NJIT during the Spring semester 2025.

- **Attractor Degeneracy in Threshold-Linear Network**

Speaker: Zelong Li (Pennsylvania State University)

Abstract. Degenerate mechanisms – different underlying cellular and molecular properties or neural circuit configurations may generate highly similar functional behaviors – has been observed and studied in the pyloric network within the stomatogastric nervous system (STNS) of crustaceans ([1], [2], [3] and etc.). Despite substantial variability in the biophysical properties of individual neurons and synaptic connections, the rhythmic oscillatory dynamics generated by the network exhibit remarkable stability. Threshold-Linear Networks (TLNs) provide a mathematical framework for understanding the surprising degeneracy phenomena emerged among their dynamical attractors. In this presentation,

we will introduce the TLN model repertoire ([4], [5], [6] and etc.) and describe a simple parameter domain within which our desired robust dynamics occurs. This domain can be effectively expanded by training the recurrent neural network, highlighting the potential for machine learning approaches to explore degeneracy in neural circuit. This is a joint work with Juliana Londoño Álvarez and Carina Curto.

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- **Distribution Shift to Representation Comparison: Operator-Theoretic Kernel Tools for Modern ML pipelines**

Speaker: Soumya Mukherjee (Pennsylvania State University)

Co-authors: Bharath Sriperumbudur (Pennsylvania State University)

Abstract. Kernel methods provide a powerful and flexible framework for analyzing probability distributions and learned representations in modern machine learning. In this poster, we present a unified operator-theoretic perspective that solves two fundamental challenges: detecting distributional shifts and comparing learned representations. First, we develop a computationally efficient two-sample hypothesis test that leverages regularization of the classical Maximum Mean Discrepancy (MMD) test statistic using the spectral properties of the associated covariance operator, enabling minimax optimality under suitable alternatives while reducing cubic computational cost via random Fourier features. Second, we introduce the Uniform Kernel Prober (UKP), a principled pseudometric for comparing model representations based on their generalization behavior over a rich class of kernel ridge regression tasks. UKP flexibly incorporates inductive biases through kernel choice, is invariant to semantically irrelevant transformations, and is computable with only unlabeled input data. Together, these contributions provide a toolkit of kernel-based operators with statistical guarantees for quantifying distribution shift and comparing representations in data-driven learning systems.

- **Variational Inference for Gaussian Mixtures via Spherical Hellinger-Kantorovich Gradient Flow**

Speaker: Aratrika Mustafi (Pennsylvania State University)

Co-authors: Anna Korba (Centre de Recherche en Économie et Statistique), Bharath Sriperumbudur (Pennsylvania State University)

Abstract. Variational Inference (VI) is a central tool in large-scale Bayesian learning, often outperforming traditional MCMC-based methods in practice. Yet, theoretical understanding of VI from a geometric standpoint has only recently begun to develop and largely remains limited to simple, low-expressivity variational families. Finite Gaussian mixtures, celebrated for their flexibility and representational power, offer a compelling alternative. However, existing theory primarily addresses optimization over component locations while assuming fixed, uniform weights. In this work, we study VI over Gaussian mixtures with both dynamic weights and locations. We propose a joint optimization framework that simultaneously updates both parameter sets, yielding provable theoretical guarantees and empirical improvements. Our formulation interprets VI as minimizing a reverse Kullback-Leibler divergence between the Gaussian convolution of a finitely supported mixing measure and the target

distribution. The optimization is performed over the space of probability measures endowed with the spherical Hellinger- Kantorovich (SHK) geometry, which naturally couples weight and location updates. We analyze the resulting gradient flow dynamics - combining Wasserstein-type transport for component locations with Hellinger-type updates for weights - and establish descent guarantees and convergence rates. Finally, we show that ignoring weight optimization introduces a significant suboptimality gap in the variational objective.

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