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The Third Joint SIAM/CAIMS Annual Meetings

(AN25)

July 28–August 1, 2025

Montréal Convention Center, Montréal, Québec, Canada

The Third Joint SIAM/CAIMS Annual Meetings

Online Component

This document was current as of July 22, 2025. Abstracts appear as submitted.

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IP1

Science 2.0 - Evolving the Scientific Method Through Learning and Reasoning Symbiosis

The abstraction of system behavior or natural phenomena into consistent mathematical models is crucial for numerous applications in science and engineering. In scientific discovery, a fundamental challenge lies in explaining natural phenomena in a way that aligns with both noisy experimental data and potentially incomplete background knowledge of universal laws. Historically, models were derived manually using a first-principles, deductive approach. This method often yielded interpretable symbolic models with remarkable universality, despite limited data support. However, this process is time-consuming and heavily reliant on domain expertise. The rise of statistical AI and data-driven approaches has revolutionized model construction, enabling rapid, automated development and deployment. Many data-driven techniques demonstrate exceptional scalability due to their use of predetermined, exploitable model structures. However, these structures often result in non-interpretable models, require extensive training data, and offer limited predictive power for out-of-set instances. This presentation will examine recent transformations in the field and ongoing efforts to bridge the gap between statistical and symbolic AI. We will discuss algorithms capable of searching for free-form symbolic models, where neither the structure nor the set of operator primitives is predetermined. Describe some of the innovative assisted/automated theorem proving machinery and their application in certifying hypothesis model conformity with background theory. Lastly, we shall touch upon recent efforts to consistently unify statistical and symbolic approaches in AI in quest of evolving the scientific method.

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IP2

Deep Unfolding Approach for Inverse Problems in Imaging : The Usecase of Limited-Angle Computed Tomography

This talk presents the recent paradigm of deep unfolding in the context of inverse problems arising in computational imaging. We address the challenge of regions of interest (ROI) reconstruction from a limited number of computed tomography (CT) measurements. Classical model-based iterative reconstruction methods lead to images with predictable features. Still, they often suffer from tedious parameterization and slow convergence. On the contrary, deep learning methods are fast, and they can reach high reconstruction quality by leveraging information from large datasets, but they lack interpretability. At the crossroads of both methods, deep unfolding networks have been recently proposed. Their design includes the physics of the imaging system and the steps of an iterative optimization algorithm. We introduce in this talk an unfolding neural network designed for ROI CT reconstruction from limited data. Few-view truncated data are effectively handled thanks to a robust non-convex data fidelity term combined with a sparsity-inducing regularization function. We unfold a block alternating proximal algorithm, embedded in an iterative reweighted scheme, allowing the learning of key parameters in a supervised manner. Through various experiments, we showcase the advantages of the proposed approach, over several state-of-the-art methods, including a model-based iterative scheme, a multi-scale deep learning architecture, and other deep unfolding networks.

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IP3

Mathematics Meets AI: Modeling Time-Series Data to Transform Health and Society

Recent advances in experimental techniques and wearable devices have enabled the collection of large-scale time-series data across a variety of domains. In this talk, I will present how the integration of mathematical modeling and machine learning (AI) offers powerful tools to analyze such data and uncover underlying mechanisms in complex biological and epidemiological systems. I will begin by introducing GOBI (Generalized ODE-Based Inference), a simple yet scalable method for inferring causal relationships and network structures from time-series data. Unlike traditional statistical approaches such as regression or Granger causality, which often produce false positives, GOBI leverages mechanistic models to enhance causal inference. I will demonstrate how GOBI resolved a long-standing controversy regarding the impact of climate change on Dengue incidence. Next, I will show how combining mathematical modeling of sleep-wake dynamics with machine learning enables the analysis of large-scale data from wearable devices. This approach has allowed us to develop personalized sleep-wake schedules that reduce daytime sleepiness and lower the risk of depression. These results have been translated into practical applications, including the bedtime guidance feature recently implemented in the Samsung Galaxy Watch. Finally, I will present Density-PINN, a physics-informed neural network framework that infers parameters and time-delay distributions in non-Markovian systems. I will illustrate how this method can identify hidden heterogeneity in antibiotic responses and variation in disease spread during pandemics. Through these examples, I will highlight how mathematics and AI, working together, can bridge the gap between data and actionable insightultimately contributing to personalized healthcare and public health policy.

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IP4

Women in Mathematics Around the World: Strategies for Gender Equality

The analysis of the gender gap in mathematics and the efforts to reduce have been part of the landscape of the mathematical community since more than 50 years, at least in North America and in Europe. In the last ten years the approach became more global, with the launching of associations of women in mathematics in all continents, the creation by the International Mathematical Union of the Committee for Women in Mathematics and significant interdisciplinary initiatives. More and more people in our scientific community -mainly women but also men - keep working to understand better the gender gap in mathematics, to fight against the invisibilisation of women in mathematics and to develop a deeper qualitative approach of remaining examples through exhibitions, films and inter-

views. Best practices are being identified and the positive changes are real, but remain very slow. My talk will concentrate on three topics - some aspects of the gender gap in mathematics, as they appear through the comparison with other scientific disciplines made possible by the global questionnaire developed by the Gender Gap in Science project - the success of the May 12 initiative Celebrating women in mathematics all over the world since 2019 - the presentation of some exhibitions, interviews and films, helping us to have a deeper qualitative approach of the obstacles to gender equality ad the strategies developed to reach it.

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IP8

Information Complexity of Convex Optimization with Integer Variables

We consider the problem of minimizing a convex function under convex constraints, where some or all of the decision variables are constrained to be integer. This has applications in areas as diverse as artificial intelligence, logistics, supply chains, national defense, chemical engineering, astronomy, to name just a few. We will assume access to first-order oracles for the objective function and separation oracles for the constraints, i.e., at any point, the oracle returns the function value, a (sub)gradient and separating hyperplane for the constraints if they are violated. We focus on the information complexity of the problem, i.e., the minimum number of oracle calls to solve the problem to a desired accuracy. We will present nearly tight upper and lower bounds for the problem, extending classical results from continuous convex optimization. We also discuss information complexity under oracles that only reveal partial first-order information, e.g., where one can only make a binary query on the function value or (sub)gradient at a given point. We will close the talk with some open questions.

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IP9

On Peaks, Plateaus and Thorny Patches: The Path to Hybrid Quantum-Classical Supercomputing

Safely on their path to maturity and scale, QPUs are now stepping into the supercomputing realm, furthering the push toward next-generation heterogeneous compute for tackling complex scientific and engineering grand challenges. The road offers impressive peaks, yet hardware limits, algorithmic bottlenecks, tricky workflow orchestration, and still-evolving software create rocky stretches, and sometimes sheer cliff drops. In this talk, well scope the current hybrid quantumHPC landscape, drawing on work from the Munich Quantum Valley (MQV) and across Europe to distill lessons learned so far and outline with a clear-eyed view whats next as we move towards a fault-tolerant, quantum-accelerated, truly heterogeneous era of supercomputing.

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IP10

Integer Distances

Euler constructed arbitrarily large sets of non-collinear points with all distances integers. Much later, Paul Erdos and Norman Anning proved that all such sets must be finite. We survey this and related problems in discrete geometry, including recent progress on Harborth's conjecture that all planar graphs can be drawn with integer-length edges, on the existence of cocircular subsets in integer-distance sets, and on non-Euclidean generalizations of the ErdosAnning theorem.

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SP1

CAIMS-SCMAI Cecil Graham Doctoral Dissertation Award Lecture: Concentration Phenomena in Several Reaction-Diffusion Equations with Kinetic Effect

Reaction-diffusion (R-D) systems serve as paradigms to understand pattern formation in biology, ecology and finance. Numerous studies have examined pattern formation in the nonlinear regime for classical two-component R-D models, such as Gierer-Meinhardt models and Gray-Scott models. Whereas, for phenomena involving cellular motility, economic growth with capital-induced labor migration or large-scale games, the incorporation of advection is essential. In this talk, we focus on two classes of R-D systems with kinetic effects: Keller-Segel (K-S) models and Mean-Field Games (MFG) systems. The K-S systems are classical models employed to explain the chemotactic process in biology. In the first part of this talk, we discuss localized pattern formation in K-S models with logistic growth. Remarkably, in the regime of small chemical diffusivity, we uncover an intricate connection between Gierer-Meinhardt models and logistic K-S systems. Surprisingly, our framework can explain economic agglomeration in the spatial Solow model with capital-induced migration. In the latter part of this talk, we focus on ergodic Mean-Field Game (MFG) systems, which are employed to characterize Nash equilibria in games involving a large number of players. We analyze the concentration behaviors of least-energy solutions and show connections with nonlinear Schrdinger equations.

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SP2

AWM-SIAM Sonia Kovalevsky Lecture: From Neurological Disorders to Additive Manufacturing: Integrating Isogeometric Analysis with Deep Learning and Digital Twins

Coupling physics-based simulation and data-driven modeling have demonstrated great power in predicting complex systems. This talk focuses on integrating an advanced finite element method, isogeometric analysis (IGA), with deep learning and digital twins to address challenging problems of neurological disorders and additive manufacturing

(AM). First, we introduce a novel phase field model coupled with tubulin and synaptogenesis concentration to simulate intricate neurite outgrowth and disorders. By integrating IGA and convolutional neural networks, we conduct thorough investigations into the functional role of various parameters affecting the neurodevelopmental disorder with comparison to experimental results. Second, to investigate intracellular transport induced neurodegenerative disorders, we develop a PDE-constrained optimization model to simulate traffic jams induced by microtubule reduction and swirl. We also build a novel IGA-based physics-informed graph neural network to quickly predict normal and abnormal transport phenomena in complex neuron geometries. Finally, in the area of AM, our research focuses on a machine learning framework for inverse design and manufacturing of self-assembling fiber-reinforced composites in 4D printing, IGA-based topology optimization for AM of heat exchangers, as well as data-driven residual deformation prediction and lattice support structure design in the laser powder bed fusion (LPBF) AM process. Our on-going efforts aim to predict stress-induced build failures using dynamic neural surrogates, where reduced order modeling is a key technique to efficiently simulate underlying physics.

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SP3

W.T and Idalia Reid Prize Lecture: PDE Systems Describing the Motion of Rigid Bodies in an Incompressible Fluid: Wellposedness, Control and Long-time Behaviour

The study of systems describing the motion of rigid bodies immersed in a fluid goes back to Euler and Kirchhoff, who considered the case of an ideal fluid subject undergoing a potential flow. The case of a single solid moving in a viscous incompressible fluid filling the whole space was considered much later, around 1980 by Weinberger and Serre. Welposedness issues for the case when the solid-fluid system is contained in a bounded container or/and of several moving bodies has been intensively studied since 2000. In this talk we first recall some of these wellposedness results . We next describe some associated control problems, aimed to provide a new approach to the understanding of the swimming of aquatic organisms. We next describe some recent results concerning the long-time behaviour of solutions. Finally, we introduce the challenging case when the rigid bodies are only partially immersed.

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SP4

John von Neumann Prize Lecture: Thirty Years of Cartesian Cut-cell Methods: Where Are We Now?

Solving a PDE in a complicated domain with a Cartesian mesh leads one to consider "cut-cells" – Cartesian cells that intersect the boundary of the domain. This type of mesh can handle complicated geometry in a robust and automatic way. The difficulties of mesh generation are replaced with those of accuracy and stability at the cut cells. Many interesting ideas have been proposed; many have fallen by the wayside. In this talk I will review a variety of approaches to these problems. I will describe our new approach called state redistribution, which stabilizes finite volume and Discontinuous Galerkin schemes in a practical post-processing step at every time step. Computations in two and three space dimensions are shown. We end with what I see as the current bottlenecks, and a discussion of open problems.

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SP5

CAIMS/SCMAI-Fields Industrial Mathematics Prize Lecture: Full Waveform Inversion: Mathematical Challenges, Computational Issues, and Applications

Full Waveform Inversion (FWI) is an advanced seismic imaging technique used to create high-resolution subsurface physical properties of the Earth by minimizing the misfit between observed and simulated seismic waveforms. It is an excellent example of interdisciplinary collaboration, bringing together core ideas from applied mathematics, scientific computing, inverse problem theory and geophysics. For the sake of computational efficiency, it is usually formulated as a PDE-constrained optimization problem constrained by seismic wave equations and solved by gradient-based iterative methods. Despite its great success in the energy industry and environmental protection, many mathematical challenges and computational issues remains to be resolved. For example, FWI suffers from various issues such as local minima, lack of low-frequency data, circle skipping, high computational cost etc. In this talk, I will provide a brief introduction to FWI, followed by a discussion of the adjoint-state method, its derivation, and its computational implications. I will review of the difficulties associated with nonconvexity, cycle skipping, and high computational cost, and describe some techniques to address these issues. Finally, I will present real-world applications of FWI in hydrocarbon exploration, emphasizing the central role of adjoint-based analysis in advancing both the theory and practice of seismic inversion.

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SP6

Past President's Address: Solving Massive Combinatorial Optimization Problems

Many design, planning and decision problems arising in engineering, sciences, finance, and statistics can be modeled as mixed-integer nonlinear optimization problems. A challenging class of mixed-integer problems arise in topological design, such additive manufacturing and the design of cloaking devices. In topology optimization, the physical response of the design is modeled as partial-differential equations (PDEs) and the design is modeled with binary variables defined on each element of the discretization of the PDE. This approach results in mixed integer PDE-constrained optimization (MIPDECO) problem that combine the computational challenges of PDEs with the combinatiorial challenges of a massive number of discrete variables. We show that despite their seemingly hopeless complexity, certain MIPDECOs can be solved efficiently (at a cost comparable to a single continuous PDE-constrained optimization solve). We discuss two classes of methods: rounding techniques that are shown to be asymptotically

optimal, and trust-region techniques that converge under refinement of the PDE. We illustrate these solution techniques with examples from topology optimization. Time permitting, we also comment on recent experience with randomized solution techniques for MIPDECOs.

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SP7

Jerald L. Ericksen Prize Lecture: Variational Analysis of a Data-Driven Formulation of the Theory of Elasticity

We study a variational, phase-space formulation of the theory of elasticity. The material is described through a set of stress-strain pairs, which form a data set in phase space. Minimization of the energy is replaced by minimization of a suitable distance of the solution from this set; compatibility and equilibrium become linear constraints. We discuss how the tools of the calculus of variations permit to address existence of minimizers, relaxation, and approximation. This is based on joint work with Franca Hoffmann, Stefan Mller and Michael Ortiz.

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SP8

I.E. Block Community Lecture : An Unexpected Journey: from Music to Art Via Math

Math is beautiful, so they say, but it can be hard for the untrained eye to appreciate. Code is beautiful, too (good code, at least!), but it's even harder for the non-expert to see. Davis presents his work on collecting and visualizing matrices, which then took an expected turn when he was asked to create artwork from music using the same techniques. His artwork reveals the stunning visual beauty found in matrices, music, and math: seemingly unrelated topics that collide to produce amazing beauty.

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SP9

CAIMS/SCMAI Research Prize Lecture: We are all different: Modeling key individual differences in physiological systems

Mathematical models of whole-body dynamics have advanced our understanding of human integrative systems that regulate physiological processes such as metabolism, temperature, and blood pressure. For most of these whole-body models, baseline parameters describe a 35-year-old young adult man who weighs 70 kg. As such, even among adults those models may not accurately represent half of the population (women), the older population, and those who weigh significantly more than 70 kg. Indeed, sex, age, and weight are known modulators of physiological function. To more accurately simulate a person who does not look like that baseline person, or to explain the mechanisms that yield the observed sex or age differences, these factors should be incorporated into mathematical models of physiological systems. Another key modulator is the time of day, because most physiological processes are regulated by the circadian clocks. Thus, ideally, mathematical models of integrative physiological systems should be specific to either a man or woman, of a certain age and weight, and a given time of day. A major goal of our research program is to build models specific to different subpopulations, and conduct model simulations to unravel the functional impacts of individual differences.

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SP10

SIAM Industry Prize Lecture: Bringing Medicines to Patients with Mathematical Biology

When applied to describe human pathophysiology, it is natural to ask how mathematical biology can contribute to human health. In this talk, I will discuss the application of mechanistic modeling in developing novel therapies and explore why this is a natural and essential endeavor. The journey from concept to approved therapy is incredibly challenging, with failure being far more likely than success. One approach to mitigate this obstacle is the utilization of mathematical models of disease that incorporate the dynamics and effects of treatments. This field is known as Quantitative Systems Pharmacology (QSP). These models can address critical questions regarding how a drug works and how that specific target may influence (or not) the progression of acute or chronic diseases. QSP models typically ordinary differential equations and are designed to accurately replicate known biological processes. By design, they can be developed, validated, and tested through a wealth of data from genetics, real-world evidence, clinical trials, and other species. In this talk, I will introduce QSP models and their impact on drug development. To illustrate this, I will present several examples, including an overview of our mechanistic modeling of COVID-19 during the pandemic that supported the development of a novel therapeutic.

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SP11

CAIMS/SCMAI-PIMS Early Career Award Lecture: High-dimensional Optimization in Machine Learning with Applications to Scaling Limits and Compute-Optimal Neural Scaling Laws

Given the massive scale of modern ML models, we now only get a single shot to train them effectively. This restricts our ability to test multiple architectures and hyperparameter configurations. Instead, we need to understand how these models scale, allowing us to experiment with smaller problems and then apply those insights to larger-scale models. In this talk, I will present a framework for analyzing scaling laws in stochastic learning algorithms using a power-law random features model, leveraging high-dimensional probability and random matrix theory. I will then use this scaling law to address the compute-optimal question: How should we choose model size and hyperparameters to achieve the best possible performance in the most compute-efficient manner? Additionally, I will introduce a scaling limit commonly seen in ML optimization

algorithms which has origins in statistical physics and I will highlight several promising research directions in scaling laws that remain underexplored but offer significant potential.

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JP1

AMS-SIAM Joint Plenary: (Machine) Learning Ocean Climate Physics Across Scales

The complexity of natural systems often stems from interactions between a wide range of spatial and temporal scales. For example, oceanic flows are frequently dominated by chaotic vortices that are approximately 100 to 200 kilometers (km) in diameter. Their size is a result of the natural propensity of vortices in flows with large aspect ratios to merge and form larger vortices. Identifying accurate and representative solutions to such multiscale systems requires the resolution of an extensive range of scalesfrom millimeters to thousands of kmwhich is impossible for any modern computer and likely implausible for in the near future. Climate scientists therefore solve the equations for the (resolved) scales that are computationally feasible and most useful for decision-making purposes, while also parameterizing the impacts of the unresolved scales (the closure problem in fluid dynamics). In this talk, I will discuss the potential for machine learning to accelerate the discovery of physics principles and governing equations for multiscale climate processes such as turbulence. I will show examples of how these discoveries can help improve climate models. I will further demonstrate the potential of AI to accelerate climate predictions and increase their reliability by generating emulators, which can reproduce decades of climate model output in seconds with high accuracy. I will discuss the promise and challenges for climate science and modeling in the age of data, computing, and artificial intelligence.

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JP2

Joint Plenary with the SIAM Conference on Control and Its Applications: Stackelberg Strategies for the Control of Partial Differential Equations

In this talk, we will present a Stackelberg strategy to control PDEs. We will act on the system with two controls: one as a leader and the other as a follower. We will discuss the different problems as the main objective is null controllability, and the follower is optimization. As an example, we present some existing results for the heat equation (See Lions, J.-L.: Some remarks on Stackelbergs optimization. Math. Models Methods Appl. Sci. 4(4), 477487 (1994), Araruna, F.D., Fernndez-Cara, E., da Silva, L.C.: Hierarchic control for the wave equation. J. Optim. Theory Appl. 178(1), 264288 (2018), Araruna, F.D., Fernndez-Cara, E., Guerrero, S., Santos, M.C.: New results on the StackelbergNash exact control of linear parabolic equations. Syst. Control Lett. 104, 7885 (2017)) and a result for the Boussinesq system (T. Takahashi, L. de Teresa, Y. Wu-Zhang, Stackelberg exact controllability for the Boussinesq system, Nonlinear Differ. Equ. Appl. (2024) 36 pp.). Then, we will present a result inverting the objectives of the leader and the follower for the heat equation (Calsavara, B.M.R., Fernndez-Cara, E., de Teresa, L., Villa, J.: New results concerning the hierarchical control of linear and semilinear parabolic equations. ESAIM Control Optim. Calc. Var. 28, 1426 (2022)). The leader will have an optimization target, and the follower will have a null controllability one. We briefly discuss a similar problem but for a wave equation (L. de Teresa, and J.-A. Villa A new hierarchical control for the wave equation, Wave Motion 134 (2025) 9 pp.)

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JP3

Joint Plenary with Conference on Computational Geometric Design: Geometry for Computational Design and Fabrication

Geometry plays an important role in the design and fabrication of freeform shapes. This talk will illustrate the fruitful interplay between theory and applications in this area. It is shown how to combine classical and discrete differential geometry with numerical optimization to develop effective fabrication-aware design tools. Special emphasis is on the use of novel quad-mesh based discrete models and on the geometrically motivated initialization and regularization of optimization algorithms. Applications include paneling solutions for geometrically complex architectural skins, design and fabrication with materials which can be easily bent but hardly stretched, mechanical metamaterials, and how to program curvature into flat sheets via curved folding. The computational results are verified at hand of physical models.

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JP4

Joint Plenary with the SIAM Conference on Applied and Computational Discrete Algorithms: Setting a Course for Post-Moore Software Performance

Software performance engineering (SPE) is the science and art of making code run fast or otherwise limiting its consumption of resources, such as power, memory footprint, network utilization, file IOs, response time, etc. SPE encompasses algorithms, parallel computing, caching, vectorization, bit tricks, loop unrolling, compiler-switch selection, tailoring code to the architecture, exploiting sparsity, changing data representation, metaprogramming, etc. Historically, gains in performance from miniaturization, codified in Moore's Law, relieved programmers from the burden of making software run fast and learning SPE techniques. I will explain why the end of Moores Law now makes SPE a critical technical skill. Since SPE is neither extensively researched nor widely taught in the universities, however, it risks devolving into an unstructured collection of ad hoc tricks. Now is the time to establish SPE as a science-based discipline, alongside traditional areas of computer science.

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CP1

Mathematical Model for the Progression of Rhegmatogenous Retinal Detachment (rrd)

Retinal detachment is the separation of the neurosensory retina from the retinal pigmented epithelium (RPE), thereby disrupting the nutrient supply to photoreceptor cells. There are three types of retinal detachment: Exudative (ERD), Tractional (TRD), and Rhegmatogenous (RRD) retinal detachment, with RRD being the most common. RRD develops when a tear or hole in the retina allows vitreous humor to flow into the sub-retinal space resulting in the separation of the neurosensory retina from the RPE. This separation, if untreated, can lead to irreversible vision loss. While ophthalmological tools can detect retinal detachment, particularly RRD, the rate of progression, especially due to constant eye movement, is poorly understood. This study develops a fluid-structure interaction model to investigate the progression of RRD. The model examines key factors, including eye movement, retinal thickness, rigidity, adhesion strength between the neurosensory retina and RPE, and the density and viscosity of vitreous humor. By quantifying detachment rates under varying conditions, the model aims to deepen our understanding of RRD dynamics and provide estimates for effective treatment timelines to prevent permanent visual impairment. Student: William Ebo Annan Advisors: Prof. Diana White Prof. Emmanuel O.A. Asamani

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CP1

Boundary Integral Simulations of Forming and Breaking Fractal Aggregates

Marine aggregates play an important role in transporting both carbon and microplastics from the surface ocean to the deep ocean. Investigations of their formation and settling rates are critical to understand their ecological impact. However, their irregular geometry, having in fact a fractal structure, complicates their study. Here we use boundary integral equations (BIE) to obtain numerically the fluid forces acting on fractal aggregates in both uniform and density-stratified ambients in the limit of zero Reynolds number. The presence of an ambient stratification requires the extension of the classical BIE and results in the inclusion of an additional term involving a volume integral, which we compute efficiently using the Fast-Multipole Method. The flow around the aggregates and the resulting surface and inner stresses are computed, as well as interactions between neighbouring aggregates. We characterize the drag as a function of aggregate size, structure, and imposed flow. We also obtain the magnitude and distribution of inner stresses when aggregates settle or are subject to shear flow to determine the most likely break points as a function of size and structure and thus inform stochastic formation models.

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CP1

Singularity Formation in Two Vortex Sheets Model for Jets

The evolution of vortex sheets is described by a nonlinear integrodifferential equation called the Birkhoff-Rott equation. The initial-value problem for the Birkhoff-Rott equation is considered ill-posed due to the Kelvin-Helmholtz instability. Moore's asymptotic analysis has predicted that a single vortex sheet with smooth initial data forms a singularity at a finite time and, in addition, the numerical study by Krasny has provided validation of Moore's result by using the point vortex approximation and the filtering technique. In this study, we consider the the Birkhoff-Rott model extended to the case of a two vortex sheets describing jets. The linear stability analysis suggests that the two vortex sheets model is also ill-posed and there exists two types of growing modes for the linearized model. We numerically investigate the formation of singularities in two vortex sheets with two types of initial conditions: the stationary solution with small perturbations given by the two growing modes of the linearized model. We see how the process of the singularity formation varies depending on the amplitude of the perturbation and the distance of two vortex sheets.

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CP1

Computational Modeling of Hemodynamics with Thick-Walled Calcified Arteries

Arterial wall calcification is a common outcome of conditions such as diabetes and atherosclerosis, yet its impact on arterial deformation and hemodynamics is not fully understood. One-dimensional arterial blood flow models provide a fast and efficient means of analysis, especially when non-axial flow can be disregarded. This study presents a model for arterial blood flow, deriving the tube law from hyperelasticity applied to a two-dimensional annular cross-section. Using this solid-fluid interaction model, we examine hemodynamic behavior in both healthy and calcified arteries. Our findings reveal that calcified arteries bear a higher mean pressure gradient along the vessel. Due to their increased stiffness, they undergo minimal deformation, resulting in a larger pulse pressure. This study assists more accurately understanding hemodynamics in the calcified arteries for future disease diagnosis and treatment.

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CP1

A Logarithmically Bounded Number of Small Rigid Bodies in a Viscous Incompressible Inhomogeneous Fluid Is Negligible

We consider a large number of inhomogeneous rigid bodies immersed in an inhomogeneous incompressible fluid contained in a bounded domain of dimension bigger or equal to two. We address the question about the asymptotic behaviour of the corresponding system of partial differential equations as the number of rigid bodies tends to infinity with a logarithmic bound and the diameter of the bodies tends to zero. We show that the rigid bodies are neglected in the limit in the sense that the limit system is given only by the inhomogeneous incompressible Navier-Stokes System. We do not require any regularity for the boundaries of the rigid bodies and the domain. Our result extends earlier work by Feireisl, Roy and Zarnescu (2023) to more general assumptions which are of physical relevance. This includes assumptions on the mass densities of the fluid and the rigid bodies, which are allowed to be inhomogeneous, can attain the value zero, and only need to be bounded in some suitable L^p-space instead of being uniformly bounded.

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CP1

Using Theory and Experiments of Spheres Moving Near Boundaries to Optimize the Method of Images for Regularized Stokeslets

The general system of images for regularized Stokeslets (GSIRS) developed by Cortez and Varela (2015) is used extensively to model Stokes flow phenomena such as microorganisms swimming near a boundary. Our project uses dynamically similar scaled macroscopic experiments to test theories for forces and torques on spheres moving near a boundary. Then we use these data and the method of regularized Stokeslets (MRS) created by Cortez et al. (2005) to calibrate the GSIRS. We test two surface discretization methods commonly used in the literature: the 6-patch method and the spherical centroidal Voronoi tessellation (SCVT) method. Our data show that a discretization method, such as SCVT, that uniformly distributes points provides the most accurate results when the motional symmetry is broken by the presence of a boundary. We use theory and the MRS to find optimal values for the regularization parameter in free space for a given surface discretization and show that the optimal regularization parameter values can be fit with simple formulae when using the SCVT method. We also present a regularization function with higher order accuracy when compared with the regularization function previously introduced by Cortez et al. (2005). The simulated force and torque values compare very well with experiments and theory for a wide range of boundary distances.

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CP2

A Metapopulation Susceptible - Infected - Hospitalized - (Intensive Care) Unit - Recovered - Deceased Model

We enhance our SIHURD model published in 2022 and propose a metapopulation infectious disease mathematical monitoring model where individuals move between discrete spatial patches. We divide the environment into a finite number of spatial patches (e.g., adjacent cities), which preserve homogeneity characteristics. We apply the enhanced SIHURD model to each spatial patch. The novelty of this model lies in introducing parameters that represent individuals' travel rates between spatial patches, which depend on their disease status. In addition, it assumes that individuals do not change their disease status while travelling between patches. Our study uses the reproduction number, R_{0_k}, for each spatial patch, $k = 1, 2, \ldots, n, (n > 1)$ integer, which represents the average number of secondary cases produced by an infected individual in a susceptible population. The system has only a disease-free equilibrium point if $R_{0_k} \leq 1$. In contrast, if $R_{0_k} > 1$, the system has an endemic equilibrium point. Reproduction numbers R_{0_k} are crucial for understanding the spread of infectious diseases and can inform measures to control outbreaks effectively. Migration between patches fundamentally alters the behaviour of the endemic equilibrium within a patch, rendering it unstable in the proposed model.

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CP2

Extremum Seeking Systems As a Method for Emulating Optimized Behaviors in Systems Biology: From Soaring Birds to Flapping Insects

We present important collection of our recent novel results in characterizing/mimicking optimized behaviors in flying organisms, namely, soaring birds and flapping insects. Our new theory, using extremum seeking methods, is quite unique as it solves decades-long problems/challenges in the literature. For instance, extremum seeking methods provide a model-free, very simple, real-time solution for quite complicated (but optimized) behaviors in nature, which fits more the biological narrative that biological organisms that are simple and incapable of high level of processing/computations, mut be using simple techniques to optimize their behavior in real-time. We hypothesize with great deal of confidence that extremum seeking methods might be the mechanisms many organisms use and it can be, to say the least, a new characterization method in sys-

tems biology and biomimicry.

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CP2

Deep Learning for Early Warning Signals of Complex Dynamical Transitions in Epidemics

The identification of tipping points, which are frequently brought about by imperceptible alterations in internal structures or external disturbances, is crucial for forecasting dynamical systems, such as vaccine-preventable infectious diseases. Based on empirical data, when either the vaccination rate or birth rate changes, the disease infection prevalence encounters a tipping point. This tipping point causes a transition between different limit cycles such as annual to biennial or more complex cycles. Identifying this transition helps control the epidemic. In this work, our aim is to design deep learning models to construct an early warning system to provide advance warning of these tipping points.

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CP2

Approximate Solution of An Epidemic Sir Model Via Laplace Transform and Q Homotopy Analysis Method.

We study an ad-hoc epidemic SIR model governed by the Caputo derivative. We use the Laplace transform and the q- Homotopy analysis method (Lq-HAM) to obtain approximate solutions to the system. We finally present some numerical simulations using Mathematica to illustrate the qualitative results. Our approach can be used even in the context of constructive fractional models and other abstract fractional differential systems.

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CP2

Analysis of Cyclic Population Dynamics of Snow Crab in the Southern Gulf of St. Lawrence Using a Stage-structured Discrete-time Population Model

The snow crab fishery is one of Canada's most profitable fisheries and is a significant economic driver in coastal communities in Atlantic Canada and Quebec. Snow crab is generally considered to be a stenothermic species, with immature crabs being more sensitive to water temperature than adult crabs, and warming due to climate change is becoming worrisome. As snow crab has a complex life cycle, developing an adequate population dynamics model for this species is challenging. Limiting the complexity of the model, at first, is therefore helpful to assess how life-history characteristics affect the population level. In this paper, we develop a discrete-time population model for snow crab based on three developmental stages for each sex : immature, adolescent and adult for the male snow crab and immature, prepubescent and adult for the female snow crab. The model, which is being developed to study the snow crab population in the southern Gulf of St. Lawrence, takes into consideration density-dependent intercohort processes (i.e. cannibalism), but predation is not considered as it is not believed to be an important factor in this region. We investigate the role of density-dependent intercohort processes and variability in recruitment in promoting cyclic population dynamics. Bifurcation analysis is performed and periodograms are computed to provide a more complete and comprehensive understanding of the dynamics of the population.

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CP2

Pre-Exposure Vaccination in the High-Risk Population Is Crucial in Controlling Mpox Resurgence in Canada

As mpox spread continues across several endemic and non-endemic countries around the world, vaccination has become an integral part of the global response to control the epidemic. In this article, we develop a compartmental mathematical model to investigate the impact of vaccination in controlling a potential mpox resurgence in Canada. The model categorizes individuals into high- and low-risk groups and incorporates pre-exposure vaccination in the high-risk group and post-exposure vaccination in the high- and low-risk groups. The vaccine-free version of the model was calibrated to the daily reported cases of mpox in Canada from April to October 2022, from which we estimated key model parameters, including the sexual and non-sexual transmission rates. Furthermore, we calibrated the full model to the daily reported cases of mpox in Canada in 2024, to estimate the current mpox vaccination rates in Canada. Our results highlight the importance of pre-exposure vaccination in the high-risk group on controlling a potential resurgence of mpox in Canada, and the minimal effects of post-exposure vaccination in the high- and low-risk groups on the outbreak. Overall, our modeling result suggests that pre-exposure vaccination in the high-risk group is crucial in controlling mpox outbreak in Canada.

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CP3

Enhancing Heat Transfer with Wavy Walls and Unsteady Flow Perturbations

Recent studies have used optimization to determine fluid flows that can efficiently cool heated objects. First we will present results on optimal fluid flows and wall shapes for heat transfer. We will then examine recently discovered steady optimal flows through a heated channel, and use a perturbation method to find nearby unsteady flows that convect more heat - up to 80% - for a given amount of power needed to move the flow. The unsteady perturbations consist of vortices, small or large, that move along the channel walls and disrupt the thermal boundary layer.

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CP3

Hydrodynamic Modeling Using Physics Informed Machine Learning Method.

Traditionally, digital twins of hydrological models solve complex systems of partial differential equations through computationally expensive and time-consuming numerical simulations. This study introduces a physics-informed machine learning framework, incorporating both data and the physics of hydrological applications, specifically we consider the computationally intensive dam-break flood problem. Our Physics-Informed Neural Networks framework aims to reduce computational costs compared to classical numerical methods based approaches embedded in various (CFD) software. We demonstrate the effectiveness of our PINNs model, trained with numerical solutions of the Shallow Water Equations, in accurately predicting the long-term dynamics of one-dimensional dam-break floods. The models performance is evaluated against a Data-Driven Neural Network and a Hybrid Neural Network, showing that the PINNs model outperforms the HNN in generalizing and predicting wave propagation. Although the Data-Driven Neural Network fits the training data closely, it fails to generalize to unseen data, underscoring the limitations of purely data-driven approaches. Our findings suggest that while data-driven models are useful, they require extensive additional data for more complex, real-world scenarios, such as two- and three-dimensional problems. PINNs, on the other hand, scales efficiently with problem dimensions, eliminating the need for mesh construction.

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CP3

Reduced Order Modelling Via Scientific Machine Learning in Computational Fluid Dynamics

We focus on some perspectives about Reduced Order Methods (ROM) for parametric Partial Differential Equations (PDEs) with a special interest in parametric problems arising in offline-online Computational Fluid Dynamics (CFD) thanks to the enhancement provided by Scientific Machine Learning (SML) in a digital twin(s) perspective. Efficient parametrisations (random inputs, geometry, physics) are very important to be able to properly address an offline-online decoupling of the computational procedures and to allow competitive computational performances. Current ROM developments in CFD include: (i) a better use of stable high fidelity methods, to enhance the quality of the reduced model too, also in presence of bifurcations and loss of uniqueness of the solution itself, (ii) capability to incorporate turbulence models and to increase the Reynolds number; (iii) more efficient parametrisation techniques, especially in presence of geometric parameters. All the previous aspects are quite relevant – and often challenging – in complex real-world CFD problems to focus, for example, on real time simulations for complex parametric industrial, environmental and biomedical flow problems, or even in a control flow setting with data assimilation and uncertainty quantification. Some model problems will be illustrated by focusing on few benchmark study cases, applied to problems of interest.

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CP3

Asymptotic Preserving Micro-Macro Decomposition Scheme for the Kinetic Boltzmann-Es-Bgk Equation

The Boltzmann equation describes the motion of a fluid for the simulation of gas dynamics over a range of Knudsen numbers. An important class of methods are asymptotic-preserving schemes, which allow the numerical method to be stable at fixed mesh parameters for any value of the Knudsen number, transitioning from kinetic to fluid regimes. To avoid the complexity of the Boltzmann collision operator, the Bhatnagar-Gross-Krook collision operator and the closely related Ellipsoidal Statistical BGK collision operator is used, which, unlike BGK, gives the correct transport coefficients. We develop an asymptotic preserving micro-macro decomposition scheme for solving the Boltzmann ES-BGK equation and implement them in parallel with MPI for efficiency. This scheme couples a microscopic kinetic equation with a macroscopic fluid equation, by equivalently writing the Boltzmann equation as a system coupling a hydrodynamic part with a kinetic part of the distribution function. A projection operator is used to separate the macroscopic and microscopic quantities. The updated microscopic quantity is coupled to the macroscopic update equation via the heat flux variable, which is obtained by taking the moment of the microscopic distribution function. The updated macroscopic variables are then used in the calculation of the projection operator which affect the microscopic update. This scheme is applied to multidimensional flows, and is an extension to previous

work done in one dimension.

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CP3

Iterated Defect Correction Approaches to Large Eddy Simulation

Large eddy simulation with correction (LES-C) turbulence models are a new family (2020) of high order turbulence models. They have been shown to be unconditionally stable and of higher formal order as well as more accurate per computational time than their natural competitors. Furthermore, LES-C models have been applied to magnetohydrodynamics (MHD) and fluid-fluid interaction problems successfully. In this talk we will discuss possibilities for iterating LES-C corrections to get even higher three step models. We show that in each of these application domains, three-step-LES-C models offer additional improvements.

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CP4

Numerical Solutions and Applications of Variable-Order Fractional Diffusion Models with Sonine Kernels

Time-variable-order fractional diffusion models with Sonine kernels provide a flexible mathematical framework for addressing complex problems across various applications. This talk explores numerical methods designed to solve these models efficiently and accurately. By allowing the diffusion order to vary dynamically, these models adapt to evolving diffusion characteristics, making them particularly effective in applications like image processing, where balancing noise reduction with the preservation of fine details is crucial. Numerical examples will illustrate the distinctive properties of these models and highlight the effectiveness of the proposed numerical solutions.

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CP4

Nonlinear Approximation of High-Dimensional Anisotropic Analytic Functions

Motivated by nonlinear approximation results for classes of parametric partial differential equations (PDEs), we seek to better understand so-called library approximations to analytic functions of countably infinite number of variables. Rather than approximating a function of interest by a single space, a library approximation uses a collection of spaces and the best space may be chosen for any point in the domain. In the setting of this paper, we use a specific library which consists of local Taylor approximations on sufficiently small rectangular subdomains of the (rescaled) parameter domain $Y := [-1, 1]^{\mathbb{N}}$. When the function of interest is the solution of a certain type of parametric PDE, recent results [Bonito et al, Nonlinear Methods for Model Reduction, 2020] prove an upper bound on the number of spaces required to achieve a desired target accuracy. In this talk, we discuss a similar result for a more general class of functions with anisotropic analyticity. In this way we show both where the previous theory depends on being in the setting of parametric PDEs with affine diffusion coefficients, and prove a more general result outside of this setting.

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CP4

Correct Implied Volatility Shapes and Reliable Pricing in the Rough Heston Model

We use modifications of the Adams method and very fast and accurate sinh-acceleration method of the Fourier inversion (iFT) (S.Boyarchenko and Levendorskiĭ, IJTAF 2019, v.22) to evaluate prices of vanilla options; for options of moderate and long maturities and strikes not very far from the spot, thousands of prices can be calculated in several msec. with relative errors of the order of 0.5% and smaller running Matlab on a Mac with moderate characteristics. We demonstrate that for the calibrated set of parameters in Euch and Rosenbaum, Math. Finance 2019, v. 29, the correct implied volatility surface is significantly flatter and fits the data very poorly, hence, the calibration results in op.cit. is an example of the *ghost calibration* (M.Boyarchenko and Levendorskiĭ, Quantitative Finance 2015, v. 15): the errors of the model and numerical method almost cancel one another. We explain how calibration errors of this sort are generated by each of popular versions of numerical realizations of iFT (Carr-Madan, Lipton-Lewis and COS methods) with prefixed parameters of a numerical method, resulting in spurious volatility smiles and skews. We suggest a general *Conformal Bootstrap principle* which allows one to avoid ghost calibration errors. We outline schemes of application of Conformal Bootstrap principle and the method of the paper to the design of accurate and fast calibration procedures.

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CP4

Waves in Klein-Gordon Time-Nonlocal Viscoelastic Porous Medium under the Effects of Moisture Diffusion.

The governing equations for a moisture diffusive viscoelastic porous medium are formulated. The time-nonlocality model is developed based on the Klein-Gordon nonlocality stress theory to predict the porous behaviour of nanostructures under extreme environments in this paper. Mathematical expression for wave speed is derived. Velocity equation is solved to show the existence of three dilatation and one shear waves propagating in the medium. Effect of moisture, nonlocality and porosity on the speed of waves

are studied. The numerical results for a particular material are illustrated graphically to observe these effects.

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CP5

A Numerical Analysis of a Stabilized Hyperbolic Equation Modelling Bio-Polymerization

This talk discusses a stabilization method for first order hyperbolic differential equations applied to DNA transcription modeling. It is known that the usual unstabilized finite element method contains spurious oscillations for non-smooth solutions. To stabilize the finite element method the authors consider adding to the first order hyperbolic differential system a Vreman stabilization term in space. Numerical analysis of the stabilized finite element algorithms and computations describing a few biological settings will be presented.

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CP5

Introducing Parsimonious Recursive Minimal Residual Method (PARMRES): Towards Gmres-Like Convergence with Reduced Overhead

Iterative solvers are instrumental to computational science, especially for solving large linear systems arising from PDE discretization. In a domain where stability and efficiency are essential, we introduce the Parsimonious Recursive Minimal Residual Method (PARMRES), an optimal algorithm that achieves GMRES-like convergence rates with significantly reduced storage and computational requirements. By deflating Fixed-Point iterations with parsimoniously recruited eigenvectors from the Krylov subspace, PARMRES minimizes overhead while maintaining robust performance. That makes it particularly well-suited for challenging cases in computational fluid dynamics (CFD). PARMRES is based on our recently proposed theoretical framework, Deflated Fixed-Point Iterations (DFPI), which unifies a broad class of iterative solvers and Fixed-Point Iterations acceleration methods, including RPM, Boost-Conv, and traditional Krylov subspace methods. One of the main results is that convergence depends mainly on stable eigenvectors in the projection space, while other components contribute little or even hinder performance. This insight drives the design of PARMRES, which parsimoniously constructs the projection space at a lowest cost to maximize performance. The theoretical basis of PARMRES algorithm will be introduced during this talk, and numerical comparisons between PARMRES and GMRES will be conducted on a variety of relevant CFD cases.

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CP5

A Symbolic Computational Approach to the Generalized Gambler's Ruin Problem in One Dimension

Consider a gambler who starts with x dollars. At each gamble, the gambler either wins a dollar with probability $\frac{1}{2}$ or loses a dollar with probability $\frac{1}{2}$. The gamblers goal is to reach N dollars without first running out of money (i.e., hitting 0 dollars). If the gambler reaches N dollars, we say that the gambler is a winner. The gambler continues to play until they either run out of money or win. This scenario is known as the gamblers ruin problem. In this talk, the power of symbolic computation is illustrated with efficient algorithms for studying the generalized gambler's ruin problem in one dimension. We also consider a new generalization of the classical gambler's ruin where we add a third step which we call the mirror step. In this scenario, we provide closed formulas for the probability of winning and expected duration of the game. When the probability of the third step is zero, we recover the formula for the probability of winning in the classical game.

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CP5

Neuromorphic Algorithms for Beyond-Von-Neumann Computing

Modern day high-performance computing (HPC) is a resource-hungry enterprise–the Frontier exascale platform states a power consumption of 20 megawatts per exaflop. This, combined with the demise of Moore's Law scaling, indicates our von Neumann CPU and GPU-based machines will not push our capabilities much beyond exascale. Some suggest that quantum computing will answer this need, but base requirements like quantum fault tolerance remain actively researched. However, neuromorphic computers are a non-von-Neumann architecture that is available right now, and they have already demonstrated an inherent advantage in energy efficiency over classic machines. These com-

puters, modeled after the brain, are inherently stochastic and thus simulate physical systems like diffusion or turbulence while consuming $\mathcal{O}(100)\times$ less power than conventional machines (Smith, Nat. Electron. 2022). The first-generation of machines demonstrated the neuromorphic power advantage for idealized systems. However, with the recent advent of second-generation machines and their novel neuron capabilities, we have the capability to develop and run neuromorphic models based on systems ranging from boundary-layer reactive aerosol transport to hypersonic flows. For these reasons, we argue that neuromorphic machines have a bright future in HPC, with potential application as on-node stochastic accelerators or low-power on-board systems for satellites and unmanned aircraft.

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CP6

Tensor Functions under Tensor-Tensor Products with Invertible Linear Transforms

The goal of this presentation is to introduce tensor functions under tensor-tensor products with arbitrary invertible linear transforms, such as the exponent of tensors, the logarithm, sine, cosine or the p-th root. We remark that this product is a generalized notion of the T-product. Moreover, we introduce several tensor means under this product. While matrix means, such as the geometric mean and the Wasserstein mean of positive-definite matrices, have been widely researched, their extension to tensors remains relatively unexplored. Understanding tensor means can lead to advancements in tasks such as tensor-based data clustering and improved modeling of higher-order relationships in scientific and engineering domains. First, we define positive definiteness, eigendecomposition and trace of third-order tensors under this tensor-tensor product. Secondly, we generalize the concept of geometric mean to tensors that are positive-definite under the tensor-tensor product and show that this geometric mean satisfies certain properties which a "mean" should satisfy. We then show that the geometric mean is a unique positive-definite solution of a specific algebraic Riccati tensor equation and that it is the midpoint of a geodesic on the manifold of positive-definite tensors for a specific Riemannian metric. Lastly, after changing the Riemannian metric on the manifold, we also define the concept of Wasserstein mean of two tensors.

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CP6

Tnl: Numerical Library for Modern Parallel Architectures

TNL (www.tnl-project.org) is a collection of building blocks that facilitate the development of efficient numerical solvers and HPC algorithms. It is implemented in C++ using modern programming paradigms in order to provide a flexible and user-friendly interface similar to, for example, the C++ Standard Template Library. TNL provides native support for modern hardware architectures such as multicore CPUs, GPUs, and distributed systems, which can be managed via a unified interface. In our presentation, we will demonstrate the main features of the library together with efficiency of the implemented algorithms and data structures.

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CP6

BlockTensorDecomposition.jl: A Block Optimization Framework for Constrained Tensor Factorization

Unsupervised learning techniques such as clustering, dimensionality reduction, and nonnegative matrix factorization have become increasingly popular and desirable approaches for interpretable data analysis. Constrained tensor decomposition problems are an expressive class of models containing nonnegative matrix factorization, and are used for decomposing arbitrary dimensional data. Practical code for solving constrained tensor decomposition problems under a unified mathematical framework is presented. New optimization techniques such as sub-block descent, partial projection and rescaling, and multiscale decomposition empirically show faster convergence to stationary solutions. The BlockTensorDecomposition.jl Julia package is engineered to be flexible for rapid prototyping and hot-swapping of key algorithmic components such as convergence criteria, how constraints are enforced, and how blocks are updates each iteration more generally. Efficacy of this framework is tested on synthetic and real-world data across a range of applications from sediment analysis and cellular biology to musical source separation.

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CP7

Key Statistical Properties of the Quantum Proportion Estimator

By incorporating the principles of quantum mechanics into computation, a number of quantum algorithms have provided brand-new ways to solve problems across various scientific disciplines. This presentation focuses on the quantum counting algorithm, which integrates two fundamental quantum techniques, the quantum Fourier transform and quantum amplitude amplification, to develop a quantum estimator for the rudimentary statistical problem of proportion estimation. Up to now, many crucial properties of this estimator remain unresolved, such as convergence in different modes, bias, and essential statistical parameters like mean and variance. We will address these open

questions from the perspective of mathematical statistics and resolve many of the aforementioned properties. This knowledge will shed light on the design of quantum statistical protocols related to proportion estimation.

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CP7

Hierarchical Matrices in Computational Chemistry: Efficient Scaling in SOS-MP2 Calculations

Hierarchical matrix techniques, particularly the H^2 matrix framework, have played a significant role in reducing the complexity of large-scale numerical computations across various scientific disciplines due to their linear-scaling memory requirements and efficient matrix-vector product complexity. In this work, we extend the application of H^2 matrix compression techniques to the domain of quantum chemistry, specifically within the Scaled Opposite-Spin Second-Order MllerPlesset Perturbation Theory (SOS-MP2) framework. By leveraging the hierarchical structure of these matrices, we introduce an efficient Hierarchical SOS-MP2 Algorithm, which significantly reduces both time complexity and memory requirements. Our proposed algorithm achieves a computational scaling of $O(N^2 \log N)$ in both time and storage costs. Numerical experiments on alkane chains and water clusters confirm that this approach maintains high accuracy while substantially accelerating calculations. These results demonstrate the effectiveness of hierarchical matrix techniques in quantum chemistry, highlighting their potential for broader applications in large-scale scientific computing.

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CP7

Fast Newton Transform: Interpolation in Downward Closed Polynomial Spaces

The *Fast Newton Transform* (FNT) addresses the computational bottleneck that arises in solving high-dimensional problems such as 6d Boltzmann, Fokker-Planck, or Vlaslov equations, multi-body Hamiltonian systems, and the inference of governing equations in complex self-organizing systems. Specifically, the challenge lies in numerically computing function expansions and their derivatives fast, while achieving high approximation power. The FNT is a Newton interpolation algorithm with runtime complexity $\mathcal{O}(N\,n\,m)$, where N is the dimension of the downward closed polynomial space, n its degree and m the spatial dimension. We select subgrids from tensorial Leja-ordered Chebyshev-Lobatto grids based on downward-closed sets. This significantly reduces the number of coefficients, $N \ll (n+1)^m$, while achieving optimal geometric approximation rates for a class of analytic functions known as BosLevenbergTrefethen functions. Specifically, we investigate ℓ^p-multi-index sets, where the Euclidean degree ($p = 2$) turns out to be the pivotal choice for mitigating the curse of dimensionality. Furthermore, the differentiation matrices in Newton basis are sparse, enabling the implementation of fast pseudo-spectral methods on flat spaces, polygonal domains, and regular manifolds. Numerical experiments validate the algorithm's superior runtime performance over state-of-the-art approaches.

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CP7

The Seed in the Initial Configuration of Linear Cellular Automata

The orbits of cellular automata (CAs), which are discrete mathematical models, are known to generate fractals, with many examples of self-similarity. When using a CA as a fractal generator, consider orbits from the single site seed, an initial configuration that gives only a single cell a positive state. In the case of a two-state CA, the seed in the single site seed is uniquely determined to be 1, because the possible states of each cell are 0 or 1. However, in CAs with three or more states, there are multiple candidates for the seed. For example, in three-state CA, the possible states are 0, 1, and 2, and the seed candidates are 1 and 2. In a four-state CA, the possible states are 0, 1, 2, and 3, and the seed candidates are 1, 2, and 3. As the number of possible states increases, the number of seed candidates also increases. In this talk, we will prove that it is sufficient to consider only the case where the seed of linear CAs is 1.

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CP7

Randomized Rank-Structured Matrix Compression with Tagging

Many applications in scientific computing involve matrices that are dense but "data-sparse,' having some exploitable low-rank structure that enables compression without significant loss of information. Rank-structured matrices are data-sparse matrices that can be tessellated into subblocks, which are either small enough to apply deterministic algorithms or else well-approximated by matrices of low rank. For large problem sizes, randomized sampling of the input matrix by a structured random test matrix, or randomized sketching, has proven effective for rank-structured matrix compression. We introduce a new sampling technique called tagging that is suitable for large black-box applications in which the entries of the input matrix are not accessed directly, but rather through fast matrix-vector or matrix-matrix multiplication. We discuss the improved efficiency of randomized sampling with tagging, as well as the accuracy of the overall compression scheme, for strongly admissible block low-rank (BLR) matrices with shared bases across admissible blocks within the same block-row or block-column, termed uniform BLR.

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CP8

Numerical Modeling of Calcium Dynamics in Urinary Bladder Smooth Muscle

Mathematical and numerical modeling of physiological systems helps understand pathological conditions and identify pharmacological targets. Urinary incontinence, or involuntary urine leakage, often results from overactive urinary bladder smooth muscles (UBSM). Intracellular calcium (Ca2+) dynamics play a key role in UBSM contraction and relaxation. This study develops a whole-cell Ca2+ model based on numerical simulations aligned with experimental data. Our simulation of electrophysiology and intracellular Ca2+ dynamics incorporates fast stochastic dynamics in tiny sub-compartments, partial differential equations (PDEs) with stochastic source terms, and a globally coupled membrane potential. We use unstructured meshes for spatially heterogeneous Ca2+ release and adaptive time-stepping for stochastic channel activity in Ca2+ release units (CRUs). Reaction-diffusion equations describe intracellular concentration fields across nanometer to micrometer scales and millisecond to second timescales. Highly stochastic CRU models drive source functions in the PDE model. The separation of fast stochastic CRU dynamics and slower PDE dynamics challenges traditional methods, so we introduce new techniques to enhance efficiency. The membrane potential couples the entire cell spatially due to its large coupling length. We developed an adaptive finite element simulator, providing an efficient computational approach to modeling intracellular Ca2+ dynamics in UBSM tissues.

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CP8

A Fractional-Order Framework for Diabetes Disease Incorporating Awareness Campaigns and Treatment Using a Two-Step Newtonian Polynomial Approach

Diabetes is rapidly emerging as a global epidemic, posing a significant threat to public health. Modeling the spread and management of diabetes is crucial for monitoring its growing prevalence and developing cost-effective strategies to mitigate its incidence and complications. This paper presents a fractional-order nonlinear model for diabetes mellitus that incorporates the cumulative effect of media-driven diabetes awareness and treatment function. The model is analyzed using a two-step Newtonian polynomial approach with the Caputo derivative. Key aspects such as equilibrium points, stability, and the existence and uniqueness of solutions are examined to ensure the robustness of the model. The obtained results are validated against previously published findings. Graphical and numerical results are obtained for different values of the fractional order. This research provides valuable insights for predicting disease trends and planning effective clinical management for diabetes patients.

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CP8

Novel Machine Learning Investigation to the Mathematical Fractional Modeling Model Analysis Breast Cancer and Chemotherapy Heart Risks

The world's second-most common cause of death for women is breast cancer. Cancer can be treated by removing cancer cells surgically, killing them, or stopping them from receiving the signal necessary for cell division. Patients who receive cancer treatment may not always have beneficial effects. Treatment for breast cancer can affect the cardiovascular system. The side effect of chemotherapy on the heart is called cardiotoxicity. We created a fractional mathematical model based on the hospital's breast cancer patients. The model is built using a set of fractional differential equations. We used a modified ABC-fractional order to explain the fractional breast cancer model. A population is subdivided into five subsets. Stages include 1 and 2 (A), 3 and 4 (B), disease-free (D), and cardiotoxic (E). We have demonstrated the existence, uniqueness, and positivity of model simulation. We run simulations and use neural networks to provide a graphical comparison study. The findings also show how various model parameters affect the system, offering greater insight and a more effective solution for real-world issues. The efficacy, stability, precision, dependability, and relevance of the proposed approach are confirmed by the error distribution using histograms, obtaining low MSE, RMSE MAE, MAPE, NSE, time series analysis, and linear regression for the breast cancer model. We conclude with computational simulations that allow us to visualize our theoretical results.

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CP8

Airy Beams Interaction in Nonlinear Optical Media

The dynamics of light beam interaction in nonlinear optical media are studied numerically and analytically. The beam dynamics are simulated by the beam propagation method. Numerical results agree with those obtained from the analytical model. Results demonstrate that reflection and transmission can be predicted and controlled by a trapped Airy beam at the interface of two nonlinear optical media. Some interesting new results will be presented in this talk.

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CP8

An Adaptive Parker-Sochacki Method for Robust Numerical Simulation

For high-resolution numerical simulation involving systems of differential equations, an explicit adaptive procedure using a foundation of the Parker-Sochacki Method (PSM) has significant advantages over many standard adaptive algorithms that use a Runge-Kutta (RK) foundation. These advantages include decreased output data storage size relative to resolution and complexity, built-in series approximations of the state space to find states between timesteps, an automatic stepwise a-priori error bound, and a simple way to increase or decrease the order of the method stepwise during the computation. At each step across the domain, the algorithm recursively generates the Taylor polynomial of the solution to the governing ODE system and also allows for straightforward incorporation of other approximation schemes to improve accuracy and efficiency. An Adaptive PSM algorithm is described theoretically and demonstrated on several examples, including a three degree of freedom trajectory system. Results are compared against standard RK adaptive algorithms and it is noted in the 3DoF example that Adaptive PSM provides roughly two orders of magnitude improvements in speed and number of steps for similar accuracy.

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CP8

Proportional-Integral-Derivative (PID) Control Through An Adaptive Parker-Sochacki Method

An algorithm for Proportional-Integral-Derivative (PID) control using a foundation of an Adaptive Parker-Sochacki Method (PSM) has significant advantages over standard PID control algorithms that use a discrete numerical foundation in simulation. Such advantages include built-in recursively generated series solutions of the state space, control variables, process variables, the proportional, integral, and derivative components, error value, and all quantities describing governing forces for the dynamical system of interest. It allows for the setpoint and tuning controls, typically taken as constants, to be modeled and adjusted as functions of time. The method requires no post interpolation as it produces continuous solutions to arbitrary degree and is adaptive both in timestep and order. The access the algorithm allows to high degree Taylor series coefficients for nearly all quantities in the system is broadly significant in its potential for enhanced understanding of stability and the impact of varying PID control parameters. Advantages of this method will be demonstrated on several examples including trajectory simulation.

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CP9

Leveraging Approximation Theory for Efficient Scientific Machine Learning

While machine learning methods are playing an increasingly prominent role in accomplishing scientific tasks, they still lack practical theory to guide decisions about their architecture, parameterization, and hyperparameter selection. In this talk, I show how to leverage approximation theory to fill this gap, using Kolmogorov-Arnold Networks as a model for explainable neural architectures (from an approximation theory standpoint). Using the lens of the composition of spline basis functions, multilayer perceptrons become a geometrically reduced version of Kolmogorov-Arnold Networks. This insight allows a natural method for algebraic and geometric refinement of neural networks, providing approximation properties that converge with the spatial resolution of the splines. I demonstrate the highlighted methods with examples that highlight their approximation capabilities for scientific tasks.

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CP9

Supremum Norm Adaptive Hybrid High Order Method for the Poisson Problem

In this work hybrid high-order methods for analyzing the Poisson problem in both two and three space dimensions is proposed. The method utilize upto scalar-valued polynomials of the same order across mesh elements and faces as degrees of freedom. At the core of the analysis is a local (element wise) discrete gradient reconstruction operator. To ensure compatibility with standard conforming finite element spaces, a linear averaging function is employed to transition the potential reconstruction operator to its conforming counterpart. Furthermore, discrete upper and lower barrier functions are constructed incorporating corrections to the conforming part of the reconstruction operator. The article thoroughly discusses the pointwise reliability and efficiency of a proposed *a posteriori* error estimator. Finally, numerical experiments are conducted to illustrate the theoretical findings.

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CP9

Adaptive Radial Basis Function Methods for Data Approximation

Radial basis functions (RBFs) are a powerful tool for constructing high-order accurate reduced representations of scattered data in arbitrary dimension and on manifolds. We present a method of constructing RBF data reductions in which the RBF centers, shape parameters, and tail are selected adaptively for each RBF. We defined a machine learning problem in which these properties are learned to minimize the data approximation error. We demonstrate the method for applications of scattered data reduction on the sphere, and compare the performance for different restrictions for adaptivity.

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CP9

Quasi-Static Griffith Fracture Evolution with Boundary Forces

We discuss the well-posedness of a variational formulation for modeling quasi-static evolution of cracks in elastic materials under boundary forces. Quasi-static evolution of fracture for displacement loads, *i.e.*, Dirichlet boundary conditions, has been studied extensively in the past couple of decades, using models based on global and local minimization. However, boundary forces, *i.e.*, Neumann boundary conditions, had been seen as problematic with the usual variational formulation, due to a straightforward non-existence argument. Recently, a variational formulation, namely dual minimization, was proposed as a method for finding solutions for fracture problem with boundary forces. Adopting this method, we study existence of quasi-static fracture evolutions under time-varying boundary forces.
Global minimizers of the quasi-static Dirichlet problem have always balanced the sum of stored elastic plus crack dissipated surface energies. Nonetheless, even though our formulation for the quasi-static Neumann problem is based on global minimization, we show that evolutions here do not necessarily satisfy this energy balance, and describe how there can be decreases in the energy. Note that decrease in the sum of stored and dissipated energies in time might be expected since the effect of kinetic energy caused by the jumps in the evolution of cracks is not considered in the quasi-static energy equation. We also give estimates on how big energy drops can be.

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CP10

Numerical Modeling of Anomalous Diffusion of Water in Porous Media Using Meshless Techniques

This study investigates the anomalous diffusion of water in porous media, a process that deviates from classical diffusion laws of fluids in porous medium. In our approach, we employ fractional calculus and analyze the Fractal and Fractional Richards Equations for modeling water diffusion. These models incorporate both singular and non-singular kernel derivatives to accurately capture the anomalous subdiffusion. To solve the system, we developed a meshless numerical method based on localized radial basis functions (LRBF) for spatial discretization. This approach is coupled with implicit time-stepping and advanced linearization techniques to efficiently address the systems nonlinearity. The parameters of the model equation and fractal/fractional derivatives are calibrated based on available experimental data. Numerical simulations are performed to validate the models using the fractal derivative and four fractional derivatives: Caputo, Atangana-Baleanu-Caputo, Fabrizio-Caputo, and San-Hao-Zhang-Baleanu fractional derivatives. We evaluate the numerical models based on laboratory experimental data. Our findings demonstrate that fractional and fractal models significantly enhance the accuracy of anomalous subdiffusion modeling while maintaining computational efficiency. This study provides a comprehensive comparative assessment of different modeling approaches, highlighting their effectiveness and adaptability in capturing subdiffusion dynamics in porous media.

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CP10

Wavy Optimal Flows for Heat Transfer from Straight Walls

In this paper, we investigate the computation of optimal incompressible fluid flows that maximize the rate of heat transfer out of the walls of a two-dimensional, straight channel given a specified flow input power Pe^2. We use a computational framework that leverages the adjoint method in combination with the BroydenFletcherGoldfarbShanno (BFGS) optimization algorithm to identify these optimal flows. The analysis is carried out for a wide range of Peclet numbers (Pe), and we demonstrate that the resulting optimal flow patterns exhibit distinct wavy structures characterized by elongated, finger-like protrusions emanating from both the top and bottom walls of the channel. These convective fingers play a crucial role in enhancing heat transfer allowing the wavy flow configurations to outperform the previously identified unidirectional optima [1], as found for Peclet values in the range 2^{13} to 2^{17}. Specifically, the wavy flows outperform the unidirectional optima by 3% to 30%, depending on the Peclet number. This study highlights the importance of flow patterns in optimizing heat transfer in convective systems and provides a comprehensive approach to finding these optimal wavy configurations using advanced optimization techniques. [1] Alben, S. (2017). Improved convection cooling in steady channel flows. Physical Review Fluids, 2(10). https://doi.org/10.1103/physrevfluids.2.104501

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CP10

On the Capabilities of Self-Similar Viscosity Models to Predict Properties of Carreau Boundary

Layer Flows

We consider the problem of the boundary layer introduced by motion between a flat plate and a non-Newtonian fluid in both the case of a static fluid over a moving plate (Sakiadis Boundary Layer) and a moving fluid over a static plate (Blasius boundary layer). For Newtonian and power-law rheologies, these flows admit self-similar solutions to the boundary-layer equations that are not admitted by more realistic rheological models. We compare the self-similar solutions to the non-self-similar solution for a more realistic Carreau viscosity model. Following previous work, we show that while the problem is no longer self-similar, the full two-dimensional flow field can be reduced to a 1-parameter family of ODEs using the Newtonian similarity transform. We show that the Carreau flow can be split into Newtonian and power-law regimes in which self-similar solutions provide an accurate prediction of wall shear. We show that self-similar solutions to Sakiadis and Blasius flows provide good predictions of wall shear compared with Carreau rheologies over a range of power-law exponents.

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CP11

Computer Assisted Discovery of Integrability Via Sparse Identification of Lax Operators

Integrablity is vital in the study of dynamical systems since it is a mathematically rich topic and often the starting point for analyzing more complex equations. However, it is difficult to even recognize if a given system is integrable a priori. Therefore, we formulate the automated discovery of integrability in dynamical systems as a symbolic regression problem. Specifically, we seek to maximize the compatibility between the known Hamiltonian of the system and a pair of matrix/differential operators known as Lax pairs. Our approach is tested on a variety of systems ranging from nonlinear oscillators to canonical Hamiltonian PDEs. We test robustness of the framework against nonintegrable perturbations, and, in all examples, reliably confirm or deny integrability. Moreover, using a thresholded l^0 regularization to promote sparsity, we recover expected and discover new Lax pairs despite wide hypotheses on the operators. We will discuss future directions for adapting our framework toward building an all purpose data-driven nonintegrability filter of complex systems.

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CP11

Two Frameworks for Higher-Order Time Discretization of Maxwell's Equations

We present two different ways to obtain higher-order time discretizations for Maxwell's equations although our strategies may be used for other time-dependent partial differential equations (PDEs) as well. A higher order spatial discretization for PDEs can be obtained by use of a polynomial basis or an enrichment of approximating spaces with carefully selected functions. This is the rationale for finite element methods (FEM), with or without discontinuous basis, and extended FEM methods. Historically, higher-order spatial finite difference (FD) discretizations were also used. However, for time discretization, higher-order FDs or FD-like schemes are an overarching theme. This includes structure preserving variational integrators. However, the PDE itself may not be tightly integrated into the formulation of such a scheme. Consequently, we propose two frameworks for such higher-order time discretizations: (1) *Time Strategy* in which one uses a higher-order FD for the time derivatives, and (2) *Space Strategy* in which we introduce higher-order spatial derivatives replacing higher-order time derivatives via the governing equations and translate to using a higher order FEM (for example). With a de Rham sequence of finite element spaces for the spatial part, we will discuss some theoretical underpinnings for error analysis in the context of Maxwell's equations. We hope this would help move forward higher-order time discretizations in a more grounded manner.

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CP11

Unconditionally Energy Gradient Stable, Linear Scheme for Tumor Growth Model Using Phase Field Model

In this work, we consider the phase field model for modelling tumor growth. To construct the governing equation, we choose the Cahn-Hilliard equation to describe cell fracture based on the generalized Fick's law. The relation between cells and nutrients is described using the chemotaxis model. The source term of the generalized Fick's law is constructed using a reversible chemical reaction network. The total energy dissipation and mass preservation properties are confirmed. To numerically solve, we adopt the convex splitting method, which is based on the Lyapunov function. Splitting the Lyapunov function into contractive and expansive parts, we can construct the unconditionally energy gradient stable scheme using the convexity of the contractive and expansive parts. We validate the energy gradient stability and mass preservation property from the numerical analysis and experiment. Moreover, we demonstrate the unique solvability of the proposed numerical scheme using block LU decomposition and eigenvalues of each operator.

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CP11

An Embedding Heat Method for Computing Geodesic Distance on Implicit Surfaces

The heat method (Crane et al., 2013) is a simple and efficient algorithm for computing geodesic distance through solving the Eikonal equation on triangulated surfaces. Based on the framework of the closest point method for surface PDEs (Ruuth et al. 2008), we present a heat method to solve the Eikonal equations on implicit surfaces in the embedding space. Our approach retains the main advantages of the original heat method (simple, fast, and robust) and bypasses numerical challenges due to mesh quality. This is a joint work with Shingyu Leung and Byungjoon Lee.

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CP12

A Novel Estimator of a Change Point Parameter in a Regression Model

Change point regression models play a crucial role in identifying shifts in the behavior of data over time, especially in fields such as finance, engineering, and signal processing. We develop a novel estimator to recover a change point parameter in a linear regression framework. The proposed method leverages jump signals in both dependent and independent variables. We obtain the convergence rate of the proposed estimator, which may be tighter than those available methods in the literature. Numerical Monte Carlo results support the theoretical results. The proposed method is also illustrated on actual data.

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CP12

Deflation for the Half-Arrow Singular Value Decomposition

A half-arrow matrix F has the form

$$\begin{aligned} F &= \begin{pmatrix} \Psi & \mathbf{g} \\ \mathbf{0}^T & \rho \end{pmatrix}, \quad \mathbf{g} \in \mathbb{R}^n, \quad \rho \in \mathbb{R}, \\ \Psi &= \operatorname{diag}(\psi_1, \ldots, \psi_n), \quad \psi_1 \geq \psi_2 \geq \ldots \geq \psi_n \geq 0. \end{aligned}$$

We consider the problem of determining which of the diagonals of Ψ are close to singular values of F and how these values can be deflated efficiently. Such deflation techniques were explored in the "conquer' stage of the divide-and-conquer bidiagonal SVD algorithms similar to those in LAPACK. This problem has important connections to the core problem as described by Paige and Strakoš that includes least squares and total least squares problems, and to truncated SVD and selective SVD methods for regularization.

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CP12

Principal Component Flow Map Learning of Pdes from Incomplete, Limited, and Noisy Data

We present a computational technique for modeling the evolution of dynamical systems in a reduced basis, with a focus on the challenging problem of modeling partially-observed partial differential equations (PDEs) on high-dimensional non-uniform grids. We address limitations of previous work on data-driven flow map learning in the sense that we focus on noisy and limited data to move toward data collection scenarios in real-world applications. Leveraging recent work on modeling PDEs in modal and nodal spaces, we present a neural network structure that is suitable for PDE modeling with noisy and limited data available only on a subset of the state variables or computational domain. In particular, spatial grid-point measurements are reduced using a learned linear transformation, after which the dynamics are learned in this reduced basis before being transformed back out to the nodal space. This approach yields a drastically reduced parameterization of the neural network compared with previous flow map models for nodal space learning. This allows for rapid high-resolution simulations, enabled by smaller training data sets and reduced training times.

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CP12

Rigged Dmd: Data-Driven Spectral Decompositions for Koopman Operators

Koopman operator theory provides a powerful framework for data-driven analysis of nonlinear dynamical systems. At its heart, the Koopman operator governs the evolution of observables on the state-space and allows one to construct reduced-order models, extract coherent features of the dynamics, and more. However, Koopman-based approaches often fail to capture important features of dynamical systems with continuous spectrum. In this talk, we show how to rigorously compute coherent features of measure-preserving dynamical systems with continuous spectrum. Our algorithm, Rigged DMD, uses a measure-preserving Dynamic Mode Decomposition to construct carefully regularized wave-packet approximations to the generalized eigenfunctions of unitary Koopman operators in rigged Hilbert spaces. We discuss the basic convergence properties of the algorithm and illustrate with a number of examples, including the nonlinear pendulum, the Lorenz system, and a high-Reynolds number lid-driven flow in a two-dimensional cavity.

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CP12

Invariant Image Reparameterisation: A Unified Approach to Structural and Practical Identifiability and Model Reduction

Parameter non-identifiability poses significant challenges when fitting mathematical models to data, especially in complex biological and engineering systems. We introduce Invariant Image Reparameterisation (IIR), an in-

tegrated approach that combines the strengths of existing methods for identifiability analysis such as symbolic methods, profile likelihood, and sloppiness analysis. IIR uses numerical evaluation of a reparameterisation condition at a reference point, along with an invariance condition that determines when this holds globally, to determine identifiable parameter combinations ordered by degree of identifiability. Our approach further enables systematic model reduction, along with uncertainty quantification through so-called Profile-Wise Analysis. We demonstrate our methodology's practical application on simple statistical and mechanistic models. IIR is available via our open-source Julia implementation.

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CP12

Spatial Placement of Greened Areas and Their Impact on Crime

Greening initiatives, aimed at community betterment, have been implemented by cities to mitigate the adverse effects of vacant and abandoned lots. This study investigates the impact of greening efforts, such as the removal of vacant buildings and the planting of trees, on community crime rates. While numerous statistical studies have examined the effects of greening, this research focuses on the spatial placement of greened areas within neighborhoods and their influence on crime, utilizing an agent-based model grounded in first principles. Although the model is not yet directly applicable to specific neighborhoods, its validity is assessed by comparing its outcomes with anecdotal evidence from previous statistical models. If validated, this model can provide insights into how the placement and size of greened areas within a neighborhood affect crime rates.

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CP14

Error Analysis of An Accelerometer-Only Algorithm to Measure Rigid Body Kinematics for Traumatic Brain Injury Detection

Advances in wearable inertial sensor technology allow for high-frequency measurement of kinematic data at select points across the human body. By using only four triaxial accelerometers distributed around the head, we may recover the acceleration field throughout the entire skull, including estimates of angular velocity and angular acceleration without the need for a gyroscope. The estimates from this accelerometer-only (AO) algorithm may be used in head injury models in order to predict or detect traumatic brain injury. Uncertainties arise when using the AO-algorithm on real sensor data. For example, the sensors may be imprecisely positioned, leading to uncertainties in the sensor positions and orientations, which then impact the predictions of the AO-algorithm. In this talk, we will present an error estimation framework for the AO-algorithm. We then demonstrate the error estimates on synthetic examples, as well as real experimental data. Consequently, our error analysis provides insights into the optimal configuration of the wearable sensors to minimize the impact of uncertainties.

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CP14

Well-Posedness and Stability Analysis of a Pde-Ode Model for the Evolution of Bacterial Persisters

Most antibiotics kill bacteria by disrupting cell wall formation during mitosis. Bacterial persisters are individuals within a population that avoid this fate by not replicating. We use a parabolic PDE to model the phenotypic switch between normal, active bacteria and persisters along with a nonlocal birth-jump process that captures epigenetic inheritance. In addition, we relate bacterial population development to resource dynamics in order to depict a more realistic bacterial growth limit. Mathematically, the model consists of a non-local PDE coupled to an ODE. We prove the well-posedness of the model using semi-group theory and the Banach fixed point theorem. We then examine the evolutionarily stable strategies of persister cells by conducting a global invasion analysis with an appropriately chosen Lyapunov functional.

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CP14

Skeletal Muscle : Mechanical Impact of Fibre Orientations

Skeletal muscles can exhibit large mechanical deformations in a short period of time. Muscle contains fibres which can be non-linearly activated. We are interested in the mechanical behaviour of muscle in cylindrical architecture. We report on the impact of different fibre orientations. These types of fibre are usually found in worms or other similar

organisms. We use a fully 3-D model of dynamic elastic deformation. Our computations are based on Finite Element Method approach. Biologically-relevant emergent features are captured in our computations.

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CP15

Integrating Sentiment Analysis into Financial Predictive Modelling

In financial markets, stock return prediction has remained a fundamental challenge, particularly in today's dynamic environments influenced by news and investor sentiment. In this study, we integrated financial news sentiment analysis into stock return forecasting models to enhance traditional econometric approaches and optimize trading strategies. To extract sentiment scores from financial news headlines, we employed a lexicon-based tool tailored for the financial domain. These sentiment indicators were incorporated into predictive models, including a sentiment-based regime-switching model for log returns, alongside advanced machine learning techniques such as random forests, neural networks, and hidden Markov models. By introducing market sentiment as a Markov process, we modelled stock return mixture distributions using parametric distribution families. Evaluation using Kolmogorov-Smirnov tests and Kullback-Leibler divergence scores confirmed that the mixture t-distribution provided the most accurate representation. Furthermore, we developed and compared two sentiment-guided trading strategies against conventional approaches. The results demonstrated significantly improvements in trading performance, reinforcing the impact of news sentiment. This research highlights the critical role of sentiment analysis in financial modelling and proposes a robust framework for integrating market sentiment into return predictions.

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CP15

Realistically Modelling Market Entry Dynamics Within Rich-Get-Richer Scheme Via Pitman-Yor Process

Understanding market entry dynamics is essential for analysing industry competition, firm survival, and market structure evolution. Traditional stochastic models, such as Poisson processes and Markov models, often fail to capture key empirical features of firm entry, including preferential attachment and heavy-tailed distributions of market share. To address these limitations, we explore the use of the Pitman-Yor Process (PYP), a nonparametric Bayesian model that generalises the Dirichlet Process by incorporating a discount parameter. This additional flexibility allows PYP to model rich-get-richer effects and power-law behaviours commonly observed in market entry data. The theoretical foundations of PYP in the context of firm entry are presented, its probabilistic properties discussed, and its advantages over classical approaches illustrated. Through numerical simulations, we demonstrate how PYP naturally accounts for market concentration effects and firm heterogeneity. Our findings suggest that PYP provides a robust framework for modelling market entry, which makes it a powerful tool both for industry and policy-makers, especially in fight against monopolies.

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CP15

Statistics-Informed Neural Network

The statistics-informed neural network (SINN) has been proposed as a machine learning-based stochastic trajectory generator [J. Comput. Phys. 474, 111819 (2023)]. With the capability of learning stochastic dynamics from time trajectory data and reproducing stochastic time trajectories faithfully and efficiently, this methodology is considered a promising tool for surrogate modeling. In this presentation, I will first introduce SINN and describe its unique structure and training scheme. Then, I will talk about extending SINN to multi-dimensions. Finally, I will discuss how SINN can be used for surrogate modeling in multi-scale multi-physics simulations.

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CP15

An Improved Simulation Method of Wishart Multivariate Stochastic Volatility Model

This article proposes a novel exact simulation method of the Wishart multivariate stochastic volatility (WMSV) model. WMSV follows $d\Sigma_t = (\Omega\Omega^T + M\Sigma_t + \Sigma_t M^T)dt + \sqrt{\Sigma_t}dZ_t Q + Q^T(dZ_t)^T\sqrt{\Sigma_t}$ and the log of asset price follows $dY_t = (r - \frac{1}{2}tr[\Sigma_t]dt + tr[\sqrt{\Sigma_t}(dW_t R^T + dZ_t\sqrt{I - RR^T})]$. This method is based on analysis of the joint moment generating function of the log-price, a terminal volatility level and an integral of volatility level with respect to time. First, the volatility marginal state is sampled by squaring a normal random matrix which follows $dN_t = N_t H^T dt + dB_t\Sigma$, with $N_0^T N_0 = x$. Then, the integral of the volatility $\int_t^T \Sigma_s ds$ is sampled given this volatility marginal state using conditional characteristic function and inversion formula. Next, conditioning on this marginal state and the integral of volatility, the characteristic function of log-price is got by a joint moment generating function. Finally, the log-price can be sampled by using inverse of characteristic functions, numerical integration and inverse transform method.

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CP15

Markov Processes for Enhanced Deepfake Generation and Detection

New and existing methods for generating, and especially detecting, deepfakes are investigated and compared on the simple problem of authenticating coin flip data. Importantly, an alternative approach to deepfake generation and detection, which uses a Markov Observation Model (MOM) is introduced and compared on detection ability to the traditional Generative Adversarial Network (GAN) approach as well as Support Vector Machine (SVM), Branching Particle Filtering (BPF) and human alternatives. MOM was also compared on generative and discrimination ability to GAN, filtering and humans (as SVM does not have generative ability).Humans are shown to perform the worst, followed in order by GAN, SVM, BPF and MOM, which was the best at the detection of deepfakes. Unsurprisingly, the order was maintained on the generation problem with removal of SVM as it does not have generation ability.

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CP17

Power Series Solution to the Hodgkin-Huxley Model of Action Potential Generation in Neurons

We investigate an exact solution to a system of coupled, nonlinear ODEs, formally known as the Hodgkin-Huxley model, using a set of power series solution techniques. The HH model was developed by Nobel Prize-winning British scientists Alan Hodgkin and Andrew Huxley to describe action potential generation in a giant squid axon. We examine various procedures for extending beyond the radius of convergence of the power series which we initially investigated for non-oscillatory solutions. Our efforts find that the signs of the coefficients of the power series representing our function alternate. This means that, for the specific and simple cases investigated thus far, the exact solution contains a singularity on the negative real axis and suggests that certain resummations can be used. More specifically, we find the power series solution through an Euler transformation of the original ODE. Finding this solution would add to a greater goal of curating a collection of tools that would assist in solving nonlinear ODEs with power series. This work was partially supported by NSF Award 1935277.

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CP17

Stochastic Dynamics of Embedded Neural Motifs in Large-Scale Networks

Neural motifs, recurring patterns in neuronal networks, serve as fundamental building blocks that shape dynamics by modulating collective behavior, enhancing information processing, and improving robustness to noise. While individual motifs have been studied, their behavior within large-scale networks under noise remains unclear, raising questions about their roles in stochastic resonance and spike-timing synchrony. We model a large-scale network of biologically plausible neurons to investigate motif influence on network behavior. Our results show that common motifs, such as feed-forward loops and bi-coupled neurons, exhibit altered dynamics when embedded in networks. These include enhanced synchrony under weak and intermediate stochastic stimuli and greater sensitivity to noise relative to isolated motifs. Functional differences, such as synchrony propensity and spike-timing regularity, are accentuated rather than diminished by background connections. We also show that asymmetries in inter- and intra-motif coupling strengths influence dynamics, with an optimal ratio maximizing coherence. Our findings highlight the functional roles of motifs in stochastic networks. By exploring local-global interactions, this work advances our understanding of neural networks and lays the groundwork for future research into motif-driven network organization in cognitive processes.

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CP17

Estimating Parametric Map of Dynamic PET Brain Imaging Using Physics-Informed Neural Networks

Quantitative analysis of dynamic PET brain images is challenging due to their high-dimensional, 4D space-time nature. Voxel-level parameter mapping using kinetic models is computationally expensive and requires large datasets, making conventional deep learning approaches difficult to apply. Efficient, noninvasive methodologies are needed to improve feasibility in small-sample studies. This study aims to develop a Physics-Informed Neural Network (PINN)-based framework for estimating parameter maps of dynamic PET brain images while working with relatively small datasets and improving computational efficiency. We utilize PiB dynamic PET imaging from the Open Access Series of Imaging Studies (OASIS-3). The approach suggested by De Benetti et al. for whole-body PET scans is adapted and optimized for brain PET imaging. Additionally, we employ the simplified reference tissue model for noninvasive quantification. To preserve the resolution of the original PET images and enhance performance on limited data, we propose a patch-level framework with tailored preprocessing and postprocessing techniques. This study demonstrates the potential of PINNs for dynamic PET imaging, offering a scalable and efficient alternative for parameter estimation in brain imaging.

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CP17

Optimal Control for Stochastic Neural Oscillators

Deep brain stimulation is a therapeutic treatment for a variety of neurological disorders such as Parkinsons disease, which is hypothesized to be due to pathological synchronization of neural activity in the motor control region of the brain. This motivates the control objective of desynchronizing neural activity using a single electrical stimulus. This study develops an event-based, energy-efficient control strategy for desynchronizing coupled neural networks using optimal control theory. In particular, by using an advanced computational solver for nonlinear partial differential equations to solve the stochastic Hamilton-Jacobi Bellman equation via level set methods for a single neuron model, we find control inputs which drive the dynamics close to the systems phaseless set. When applied to coupled neural networks, these inputs achieve effective randomization of neural spike timing, leading to significant network desynchronization. Compared to its deterministic counterpart, our stochastic method can achieve considerable energy savings.

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CP18

Engineering Optimal Parallel Task Scheduling

The NP-hard scheduling problem $P||C_{\max}$ encompasses a set of tasks with known execution time which must be mapped to a set of identical machines such that the overall completion time is minimized. In this work, we improve existing techniques for optimal $P||C_{\max}$ scheduling with a combination of new theoretical insights and careful practical engineering. Most importantly, we derive techniques to prune vast portions of the search space of branch-and-bound approaches and propose improved upper and lower bounding techniques. Moreover, we present new benchmarks for $P||C_{\max}$, based on diverse applications, which can shed light on aspects that prior synthetic instances fail to capture. In extensive evaluations, we observe that our pruning reduces the number of explored nodes by 90× and running times by 12×. Compared to a state-of-the-art ILP-based approach, our approach is preferable for short running time limits and for instances with large makespans.

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CP18

Mitigation of Finite-Precision Error in the Resummation of Power Series Solutions

Power series are an analytical tool that can provide accurate (and sometimes exact) solutions to nonlinear ordinary differential or transcendental equations. However, it is typically the case that such power series diverge at a radius of convergence within the (physical) domain of interest, due to singularities outside and/or at the boundary of the physical domain. To bypass the radius of convergence and analytically continue a power series as a convergent resummation, a judicious choice of expansion variable (i.e., "gauge function) may be chosen which maps the closest singularities in an appropriate direction. Unfortunately, the operations used to transform an original power series into such a resummation often amplify and/or accrue finite precision error when implemented on a computer. In this talk we demonstrate how to avoid (or at least mitigate) such error, without increasing the precision of your machine (i.e., while staying in double precision).

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CP18

A Size O(N) Relaxation of the Oversampled Fourier Phase Retrieval Problem With Small Expected Optimality Gap

We present a sum-of-squares (SOS) relaxation for the oversampled Fourier phase retrieval problem. By optimizing over the convex SOS cone directly, our relaxation avoids the need for semidefinite programming and variable lifting. For a phase retrieval instance containing N unknowns, the resulting relaxation has only $O(N)$ variables, a significant improvement compared to the $O(N^2)$ required by standard lifting methods. We show that the relaxation returns a nontrivial lower bound with a small expected optimality gap for oversampled Fourier phase retrieval instances that arise in experimental settings. We present numerical evidence that the relaxation is tight for many instances of interest. To solve the relaxation, we use a matrix-free interior point method capable of handling phase retrieval instances with more than one million unknowns.

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CP18

Using New Representations to Derive and Prove Combinatorial Formulas

Some papers analyze or compare algorithms by generating random permutations as inputs and comparing some numbers, without having a complete theoretical understanding of why some algorithms perform better than others, on average. Because generating all permutations of higher order is very expensive and sometimes impossible due to computational and time limitations, combinatorial formulas are needed to understand the behavior of such algorithms. Using new representations helped in obtaining combinatorial formulas related to outputs and performance of algorithms. Some of the results are related to distributions of elements derived from permutations and subsets of permutations. Having combinatorial formulas that give exact results could help programmers decide which algorithms to use for specific types of data. My results could be used to analyze

other theoretical aspects related to permutations and average behavior of sorting algorithms.

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CP19

Finite Population Effects in a Moving Optimum Model

In the face of anthropogenic climate change, populations are under new selective pressure to rapidly adapt or else go extinct. Moving optimum models have provided a theoretical framework for understanding how populations respond to such changing conditions. These models generally describe the population in terms of the distribution of a quantitative trait x, which evolves in response to an optimal trait shifting at a constant speed c. One such model describes changes in the density $v(t, x)$ of individuals with trait x at time t according to the equation:

$$v_t = \frac{\sigma^2}{2} v_{xx} + \left[1 - \frac{(x - ct)^2}{2} - \int_{\mathbb{R}} v(t, y) dy\right] v,$$

where σ^2 is variance in the trait due to mutation. A key assumption of most moving optimum models is that of an infinite population size, in which stochasticity from random sampling events is ignored. However, stochastic simulations show that even for large population sizes, deterministic predictions can dramatically overestimate the success of an asexually-reproducing population. This can be attributed to the low density of individuals carrying traits in the tail of the distribution, from which future generations are known to descend and thus drive evolution of the population. Using approximation methods previously applied to front propagation models, we seek to develop a deterministic correction for the effects of stochasticity on the success of a population adapting to a constant environmental change.

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CP19

Stochastic Differential Equation Models of Chemotaxis Driven by Fractional Brownian Motion

Chemotaxis, the directed movement of cells and microorganisms in response to chemical signals, is a fundamental biological process. The seminal mathematical model by Keller and Segel, which focuses on the aggregation dynamics of Dictyostelium discoideum, provides a foundational framework for understanding this phenomenon. Current modeling techniques merge elements of Brownian motion with gradient-driven motility, paralleling the mechanisms in stochastic gradient ascent algorithms used in optimization tasks. Fundamentally, chemotaxis is a natural optimization process that strives to position cells in areas of highest chemoattractant concentration. However, recent experimental findings challenge this traditional view. In the absence of chemotactic cues, many cell types display a motility pattern akin to fractional Brownian motion, characterized by correlated incrementscontrary to simple Brownian motion predictions. This revelation is pivotal for our understanding of cell migration towards chemoattractant sources. Our presentation will provide evidence from computational simulations that cells with positively correlated movements navigate their environments more effectively. Additionally, our computational analysis will shed light on the relative importance of mechanisms that combine external signals with internal cell polarization. This work was supported in part by an ANID FONDECYT Regular grant (No. 1221220).

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CP19

Mathematical Model of the Learning Mechanism in True Slime Molds

It is believed that the nervous system plays an important role in human learning ability. On the other hand, it has been reported that unicellular organisms may possess the learning ability, even though they do not have a nervous system. Boisseau et al. (2016) demonstrated the hallmarks of habituation, a type of learning, in the plasmodium of *Physarum polycephalum*, true slime mold, which is a unicellular organism. In this study, we made a mathematical model to understand the mechanism. We consider the plasmodium to be composed of two parts: a front part and a rear part. We formulated that the expansion velocity of the plasmodium tip is proportional to the pressure difference between the front and rear parts, as its migration is driven by internal sol flow, approximated by Hagen-Poiseuille flow. In addition, we formulated a simple reaction-diffusion model of a chemical that influences sol pressure. Then, the temporal dynamics of sol pressures were derived from the reaction-diffusion model. Finally, we obtained a model of linear ordinary differential equations with three dependent variables: the plasmodium tip position, and the sol pressures at the front and rear parts. Our model reproduced the experimental results of Boisseau et al. (2016). We found that the dimensional reduction structure, which transforms two variables—the sol pressures at the front and rear parts—into one variable, the expansion velocity, plays an important role in plasmodium learning.

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CP19

Finding Math in the Revitalization of a Fishpond in Hawaii

Kuhialoko, located on the island of Oahu, Hawaii, was once a vital food producing area, sustaining fishponds and taro fields. Over time, its use shifted from aquaculture to rice and watercress farming before becoming a dumping site for construction debris. Today, a community-led effort integrates native science with western science to revitalize the area and promote food sovereignty. In collaboration with Kuhialoko, University of Hawai?i students and faculty, through the NSF funded Ola I Ka ?Aina project, engage in ?aina (land)-based research while applying statistical methods to monitor the revitalization progress. In summer '23, the project established baseline environmental conditions, deployed a multiparameter sonde for water quality monitoring, and engaged student researchers in data collection. Restoration efforts from fall '23 to spring '25 have focused on removing invasive grasses, mitigating erosion through native plantings, and installing artificial floating islands to improve water quality and biodiversity. Mathematical modeling and quantitative analysis play a key role in monitoring dissolved oxygen (DO) dynamics. Two curriculum-integrated activities"Understanding DO Levels Before and After Invasive Grass Removal" and "Understanding DO Patterns Using Hawaiian Moon Calendar"connect ?aina-based research with statistics, laying the foundation for deeper mathematical modeling of the fishpond as a dynamic system.

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CP19

Contrasting Mathematical Models for Animals Huddling for Warmth

Many species of animals have been observed to huddle for warmth, particularly rat pups and penguins. Both these very different species have been observed to continuously move throughout the huddle so that everyone gets comparable protection from the cold. In this talk, we will present different models for animal huddling and show how their motivations can lead to similar milling behavior, while at the same time yielding strikingly different macroscopic movement patterns. We will showcase physics-inspired models for temperature exchange between animals coupled with models for their movement and discuss why animals may have evolved to have this behavior.

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CP20

Dynamic Behavior under a Diffusion-Ratio Limit in a Generalized Free-Interfacial Combustion Model

We consider a free-interfacial mathematical model of solid combustion that involves the ratio a_p of the diffusivity in the burned material to the diffusivity in the unburned material, where $0 < a_p < 1$. For the case in which diffusivities in the reactant and product are equal, we let a_p in this generalized model approach 1. On the other hand, the case of negligible heat diffusion in the product can be described with a one-sided free-boundary model. The results of asymptotic and numerical analyses on such a model are reported in [L. K. Gross and J. Yu, SIAM J. Appl. Math., 65 (2005), pp. 17081725]. In the present work, we show that in the limit as a_p approaches 0, the weakly nonlinear behavior of the generalized model does not quantitatively match the behavior of the one-sided model. Similar phenomena can be observed in Stefan models and in fluid dynamics. We provide evidence and illustrations of the expected discrepancies, both asymptotically and numerically.

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CP20

Opinion Dynamics with Continuous Age Structure

We extend a classical model of continuous opinion formation to explicitly include an age-structured population, considering both an individual level stochastic differential equation (SDE) model and a mean-field partial differential equation (PDE) model. The inclusion of ageing, births, and deaths allows new effects to be observed, such as: changing opinion variance across ages; the emergence of new opinion clusters; a moving consensus; and periodic combinations and re-emergences of clusters. We rigorously prove the existence of stationary states in the PDE model and discuss their (non)uniqueness, as well as demonstrating several connections between this and other existing models.

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CP20

Higher-Order Network Structure Inference: A Topological Approach to Threshold Selection

The proliferation of large-scale relational data presents challenges in identifying essential network properties, and as such, methods to threshold or remove nodes and concepts are becoming more prevalent. Existing network thresholding methods often neglect higher-order interactions, potentially leading to incomplete representations of relations among the data. We introduce a new thresholding algorithm which uses methods from topological data analysis to identify locally optimal threshold parameters in a given domain. Leveraging persistent homology and linear programming, the procedure computes the stability of a networks homological structure against variations over the parameter domain. Further hyperparameters allow the user to require certain structure in the selected network, such as a minimum number of n-dimensional features. The flexibility and power of this approach empower

researchers to tailor thresholding procedures to specific analytical goals, providing a valuable tool for exploring and understanding intricate relationships in large-scale relational data.

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CP20

Endemic Solutions to a Spatiotemporal Sirs Model

In recent years, integrating spatial data into epidemiological models has emerged as a promising approach to deepen our understanding of infectious disease dynamics. Now, five years after the onset of COVID-19, attention has shifted from predicting pandemic outbreaks to exploring whether a global pandemic might transition into an endemic state. In this work, we develop a reaction-diffusion model that captures the interplay between human mobility across space and disease dynamics over time. Beginning with a volumetric SIRS agent-based model, we derive its continuum limit as a coupled system of partial differential equations defined on a two-dimensional spatial domain. Notably, our model suggests the novel possibility of endemic solutions in which dissipated peaks reemerge in different geographical regionsa behavior that contrasts with outcomes from analogous one-dimensional or spatially homogeneous models. Furthermore, this study underscores the potential benefits of applying established numerical and asymptotic techniques for nonlinear PDE analysis to inform future public health decision-making.

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CP20

Traveling Wave Solutions of a Reaction-Diffusion System Modeling Social Outbursts with Police Management Strategies

Despite legal recognition of protest activity, the historical interaction between the government and protesters has been complex. A system of reaction-diffusion equations is introduced to model the interplay between the dynamics of protesters, social tension, and law enforcement. We establish the existence and stability of traveling wave solutions in this system, supported by both theoretical analyses and numerical simulations. This study is motivated by the "wave-like dynamics of rioting activity during the French riots in 2005. Changes in certain parameters cause a qualitative difference in the solution to the system, leading to situations that correspond to different protest management strategies. We delve into the impact of two distinct protest management approaches on the qualitative and semi-quantitative characteristics of the traveling waves.

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CP20

Temporal Pattern Classification of Internet Meme Propagation: A Hybrid Machine Learning Approach

Quantitative analysis of internet memesdigital cultural phenomena that propagate through online networksremains an understudied domain in computational social science. Building upon established research that modeled meme popularity through ordinary differential equations, this study presents a novel machine learning approach to classify and predict meme popularity trajectories. Previous work identified four distinct post-peak patterns: smooth decay, oscillatory decay, plateau, and sustained growth. We significantly expand the empirical foundation by constructing a comprehensive dataset of 2,000+ memes, leveraging Google Trends time-series data. Our methodological framework employs a two-stage machine learning pipeline: first, implementing k-means clustering (k=4) for unsupervised pattern discovery, followed by Support Vector Classification (SVC) for supervised learning. This approach enables both validation of previously identified trajectory patterns and development of a predictive model for meme popularity evolution. The resulting classification model demonstrates robust predictive capabilities, with implications for understanding viral content dynamics in digital ecosystems.

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CP21

Global Dynamics of a Tumor Growth Model with Three Mechanisms

Understanding the emergence of chemotherapy resistance in cancer patients, whether driven by Darwinian evolution, gene expression changes, or the transfer of microvesicles from resistant to sensitive cells, is crucial as it significantly impacts treatment outcomes by promoting the survival and spread of resistant cells. We have developed a mathematical model to describe the evolution of tumor cells that are either sensitive or resistant to chemotherapy and to make it more realistic by including a separate equation for the number of microvesicles. This model accounts for three resistance mechanisms: Darwinian selection, Lamarckian induction, and resistance via microvesicle transfer, simulating infectious spread. Our analysis identifies three key threshold parameters that determine the stability and ex-

istence of different equilibria within the system. We provide a comprehensive description of the global dynamics, including the existence of global attractors depending on these threshold values. In addition, we explore the effects of varying drug concentrations and characterize potential bifurcation sequences that lead to successful treatment or therapeutic failure. Lastly, we identify the factor that exerts the most significant influence on cancer cell growth.

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CP21

Endemicity and Eradication of Diseases In the Presence of Vaccination and Reinfection in a SEIRV Model

The COVID-19 pandemic marked the need for advanced modeling of reinfectious diseases, highlighting challenges in controlling the spread of infectious diseases even amidst vaccination efforts. Hence, we extend the widely studied SEIR framework to simultaneously incorporate vaccination and reinfection, resulting in a novel SEIRV model. This allows us to analyze the impact of reinfection on disease eradication, the control reproduction number R_v, and bifurcations. While analytic forms for endemic equilibria are intractable for this model, making analyzing backward bifurcations challenging, we show that it is possible to prove their existence in general. We also derive an approximation for endemic equilibria and the bifurcation threshold R_v^C (determining when a backward bifurcation occurs), particularly when the vaccine is fully efficient. Additionally, we develop an algorithm to compute R_v^C to arbitrary precision without requiring assumptions about vaccine efficiency. We establish the global asymptotic stability of the disease-free equilibrium, providing insights into herd immunity thresholds, and prove the local asymptotic stability of the endemic equilibrium when $R_v > 1$, under specific conditions. Numerical simulations confirm our results, validating stability conditions and the existence of a bifurcation. These findings provide insights for modeling reinfectious diseases in the presence of vaccination, offering valuable tools for public health decision-making.

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CP21

Virtual Clinical Trial Reveals Significant Clinical Potential of Targeting Tumour-Associated Macrophages and Microglia to Treat Glioblastoma

Glioblastoma is the most aggressive primary brain tumour, with a median survival of fifteen months with treatment. Standard-of-care (SOC) consists of resection, radio- and chemotherapy. Clinical trials involving PD-1 inhibition with nivolumab combined with SOC failed to increase survival. A quantitative understanding of the interactions between the tumour and its immune environment driving treatment outcomes is currently lacking. Ill present a mathematical model of tumour growth that considers CD8+ T cells, pro- and antitumoral tumour-associated macrophages and microglia (TAMs), SOC, and nivolumab. Using our model, we studied five TAM-targeting strategies currently under investigation for solid tumours. Our results show that PD-1 inhibition fails due to a lack of CD8+ T cell recruitment during treatment explained by TAM-driven immunosuppressive mechanisms. Our model predicts that while reducing TAM numbers does not improve prognosis, altering their functions to counter their protumoral properties has the potential to considerably reduce post-treatment tumour burden. In particular, restoring antitumoral TAM phagocytic activity through anti-CD47 treatment in combination with SOC was predicted to nearly eradicate the tumour. By studying time-varying efficacy with the same half-life as the anti-CD47 antibody Hu5F9-G4, our model predicts that repeated dosing of anti-CD47 provides sustained control of tumour growth.

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CP21

Long-Lasting and Slowly Varying Transient Dynamics in Discrete-Time Systems

Mathematical models of ecological and epidemiological systems often focus on asymptotic dynamics, such as equilibria and periodic orbits. However, many systems exhibit long transient behaviors where certain variables of interest remain in a slowly evolving state for an extended period before undergoing rapid change. These transient dynamics can have significant implications for population persistence, disease outbreaks, and ecosystem stability. In this work, we analyze long-lasting and slowly varying transient dynamics in discrete-time systems. We extend previous theoretical frameworks by identifying conditions under which an observable of the system can exhibit prolonged transients and derive criteria for characterizing these dynamics. Our results show that specific points in the state space, analogous to transient centers in continuous-time systems, can generate and sustain long transients in discrete-time models. We further demonstrate how these properties manifest in predator-prey models and epidemiological systems, particularly in contexts where populations or disease prevalence remain low for an extended period before experiencing a sudden shift. These findings provide a foundation for understanding and predicting long transients in discrete-time ecological and epidemiological models.

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CP22

Primal Necessary Conditions for Weak Minima for Inequality-Constrained Multiobjective Optimization Problems with Locally Lipschitz Data

In this talk we deal with a multiobjective optimization problem (P) with inequality constraints. All the functions involved are assumed to be locally Lipschitz on an open set of a Banach space. The goal of the talk is to provide primal second-order necessary conditions for the existence of a local weak minimum for the nonsmooth multiobjective optimization problem (P). Our conditions make use of Zingwill Second-Order Constraint Qualification and are formulated in terms of generalized derivatives. We do not suppose any kind of differentiability of any order of the objective and inequality constraint functions. Our results are compared to the existing ones. Some examples are discussed.

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CP22

Low-Rank Gradient Flow a First Order Algorithm for Non-Convex Optimization

We introduce a novel class of first-order methods for unconstrained optimization, termed Low-Rank Gradient Flows (LRGFs). The primary innovation lies in constructing a low-rank quadratic surrogate for the cost function at each optimization step, followed by an analytical solution for the gradient flow on this surrogate model. Each step concludes with a line search along the curve representing the gradient flow, for which a simple formula is readily available. The computational cost per step is comparable to that of nonlinear conjugate gradient algorithms. A distinctive feature of LRGF is its curvilinear line search, which enables it to navigate the cost function's geometry more effectively than traditional methods that rely solely on straight-line searches. This enhanced flexibility allows LRGF to avoid local minima more frequently. For higher-dimensional problems, convergence is further accelerated through a multilevel strategy based on reduced-order models.

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CP22

Time-Inhomogeneous Birth-Death Process-Based Optimal Control for Antibiotic-Induced Resistance Mitigation

Based on published estimates by the Lancet in 2019 [1], antimicrobial resistance (AMR) is a major public health threat of the 21st century. Understanding AMR evolution is critical for mitigating this issue. Mathematical models, particularly Markov chains, have gained considerable attention for understanding this evolution. The resulting analytical and numerical studies not only validate relevant experimental results but also offer insights into the rescue mechanism of an organism in deteriorating environments. However, most existing models assume standing genetic variation or the introduction of a new bacterial strain from an external source and do not consider the possibility of pure drug-induced or random mutation of reference bacterial strains. Thus, we propose a pharmacodynamics-based continuous-time Markov chain considering the emergence of a bacterial strain via random or drug-induced mutations. Particularly, the proposed model is tractable as a generalized birth–death process with immigration. Considering dose-dependent mutation over a fixed treatment duration, informed by the first-passage time of the sensitive wild-type bacteria strain to state zero, we analyze the optimal treatment strategy to minimize *de novo* resistance with low drug concentration. Moreover, we explore the optimal biostatic–biocidal combination therapy to eradicate bacteria.

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CP22

Fast Optimization for an Airborne Array Towards Power Maximization with Dynamic Nulls

We explore optimization techniques and antenna synthesis strategies for real time low-frequency beamforming and interference nulling with an airborne antenna array. The focus is on utilizing the airborne network as a relay to transmit around attenuating obstacles, such as forests, with the goal of outperforming a direct link. Unlike traditional antenna design, where alignment accuracy of elements and mechanical tolerances are carefully accounted for, this airborne network is naturally sensitive to tilting and position errors due to environmental factors so we must account for this in our optimization.

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CP22

Unifying Trust-Region Algorithms with Adaptive Sampling for Nonconvex Stochastic Optimization

Continuous simulation optimization is challenging due to its derivative-free and often nonconvex noisy setting. Trust-region methods have proven remarkable robustness for this class of problems. Each iteration of a trust-region method involves constructing a local model via interpolation or regression within a neighborhood of the current best solution that helps verify sufficient reduction in the function estimate when determining the next iterate. When the local model approximates the function well, larger neighborhoods are advantageous for faster progress. Conversely, unsuccessful approximations can be corrected by contracting the neighborhood. Traditional trust-region methods can be slowed down by incremental contractions that lead to numerous unnecessary iterations and significant simulation cost towards convergence to a stationary point. We propose a unified regime for adaptive sampling trust-region optimization (ASTRO) that can enjoy faster convergence in both iteration count and sampling effort by employing quadratic regularization and dynamically adjusting the trust-region size based on gradient estimates. This unification with other regularization frameworks enables almost sure $\mathcal{O}(\epsilon^{-1.5})$ iteration complexity and $\tilde{\mathcal{O}}(\epsilon^{-4.5})$ sample complexity compared with the state-of-the-art $\mathcal{O}(\epsilon^{-2})$ and $\tilde{\mathcal{O}}(\epsilon^{-6})$, respectively.

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CP23

A Well-Balanced Low Mach Solver for Atmospheric Flows

We consider numerical methods for the dynamical core in numerical weather prediction (NWP). Thus, we are interested in schemes for the Euler equations at low Mach numbers with a gravity source term. Currently, the trend in NWP is to increase the resolution. Thus, high order Discontinuous Galerkin (DG) methods are competitive, and also well suited for High Performance Computing due to their high arithmetic intensity. Due to stiffness, implicit discretizations are needed. The design goal is thus a suitable highly parallel stable implicit DG implementation. To deal with the gravitational source term, a well-balanced method is needed. Additionally, one wants a numerical flux suitable for low Mach numbers, and some form of nonlinear stability such as entropy stability. DG methods that have each of these properties individually have been suggested, but so far, a method with all of these properties simultaneously is missing. Currently, Environment and Climate Change Canada (ECCC) is doing a redesign of their dynamical core along these lines in the code WxFactory. We present the implementation of a well-balanced DG method suitable for low Mach numbers and provide numerical results showing the performance on atmospheric test cases.

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CP23

Shocks Without Shock-Capturing: Extreme Scale Solutions to the Compressible Navier-Stokes Equations Via Inviscid Geometric Regularization

Shock waves require bespoke treatments in the numerical simulation of compressible flows. Inviscid flows give rise to singularities, precluding the existence of strong solutions of the PDE. Instead, solutions of the compressible Euler equations are defined as vanishing viscosity limits of viscous regularizations like the Navier-Stokes equation. Any physical fluid has some amount of viscosity. However, if the resulting shock width is smaller than the mesh width, it is prone to cause Gibbs oscillations and instabilities in numerical methods. This forces a choice between excessive computational cost due to large computational meshes and excessive energy dissipation due to artificially large viscosity. This work relies upon information-geometric regularization (IGR), which now enables the use of standard numerics that solve the flow equations without numerical dis-

sipation. Example simulations demonstrate a capability to reproduce shock relations while maintaining fine-scale flow structures faithfully. Extreme-scale simulations are postulated and, in part, shown. Such simulations were otherwise out of reach due to the memory footprint, computational cost, and numerical accuracy of traditional shock-capturing methods for the otherwise same physical problem.

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CP23

Small-Scale Anisotropy in Large Eddy Simulations of Atmospheric Turbulences

Understanding the isotropy of kinetic energy dissipation is critical to accurately modeling atmospheric turbulence. The atmosphere is turbulent and multi-scale, and numerical models cannot resolve the smallest scales of turbulence, so large eddy simulation (LES) must parameterize them. This research investigates the isotropy of the eddy dissipation in LES of atmospheric turbulence. We use the Weather Research and Forecasting (WRF), which is a numerical model that solves the equations of motion for atmospheric dynamics. For this analysis, three cases were conducted: (1) a canonical convective boundary layer case with surface heating, (2) a localized plume driven by a circular heat source on the ground, and (3) a shear-driven simulation with a hyperbolic tangent potential temperature profile for the initial condition, triggered by a hot bubble in the center of the domain. Metrics derived from energy dissipation rates were used to analyze the test cases and quantify the anisotropy. These results clarify the limitations and strengths of the LES in simulating atmosphere turbulence. In addition, the dependence on resolution simulation as the smaller-scale turbulence is resolved was investigated.

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CP23

Shocks Without Shock-Capturing: An Inviscid Information Geometric Regularization

Shock waves in high-speed gas dynamics cause severe numerical challenges for classical and learning-based solvers. This talk begins with the observation that shock formation arises from the flow map reaching the boundary of the manifold of diffeomorphisms. We modify its geometry such that geodesics approach but never reach the boundary. The resulting information geometric regularization (IGR) has smooth solutions while avoiding the excessive dissipation of viscous regularizations, accelerating and simplifying the simulation of flows with shocks. We prove the existence of global strong IGR solutions in the unidimensional pressureless case and illustrate its practical utility on multidimensional examples with complex shock interactions.The modified geometry of the diffeomorphism manifold is the information geometry of the mass density. It is thus the starting point of information geometric mechanics that views the solutions of continuum mechanical PDEs as parameters of probability distributions originating from statistical physics.

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CP23

Unsteady Perturbation Solutions of 2D Anisotropic Boussinesq Systems in a Periodic Domain

This talk presents some unsteady solutions of the perturbed anisotropic Boussinesq system in a two dimensional periodic domain. In this Boussinesq system, the velocity has only the horizonal diffusion and the temperature has only the vertical diffusion. This corresponds to the Geophysical Reynolds-Averaged Navier-Stokes Equations, where the horizontal turbulent viscosity is far larger than the vertical turbulent viscosity. This work focuses on the perturbation around a particular solution with zero velocity and a linear temperature profile in the vertical coordinate. Some mathematical analysis has been performed to derive the stable steady state solutions of the perturbation system with thermal stratification. In contrast, this work presents some unsteady perturbation solution using numerical simulations, including periodic perturbation solutions in time.

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CP24

Stabilized Finite Element Methods for Steady Flows in Porous Media

This study investigates the complex fluid flow dynamics through microscopic rock pores, particularly in challenging subsurface reservoirs with limited natural flow. The Brinkman equations are a fundamental framework for modeling flow in porous media. Using these equations, we analyze fluid behavior in micro-layered rock structures. To ensure numerical stability, we propose a mixed formulation augmented by the rate of deformation tensor. We develop stabilized finite element methods to address the incompatibility of finite element spaces. Theoretical analysis explores key properties such as coercivity and continuity, offering error estimates to establish robustness. These methods align with mathematical analysis in achieving convergence rates by incorporating stabilization terms, even when using low-order basis functions. Additionally, the methods are extended to simulate pore-scale flow in porous media, with numerical experiments validating their accuracy and effectiveness. Remarkably, as inlet velocity increases, a substantial amplification in the average pressure difference is observed, surpassing predictions made by the Stokes equa-

tion.

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CP24

A Theory and Data Integrated Method for Inertial Microcavitation Rheometry in Soft Materials

Inertial Microcavitation Rheometry (IMR) can characterize soft, tissue-like materials in the ultra-high-strain-rate regime. Characterization involves comparing laser-induced cavitation experimental bubble radius histories to forward numerical simulations of Rayleigh-Plesset-type equations. We propose a unified framework that integrates recent theoretical and data-driven advances into a sequential approach. First, we use a parsimonious IMR technique that relies on the first bubble collapse time to obtain an initial selection of constitutive material models and associated parameter(s). Then, using the initial selection, a Bayesian model selection approach is used to inform the prior distributions for the models and their parameter spaces. The Bayesian approach determines the most descriptive constitutive model of the experimental data, estimates its parameter values, and quantifies uncertainty. Data assimilation is then used to obtain a refined parameter range. During the meeting, we will also compare the proposed method to the original IMR to evaluate its capability for in situ material characterization.

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CP25

From Pinns to Penns: Hybrid, Physics-Embedded Neural Networks for PDEs

We present a Physics-Embedded model, which combines the Physics-Informed framework and traditional numerical operators such as the finite element method, to solve Partial Differential Equations. This innovative approach allows the strong imposition of Dirichlet boundary conditions in a seamless manner, and it unables the resolution of complex, non-analytical problems without the need for training data. Our hybrid model relies on numerical differentiation, and we derive an efficient numerical gradient kernel based on Finite Element approximation. We demonstrate that this numerical gradient is up to two orders of magnitude faster than automatic differentiation, since its numerical cost is independent of the complexity of the trained model. After a mathematical and numerical discussion on the improvements of our hybrid approach compared to automatic differentiation-based PINNs, we apply this framework to several academic benchmarks, demonstrating its accuracy and its numerical efficiency. Finally, we apply our Physics-Embedded model for a three-dimensional solid mechanics case on a challenging geometry, thus demonstrating the extended ability of our hybrid approach compared to conventional PINNs.

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CP25

Fast Ai-Based Algorithm for Routing Robotic Wheelchairs in Obstacle-Rich Environments

The PRM, an AI-based algorithm, has proven to be highly effective in solving robotic routing problems with numerous obstacles. Notably, PRM can be successfully applied to robotic autonomous wheelchairs. When equipped with sensors, navigators, on-board computers and smart algorithms, such wheelchairs can operate autonomously, helping people with disabilities avoid obstacles and follow optimal paths. However, when faced with densely crowded areas, the PRM often suffers from excessive computation time and produces suboptimal solutions. To address these limitations, we present an improved algorithm that combines the strengths of PRM and A*, and offers notable improvements in computation time, convergence speed, and path length compared to existing methods. The key innovation is the algorithms adaptability to dense environments. Namely, when encountering obstacles, the algorithm leverages A*s predictive power by looking ahead, choosing the least crowded direction, and identifying detour options in less crowded sub-areas, rather than processing each obstacle individually and processing the entire large map. This approach allows the robot to update its path in real-time, ensuring faster and obstacle-avoiding navigation. Experimental validation was conducted using real data and simulated maps. The results demonstrated the algorithms effectiveness and practicality, especially in obstacle-rich environments, both randomized and realistic.

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CP25

Hybrid Neural-Eta Method for Solving Oscillatory ODEs and PDEs

This work introduces a novel approach in scientific machine learning for solving ordinary and partial differential equations (ODEs and PDEs) in dynamical systems. By leveraging neural networks and Eta-based functions, the proposed method assumes solutions can be represented as weighted sums of these functions. The weights, optimized using backpropagation, are part of the neural network and minimize the residuals of the system's equations. The neural network input incorporates values of Eta-based functions at randomly selected points, which are iteratively updated to adapt to the systems dynamics. To enhance accuracy, the method dynamically adjusts these points and the Eta-based function frequencies. This innovative approach harnesses advancements in computational power, neural networks, and statistical learning to efficiently address complex ODEs and PDEs. Numerical examples showcase its effectiveness, demonstrating its potential for applications across scientific and engineering disciplines.

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CP25

Consensus-Based Bi-Level Optimization: On An Endeavor Between Federated Learning, Stochastic Interacting Particle Systems, Optimization, and Robustness

Bi-level optimization problems, where one wishes to find the global minimizer of an upper-level objective over the globally optimal solution set of a lower-level objective, arise in a variety of scenarios throughout science and engineering and machine learning. In this talk, we discuss consensus-based bi-level optimization (CB^2O), a multi-particle metaheuristic derivative-free optimization method designed to solve nonconvex bi-level optimization problems. Our method leverages within the computation of the consensus point a carefully designed particle selection principle implemented through a suitable choice of a quantile on the level of the lower-level objective, together with a Laplace principle-type approximation w.r.t. the upper-level objective. We give an existence proof of solutions to a corresponding mean-field dynamics, for which we in particular establish the stability of our consensus point w.r.t. a combination of Wasserstein and L^2 perturbations. For such solution, we provide a global convergence analysis in mean-field law showing that the solution of the associated nonlinear nonlocal Fokker-Planck equation converges exponentially fast to the unique solution of the bi-level optimization problem. The practicability and efficiency of our CB^2O algorithm is demonstrated through extensive numerical experiments in the settings of constrained global optimization, sparse representation learning, and robust (clustered) federated learning in adversarial settings.

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CP26

Exponential Decay in a Delayed Wave Equation with Variable Coefficient

In this talk, we consider a wave equation that incorporates strong damping and a time delay term, both with weighted coefficients. Previous studies, such as *[S. Nicaise, C. Pignotti, Stability and instability results of the wave equation with a delay term in the boundary or internal feedbacks, SIAM J. Control Optim., 45 (2006)]*, have established exponential stability under the condition that the weight of the damping (or strong damping) dominates the weight of the delay term. This idea has also been extended to cases involving weighted coefficients, as demonstrated by *[A. Benaissa, S. Messaoudi, A. Benguessoum, Energy decay of solutions for a wave equation with a constant weak delay and a weak internal feedback, Electron. J. Qual. Theo., (2014)]*. Our study introduces a new perspective: we achieve exponential stability and, remarkably, identify scenarios where the delayed term does not need to be dominated by the damping term, yet the system remains exponentially stable. A numerical example will be presented validating our result.

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CP26

Solving Scalar Hyperbolic Conservation Laws on 2D Manifolds with analysis of Flux Induced Foliation

We present a formulation for solving scalar hyperbolic conservation laws on 2D manifolds with co-dimension one, focusing on problems that involve discontinuous solutions such as Burgers' equation, traffic flow problem and Buckley-Leverett equation. A central aspect of this work is the design of the surface flux divergence to satisfy the geometric conservation (GC) condition through a specified flux directional vector $\vec{\boldsymbol{V}}$ and the detailed analysis of the flow dynamics via the characteristic foliation induced by such vector. The surface PDEs is solved numer-

ically using a cp-WENO scheme, which couples the Closest Point Method (CPM) with a nonlinear Weighted Essentially Non-Oscillatory (WENO) finite difference framework. Numerical results show that the proposed formulation accurately captures discontinuities and effectively handles shock-dominated solutions, highlighting its robustness and potential for broader applications in computations on manifolds.

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CP26

Self-Similar Vortical Flows

Vortex spirals and vortex cusps are important features of self-similar vortical flows near stagnation points. Vortex sheets produced at triple points of Mach reflection have distinguished signs that determine whether interaction with walls or symmetry axes can be attached cusps or detached jets. Progress on analysis, modelling and numerics for such phenomena is discussed, along with applications to shock reflection or non-uniqueness of vortical flows.

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CP27

Raking Methods and Applications to Health Metrics

Raking is widely used in survey inference to adjust the observations in contingency tables to the given marginals. We propose a statistical approach, and a corresponding optimization algorithm, that is able to handle uncertain observations and margins and results in an efficient uncertainty quantification of the posterior (raked) estimates. Empirical results show that the approach obtains, at the cost of a single solve, nearly the same uncertainty estimates as computationally intensive Monte Carlo techniques that pass thousands of observed and of marginal samples through the entire raking process. In many real situations, prior information in the form of ordinal constraints is available, and the adjusted observations table after raking must satisfy these constraints in order to be interpretable. We also propose a modified raking method that allows ordinal constraints and has nearly the same running time as the conventional raking method. We illustrate the proposed approach on mortality rate data.

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CP27

Numerical Methods for Distributed Delay Differential Equations Including Random Parameters

We consider systems of delay differential equations (DDEs) with a distributed delay, where physical parameters are replaced by random variables to perform an uncertainty quantification. Hence the solution of a system of DDEs becomes a random process. We expand the random process in the generalized polynomial chaos, which implies a series including unknown coefficient functions and predetermined orthogonal basis polynomials. The coefficient functions can be computed by either a stochastic Galerkin method or a stochastic collocation method. We apply the stochastic Galerkin approach, which yields a larger coupled system of DDEs with distributed delay satisfied by the coefficient functions. Consequently, we investigate the properties of the stochastic Galerkin system. Now methods for initial value problems of differential equations with distributed delay have to be used. On the one hand, an equivalent system consisting of ordinary differential equations or DDEs with discrete delays is available in the case of several traditional distributions. On the other hand, the integrals defining the distributed delay can be discretized by a quadrature formula, where a system of DDEs with discrete delays has to be solved. We present results of numerical computations using a test example.

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CP27

Zig-Zag Sampling for Bayesian Inference in Parametric PDEs

Bayesian inference provides a rigorous framework for quantifying uncertainty in models governed by partial differential equations (PDEs), which arise in many applied fields such as solid mechanics, fluid dynamics, and geophysics. A significant challenge in these problems is the high dimensionality induced by spatially distributed parameters modeled as random fields whose inference typically demands a prohibitive number of forward model evaluations when using standard Markov chain Monte Carlo (MCMC) techniques. In this work, we explore the use of the Zig-Zag sampler, a non-reversible Markov process with linear deterministic dynamics, as an efficient alternative for sampling the posterior distribution in high-dimensional, non-linear Bayesian inverse problems constrained by PDEs. The Zig-Zag sampler has excellent properties in theory its application to non-linear inverse problems is complicated by the requirement of a global upper bound on the gradient of the posterior distribution a quantity that is usually not available. To overcome this limitation, we introduce a surrogate model to approximate the posterior gradient, thereby enabling a global estimation of the necessary bound. Any bias introduced by the surrogate is controlled through a Pois-

son thinning procedure, which corrects the dynamics of the approximate process. Our numerical experiments demonstrate that the Zig-Zag sampler more efficiently achieves a target accuracy than traditional MCMC approaches.

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CP28

Optimized Schwarz Methods in Time for Discrete Transport Control

Control problems in which the underlying systems are governed by hyperbolic partial differential equations (PDEs) arise in many applications, such as inverse problems and data assimilation. The numerical solution of such problems is challenging for two different reasons. First, the intensive computations required to simulate hyperbolic phenomena to a high resolution inside the optimization loop means that one must use scalable and efficient solvers that can take advantage of modern parallel architecutres. Second, once the hyperbolic PDE is discretized, numerical dispersion fundamentally changes the behaviour of the problem; thus, iterative algorithms applied to the discrete model behave very differently from what can be predicted based on properties of the continuous problem. In this talk, we present an optimized Schwarz method for solving the transport equation, where we subdivide the time horizon into several sub-intervals and solve the resulting sub-interval control problems in parallel. We prove that for a good choice of parameters, our method converges to the exact solution in a finite number of iterations when applied to the PDE the continuous setting. However, this is no longer true for the discretized PDE; moreover, the best parameter for fast convergence changes depending on whether relaxation is used, and whether the iteration is accelerated by a Krylov subspace method. Numerical examples are presented to illustrate this behaviour.

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CP28

Nonlinear Preconditioning for the Phase-Field Fracture Model

The phase-field fracture model is a variational formulation of quasi-static crack evolution in brittle material. The model is not globally convex, but there is a natural splitting of the variables into two convex subproblems which may be solved sequentially. This is referred to as alternate minimization. Recent work [A. Kopanicakova, H. Kothari, R. Krause, Nonlinear field-split preconditioners for solving monolithic phase-field models of brittle fracture, 2023] has equated this to a multiplicative Schwarz preconditioner and combined it with an inexact Newton step to improve efficiency. This talk examines attempts to replicate these results, generalize them with alternatives to the Newton step, and apply them to real world examples.

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CP28

Numerical Approximation of P-Laplace Eigenpairs

We approximate eigenpairs of the p-Laplace operator with zero Dirichlet boundary conditions using a finite element method. In this talk we will discuss the $p \to \infty$ limit and its connection to the underlying geometry of our domain. Working with large p values presents numerical challenges which require careful treatment. We present computational results in 1D, planar domains, and surfaces lying in $\mathbb{R}^3$.

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CP28

On the Numerical Solution of Initial-Boundary Value Problem To One Nonlinear Parabolic Equation

Investigations of some diffusion models bring us to the following initial-boundary value problem to nonlinear parabolic equation:

$$U_t = (k(x,\ t,\ U)\,U_x)_x + f(x,\ t,\ U,\ U_x), \quad (x,\ t) \in \Omega \times (0,\ T],$$

$$U(x,\ 0) = \varphi(x), \quad x \in \bar{\Omega},$$

$$U(0,\ t) = \phi_0(t), \quad U(1,\ t) = \phi_1(t), \quad t \in (0,\ T],$$

where $U = U(x,\ t)$ is unknown function, k, f, φ, ϕ_0 and ϕ_1 are given functions, $T = const > 0$, $\Omega = (0,\ 1)$. To this problem we construct the difference analogue, for which under some restrictions on functions k, f, φ, ϕ_0 and ϕ_1 we prove the theorems of existence and uniqueness of the solution. Also, for the difference analogue we construct the iteration scheme and prove convergence of the iteration scheme to the solution of the difference analogue. If solution U of the source problem is smooth enough, we also prove the convergence of the solution of the difference analogue to the solution of the source problem.

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CP29

Synthetic Method of Analogues for Emerging Infectious Disease Forecasting

The Method of Analogues (MOA) has gained popularity in infectious disease forecasting due to its non-parametric nature. MOA matches local behaviors in a time series to historical data, using subsequent values from the best matches

to generate forecasts. This approach avoids heavily parameterized models that may misrepresent disease dynamics. However, MOA is limited when historical data is sparse, as seen in the early COVID-19 pandemic. We propose the Synthetic Method of Analogues (sMOA), which replaces historical data with a library of synthetic disease trajectories. This circumvents the need for explicit parameter estimation by matching ongoing time series data to a comprehensive library of synthetic segments for both counts and deaths. Focusing on counts, we demonstrate that sMOA achieves competitive performance, outperforming 75% of models from the COVID-19 Forecasting Hub. Furthermore, we extend sMOA to forecast both counts and deaths, exploring whether leveraging their relationship enhances predictive accuracy. By adopting this bivariate approach, we aim to improve sMOA's utility in public health decision-making. Developing forecasting methods that do not rely on historical data while maintaining accuracy during novel pandemics is crucial for strengthening preparedness and response.

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CP29

Improving Cancer Immunotherapy Outcomes Through Mechanistic Digital Twin Models

Our mechanistic mathematical models have demonstrated marked success in describing robust relationships that link measurable clinical data with the key factors involved in cancer progression and therapeutic response to study why immune checkpoint inhibitor (ICI) immunotherapy succeeds or fails on an individual patient basis. We have now extended our previous model to study the differences between tumors that have delayed response by imaging and those that never respond. These are only distinguishable retrospectively in the clinic, which can lead to incorrect treatment decisions or cause costly delay in treatment adaptation. The new model describes a more diverse range of tumor response patterns by including sensitive and resistant tumor cell populations, key aspects of the distinct interactions and feedback each population has with immune cells, and resulting changes in phenotypic distributions within the tumor over time. However, some readily available clinical measures that likely associate with outcomes are not easily included into mechanistic equations. Solving this new model using physics-informed neural networks on data from an in-house patient cohort treated with ICI enables us to include this additional data, improving predictive accuracy while retaining mechanistic explanations of outcomes. We are using this innovative approach to study the differences between tumor responses with more nuances to facilitate timely and informed treatment decisions.

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CP29

Mathematical Modelling and Analysis of the Dynamics of Host-Reservoir Transmission of Ebola

We develop in this work, a mathematical model to assess the impact of the reservoir on the dynamics of Ebola virus disease (EVD). Our model couples a human-to-human model with a bat-to-bat model and the indirect environmental contamination through a spillover process (that is. process by which a zoonotic pathogen moves from an animal host (or environmental reservoir) to a human host) from bats to humans. The coupled models and the submodels exhibit each a threshold behaviour with the associated basic reproduction numbers being the bifurcation parameters. The existence of equilibria and their global stability are established by combining graph theory. LyapunovLaSalle techniques and monotone operator theory. Control strategies are evaluated by using the target reproduction numbers. The spillover event is proved to be highly detrimental to EVD by allowing the disease to veer from bats to humans even though the disease was not initially endemic in the human population. The efforts required to control EVD are assessed through S-control. Precisely, we show that the spillover effect contributes to boost the disease outbreak. This propones that the consumption and manipulation of fruit-bats play a major role in sustaining EVD in a given community.

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CP29

Bayesian Parameterization of Coupled Behaviour Disease Model(s)

Mathematical models have been widely used to understand the dynamics of diseases from infectious diseases to oncology. Many infectious disease models have generally helped to understand the behaviour of diseases and subsequently in making predictions. However, recent data shows that

the dynamics of these diseases are influenced by the behaviour of the host population. With evidence of imitation dynamics amongst the host population affecting the transmission of the disease. This work establishes that coupled behaviour-disease models give more information about the disease and improve the predictive power(s) of the models. We illustrate this concept by applying a formulated coupled behaviour-disease model for the first year of the COVID-19 virus from selected countries and cities while parameter estimation is performed using an Approximate Bayesian Computation (ABC) approach. We examine the predictive power of a conventional deterministic SIR model and a coupled behaviour-disease model which takes into account the seasonality of the COVID-19 virus. Using an adjusted AIC statistical measure for model performance, we obtained a similar performance for both models with respect to fitting but observe the coupled model outperformed the disease model in forecasting. Also, the peak magnitude and duration for the second peak within the prediction period had the coupled model match closely with the data unlike the disease model.

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CP29

Mathematical Models of Synchrony: From External Forcing to Stage-Structure

Synchrony in life history events among individuals is widespread in ecological and evolutionary systems, manifesting in masting reproduction, swarm colonization, and coordinated attacks. This talk focuses on seed mastingsynchronized, intermittent reproductionas a key example of such coordinated behaviour. I begin by exploring multiple mechanisms for creating event synchrony in natural populations, including external environmental forcing to age-specific density-dependent population growth. The latter is an ecological model inspired by synchrony observed in epidemiology models with recurrent outbreaks. This approach inherently generates synchrony (cycles). We show that the dynamics of this system undergo a bifurcation: when competition is high, and juveniles and adults undergo a low number of progressive stages, the system exhibits a stable endemic equilibrium with transient cycles. As parameters cross a critical threshold, the equilibrium becomes unstable, giving rise to stable limit cycles and robust population-level synchrony. This transition provides an endogenous mechanism for periodic reproductive bursts. Using these synchronous ecological models, we explore the implications for masting's evolutionary drivers, including predator satiation and pathogen escape. We show that masting is largely selectively neutral, indicating that current evolutionary hypotheses must be expanded to explain the initial emergence of synchronous reproduction.

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CP30

Determining Climate Risks with NASA Earthdata Cloud

Predicting and managing environmental risks of various climate-related disasters (e.g., wildfires, drought, and floods) is challenging and critical worldwide. These natural risks are intrinsically linked to the dynamic spatial and temporal distributions of surface water, precipitation, vegetation, and land use. These distributions can be modelled for forecasting and analysis (enabling quantification of environmental risks) using hundreds of petabytes of relevant Earth science data available through the NASA Earthdata Cloud. This presentation walks through analyses of climate risk scenarios (e.g., floods and wildfires) facilitated by geospatial data products from NASA's Earthdata Cloud. The case studies—co-developed by 2i2c and MetaDocencia—highlight the interplay of distributed data with scalable numerical strategies ("data-proximate computing") implemented using scientific Python libraries (e.g., NumPy, Pandas, Xarray, etc.). Computationally, the scenarios rely on constructing quantitative estimates of changes in hydrological water mass balance over various defined regions of interest. This presentation provides an overview of publically available tutorial materials co-developed by 2i2c and MetaDocencia as part of NASA's Open Science initiatives to reinforce principles of Open Science and reproducibility.

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CP30

On the Vulnerability of Boreal Forest Ecosystems to Climate Change: a Hybrid Modelling Approach

In this contributed lecture, I will present recent results and perspectives of a research project on the vulnerability of the boreal forest to extreme events arising from climate change. The biological evolution of the forest is modeled by a reaction-diffusion system with hysteresis admitting remarkable nonlinear dynamics, since it does not possess the global attractor, although it presents an infinite number of heterogeneous stationary solutions that weakly attract very particular trajectories. Under the effect of a small perturbation of the hysteresis process, the heterogeneous stationary solutions are proved to bifurcate towards discontinuous patterns admitting two discontinuity jumps. The continuous dynamics of the forest are then coupled with a discrete probabilistic process reproducing the impacts of megafires. The resulting hybrid model exhibits rich dynamics, which help better understand the ecological transitions of the boreal forest. The model is calibrated by confrontation with paleoecology data produced in the province of Qubec, Canada, in order to experiment various scenarios of forest migration, depending on the intensity of the perturbation of its environment. This research is supported by the Institute of Mathematics for Planet Earth of the French National Centre for the Scientific Research and by the French National Research Agency (TOUNDRA project, ANR-24-CE56-3042).

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CP30

Bifurcations in a Coupled Delayed Action Oscillator Model of the El Nio Southern Oscillation

Drastic fluctuations in sea-surface temperature (SST) may cause massive rainfall which causes severe floods, as well as extreme drought which increases the occurrence of forest fires. In 1988, Suarez and Schopf introduced the delayed-

action oscillator (DAO) model to describe the irregular fluctuations of the SST on a region in the central equatorial Pacific that has a strong ocean-atmosphere coupling. Their model incorporates the effects of oceanic wave transit and helps to explain the El Nio-Southern Oscillation (ENSO) phenomenon. In 2007, Boutle et al. studied the influence of the annual cycle, global warming, and stochasticity in the DAO model. In the same study, a model of a coupled DAO was introduced which describes the scenario where there are two coupled regions along the equatorial Pacific with strong ocean-atmosphere coupling. Numerical simulations show that the behavior obtained from the coupled DAO is more similar to that of the El Nio than the behavior from the single DAO. In this work, we revisit the coupled DAO model and explain why it is better at describing the fluctuations in SST. Moreover, we examine the different limit-cycle solutions to the coupled DAO model and their bifurcations.

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CP30

Modelling Climate and Morphology Drivers of Wetland Methane Emissions

Wetlands are characterised by the interaction of soil with seasonal or permanent water bodies and serve a crucial role in water filtration, flood prevention and support of diverse ecosystems. However, their ability to sequester and store carbon also secures their place as the largest natural source of methane emissions. These emissions are strongly dependent on the relative depth of the water body to the soil, with submerged soil providing the anaerobic conditions favourable to methanogenesis and detrimental to methane consumption. We present a mathematical model to describe the movement of the water table, considering its dynamics at the daily timescale as a balance of stochastic recharge by (Poisson) rainfall events and associated surface run-off from the watershed, with exfiltration, evapotranspiration and groundwater flows. We couple this model to a set of ODEs describing methane production, oxidation and emission, parameterised by this water table depth, and obtain probability distribution functions for annual methane emissions. In search of improved estimates for wetland methane emissions, we consider how the inherent variations in water table depth due to the soil profile leads to changing emission profiles across the wetland. Moreover, we employ our model to explore the influence of different weather conditions, particularly rainfall and temperature, on wetland methane emissions, illustrating how sensitivity to water table depth increases with temperature.

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CP30

Mitigation Across Five Regions in a Coupled Social-Climate Model

We construct and analyze a coupled social-climate model with region-level parameterization, based on forecasts of costs of renewables, climate change impacts, and estimates of the strength of social norms. The first part of our analysis reveals that social learning rates play a significant role in influencing the uptake of mitigation and, therefore, temperature trajectories. We also find that all regions are able to reduce the peak temperature value by increasing learning rates, but in doing so can have contrasting effects on the times at which these peaks occur. The second part of our analysis deals with characterizing the nature of the climate change mitigation game with five regional players. Initial findings suggest that the strategy to mitigate offers a lucrative payoff to all regions, while the incentive to free-ride on others mitigation efforts differs across regions.

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CP30

Innovating with Machine Learning: Science-Driven Solutions for Environmental Challenges

In recent years, the use of machine learning (ML) algorithms has expanded across various disciplines. While these algorithms can yield remarkable results when trained on high-quality, abundant data, they often face significant challenges in fields where data is sparse or difficult to access. Environmental sciences, for instance, presents a unique challenge in this regard, where limited data can render traditional ML models less effective. In this talk, I will emphasize the importance of integrating scientific principles into the development of ML algorithms tailored to environmental challenges. Focusing on two distinct issueswildfire perimeter mapping and monitoring methane emissions from oil sands tailingsI will demonstrate how combining mathematics, biochemistry, lab experiments, diverse data sources, and ML models can provide innovative, real-time solutions. The lecture will explore the scope, framework, and outcomes of these science-driven ML approaches, illustrating their potential to transform environmental monitoring. Specifically, I will show how, in situations where data collection is limited, we can train our models to be smarteracting as powerful tools for emission tracking or even predicting evacuation needs in the event of nearby wildfires.

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CP31

An Optimization Approach to Mitigating Transient and Steady-State Inequalities in Innovation Adoption

Policymakers are concerned about maximizing innovation adoption and minimizing inequality across communities in a population. The challenge is fostering inclusive diffusion while ensuring an equitable distribution, given variations in community income levels. However, achieving both goals simultaneously can be challenging. Early adoption by wealthier individuals, driven by homophily, the tendency to interact with those who share similar traits, and learning through cost-benefit evaluation during interactions with adopters, can exacerbate inequality by concentrating adoption in high-income communities. However, focusing on reducing inequality can slow adoption, giving low-income communities more time to adopt. In both cases, the solution remains sub-optimal. Therefore, we propose an adoption diffusion model to analyze the optimal solution to this min-max problem. The model incorporates willingness, which is a function of the adoption decisions of proximate individuals, and affordability, which is a function of ones income and the innovation price. The interplay between them determines adoption levels, timing, and disparities in transient and steady states. We conduct a sensitivity analysis to demonstrate how homophily and learning shape disparities as feedback mechanisms that influence adoption trajectories. Our findings provide insights for policymakers into intervention strategies to leverage initial adopters to achieve goals simultaneously in a constrained time frame.

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CP31

Stochastic Modeling and Optimization of the Storage Process in the Context of Renewable Energies

Within the European Union, many countries are gradually replacing fossil fuels with renewable energy sources in the electrical power production process. The resulting transformation takes various shapes. Photovoltaic systems, along with batteries play a major role in this development. Batteries are used to store excess power or provide redundancy in case when photovoltaic power is unavailable. This significantly changes the consumers interaction with the public power grid towards bidirectional energy exchange, resulting in new challenges for distribution network operators. We analyze the energy-storage process in a low-voltage network, where households are equipped with photovoltaic systems and batteries. The latter undergo a continuous charging and discharging process. The joint probability distribution of the battery array is of particular interest. Also, we are analyzing ways to optimize the households energy cost (or total energy drawn from the grid) by taking price, feed-in compensation, and weather information into account in order to come up with cost optimal feed-in and consumption policies. The optimization problems make extensive use of the paradigm of Dynamic Programming, as expressed in the well-known Bellman equation. Finally, this game can also be analyzed from the power providers perspective. She/he can ask herself/himself about her/his degrees of freedom in responding to the consumer actions.

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CP31

Portfolio Time Consistency and Utility Weighted Discount Rates

Merton portfolio management problem is studied in this paper within a stochastic volatility, non constant time discount rate, and power utility framework. This problem is time inconsistent and the way out of this predicament is to consider the subgame perfect strategies. The later are characterized through an extended Hamilton Jacobi Bellman (HJB) equation. A fixed point iteration is employed to solve the extended HJB equation. This is done in a two stage approach: in a first step the utility weighted discount rate is introduced and characterized as the fixed point of a certain operator; in the second step the value function is determined through a linear parabolic partial differential equation. Numerical experiments explore the effect of the time discount rate on the subgame perfect and precommitment strategies.

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CP31

Semidefinite Programming and Critical Phenomena

In recent years, revolutionary advances in computational methods have transformed the study of critical phenomena. The critical exponents in models such as the 3D Ising and O(N) vector models have been computed with unprecedented precision using the numerical conformal bootstrap – a method that combines ideas from quantum field theory with advanced numerical optimization. The physics problem translates into an optimization task over a family of SDPs defined on a non-convex parameter space. In our journey to solve challenging physics problems, we have achieved dramatic improvements in the algorithms for these SDPs, which also have applications beyond our field. In this talk, I will review these recent developments and discuss the broader implications of our work.

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CP32

Krylov Methods on Quantum Computers: Chal-

lenges and Opportunities

Recent years have seen major breakthroughs in quantum computing hardware. But even with these advances, the question remains: What will quantum computers be good for, at least in the near-term? One proposal has suggested that quantum analogs of Krylov subspace methods could be used to solve exponentially large eigenvalue problems occurring in chemistry and condensed matter physics. But these quantum Krylov methods have significant downsides, requiring the solution of a highly ill-conditioned generalized eigenvalue problem perturbed by large amounts of noise. This talk provides a mathematical explanation for why, in spite of these limitations, quantum Krylov methods often still produce accurate eigenvalue estimates. The talk will conclude with a discussion of more recent work.

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CP32

Wasserstein Convergence and Bias estimates for Kinetic Langevin Integrators

Underdamped (kinetic) Langevin dynamics is becoming a popular tool for sampling in statistical machine learning and molecular dynamics due to the fact that it has desirable non-asymptotic properties. For some target measure a continuous Langevin diffusion can be constructed to have the target as the invariant measure. In MCMC, Langevin diffusions are discretized to generate samples from the target. The choice of discretization is very important for the quality of the samples. Popular numerical integrators include Euler-Maruyama, BAOAB and the stochastic Euler scheme. The quality of a numerical scheme is measured through its bias and its convergence rate. This talk will focus on a framework to provide Wasserstein convergence rates for many different discretizations from machine learning and molecular dynamics which hold for a large range of stepsizes. We will also discuss the property ?-limit convergent (GLC) to characterize underdamped Langevin schemes that converge to the overdamped dynamics in the high friction limit and which have stepsize restrictions that are independent of the friction parameter; we show that this property is not generic by exhibiting methods from both the class and its complement. We further provide second-order asymptotic bias estimates for the BAOAB scheme, which remain accurate in the high-friction limit by comparing it to modified stochastic dynamics which preserves the invariant measure.

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MS1

Guaranteed Sampling Flexibility for Low-Tubal-Rank Tensor Completion

Tensor completion is an important topic in high-dimensional data analysis, with Bernoulli sampling and t-CUR sampling being two commonly used approaches. While Bernoulli sampling is widely studied, t-CUR sampling targets low-tubal-rank tensors through subtensors, yet both methods lack the adaptability required for many practical scenarios. In this talk, I introduce Tensor Cross-Concentrated Sampling (t-CCS), a novel sampling framework that extends the concept of cross-concentrated sampling from matrices to tensors. By bridging the gap between Bernoulli and t-CUR sampling, t-CCS offers enhanced flexibility and computational efficiency. I will present a sufficient condition for the successful recovery of low-rank tensors using t-CCS samples. Additionally, I will share a theoretical framework validating t-CUR via uniform random sampling and provide a detailed sampling complexity analysis for tensor completion under Bernoulli sampling. To complement the t-CCS framework, I will introduce the Iterative t-CUR Tensor Completion (ITCURTC) algorithm, an efficient non-convex approach designed for t-CCS-based tensor completion. Through extensive experiments on both synthetic and real-world datasets, I will demonstrate the practical effectiveness of the t-CCS model and the ITCURTC algorithm.

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MS1

Application and Evaluation of a New Notion of Discrete Graph Curvature on Real-World Networks

The extension of curvature, which is historically defined in continuous spaces, to discrete objects such as graphs presents new opportunities and challenges for application. In this work, we review recent notions of graph curvature parameterized by different distances on a graph. We explore the relationship between node-level curvature and well-established node-centrality measures on synthetic and real-world graphs in order to better understand their relationship, and what novel information the curvature can reveal about a network. We end with a discussion of outstanding questions and applications.

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MS1

Identification of Paths for Dynamic tTransport via Mean-field Control

The task of sampling from a target probability distribution is fundamental to modern applied mathematics and machine learning. Sampling is the key ingredient in

Monte Carlo methods, enables uncertainty quantification in Bayesian inference, and underlies generative modeling. One sampling approach, which achieves state-of-the-art performance in generative modeling and is receiving growing interest in density-driven sampling as well, is that of dynamic transport (DT): the idea is to evolve samples from a tractable reference distribution (e.g., Gaussian) using an ODE or SDE such that the transformed samples correspond to the desired target distribution. DT induces a path of distributions, corresponding to the distributions of the intermediate states of the dynamics, between the reference and the target, and in some DT approaches it is possible to specify this path explicitly. Understanding of how to choose paths well, however, is lacking, and some commonly used paths can produce "teleportation behavior' that is completely undesirable for transport. In this work we identify suitable paths for dynamic transport via solution of mean-field control problems. We ground our approach in potential mean-field games, which have recently been shown to describe a large number of DT approaches, and carry out the identification of paths computationally via optimal recovery on reproducing Kernel Hilbert space.

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MS1

Towards Equity in Education: A Discussion on Tools in Education Data Mining

Educational data mining and machine learning are useful fields that provide insights in predicting student performance and achievement. Current issues facing researchers in the field of educational data mining include interpretability of prediction models, lack of uniform standards for datasets used for training prediction models, and optimizing algorithms according to the characteristics of educational datasets. By using current machine learning and data mining techniques, along with leveraging large datasets that include data from social mobility (ability of an individual to improve their socioeconomic standing) studies, predictive models can be adapted to provide more interpretable models. A variety of data mining and machine learning techniques, including semi-supervised and active learning algorithms, are explored in this talk.

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MS2

Structured Output Regularization: A Versatile Framework for Efficient Transfer Learning

Traditional transfer learning typically reuses large pretrained networks by freezing their weights and adding task-specific layers. While this approach is computationally efficient, it limits the model's ability to adapt to domain-specific features and can lead to overfitting with very limited data. To address these limitations, we propose Structured Output Regularization (SOR), a simple yet effective strategy that freezes the internal network structures (e.g., convolutional filters) while introducing a single L_1-regularized scaling parameter for each structures output. By allowing these outputs to be adaptively scaled or pruned, our method tailors the model to specific data and can reduce the final model complexity, with minimal additional parameters. On a toy dataset, we demonstrate that SOR can maintain strong transfer performance while significantly reducing model size. Furthermore, we evaluate SOR on three medical imaging classification tasks where data are typically scarce and achieve competitive results using VGG16, DenseNet121, and EfficientNetB4 bases compared to established benchmarks. Our method is easily applicable to various network components, such as convolutional filters, recurrent units and self-attention layers, enabling broad applicability for transfer learning tasks.

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MS2

Automatic Hierarchical Clustering-Based Image Semantic Segmentation for Hyperspectral Fluorescence Images

While hyperspectral imaging is commonly used in geospatial research and in astronomy, it applications for healthcare are emerging. Among multiple imaging modalities, fluorescence microscopic hyperspectral imaging (FMHSI) of unstained biological tissue is a foundational tool in diagnostic pathology and biomedical research, which enables the acquisition of datasets with high spectral and spatial resolutions. Semantic segmentation of FMHSI images is essential for obtaining labelled HSI data. We aim to develop an automatic unsupervised hyperspectral image semantic segmentation approach that produces high-quality segments for high-level vision tasks such as remote disease diagnosis and pathology-assisted surgery. Our multi-step algorithm starts with image denoising and dimension reduction using filtering and superpixels. An automatic hierarchical clustering-based image segmentation method is then applied to create image segments based on the spectral and spatial information. Finally, an adjacent region merging process is performed to refine the segmentation and output the final set of tissue sections. We will open-source the algorithms and develop an application that empowers users to gain deeper insights into the intricacies of FMHSI data. Moreover, the approach and app are promising for enhancing the comprehension and diagnosis of eye diseases, including Spaceflight-Associated Neuro-ocular Syndrome.

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MS2

A Data-Driven Approach for Hyperspectral Image Analysis of Eye Tissues

Biomedical hyperspectral fluorescence imaging is a powerful, noninvasive modality that enables detailed analysis of biological tissues by capturing rich spectral information at each pixel. This technique provides valuable insights into tissue composition and pathology, making it particu-

larly useful for medical diagnostics and research. Our work focuses on leveraging this technology to enhance the understanding of ocular health by accurately segmenting hyperspectral images of key eye structures, including the retina, choroid, sclera, and muscle fibers. To achieve this, we have developed and refined advanced algorithms to optimize hyperspectral fluorescence data analysis, integrating machine learning techniques to improve segmentation accuracy and efficiency. Our method enhances tissue differentiation, reduces reliance on invasive procedures, and enables early detection of ocular abnormalities. Our presentation aims to demonstrate the efficacy of these advancements, thereby contributing to the advancement of biomedical hyperspectral fluorescence imaging research and its implications in ocular health studies.

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MS3

QCLAB: A Matlab Toolbox for Quantum Linear Algebra

We introduce QCLAB, an object-oriented MATLAB toolbox for constructing, representing, and simulating quantum circuits. As quantum computing continues to advance rapidly, access to robust computational tools remains essential while quantum hardware matures. Designed with an emphasis on numerical stability, efficiency, and performance, QCLAB provides a reliable platform for prototyping and testing quantum algorithms. Its seamless MATLAB integration and focus on numerical robustness make it particularly valuable for applications in numerical linear algebra. This talk, featuring a hands-on MATLAB tutorial, introduces both the fundamentals of quantum computing and the core functionalities of QCLAB. To offer concrete insights, we will focus on Quantum Phase Estimation (QPE) - a fundamental quantum algorithm for efficiently determining the eigenvalue (or phase) of an eigenvector of a unitary operator. By not only exploring the theory behind this algorithm but also implementing it with QCLAB, the audience will gain practical experience and be encouraged to engage actively with this exciting research area. With both beginners and experts in mind, this session is designed for researchers looking for an accessible entry point into quantum computing and experienced practitioners seeking a tool for rapid prototyping of quantum algorithms.

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MS3

U(N) Quantum Signal Processing and Infinite-Dimensional Linear Algebra

I will present two recent results on generalizing quantum signal processing (QSP) and singular value transform algorithms to high dimensions. One is a theory of U(N) quantum signal processing and singular value transform with application to optimal amplitude estimation. The second result is on generalization of QSP to hybrid continuous-discrete-variable systems which allows manipulation of an infinite-dimensional system realized by a quantum harmonic oscillator. Applications to quantum state transfer and quantum simulation will be presented.

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MS3

Condensed Matter Physics and Beyond-classical Random Circuit Sampling on an Analog-digital Quantum Simulator

Simulating the dynamics of many-body quantum systems is challenging for classical computers. Exact simulations scale exponentially in both time and memory with the number of particles to be simulated, while methods based on tensor networks (or tensor trains) scale exponentially in the amount of entanglement in the system. On the other hand, quantum dynamics simulations are well-suited to a quantum computer, with costs scaling only polynomially in the number of particles. One particularly promising route in the near term is analog quantum simulation. Instead of using the quantum computer to implement discrete gates (ie discrete linear transformations), one sets up the computer so that its natural behavior as a physical system automatically implements the time evolution (application of $\exp(-iHt)$ for an exponentially large matrix H). In this work, we show new capabilities in quantum simulation that come from combining digital quantum gates with analog evolution. We demonstrate: (a) Accurate calibration of the analog evolution, giving an error per qubit per cycle of less than 0.1%. (b) Approximate adiabatic preparation of the ground state of an interacting many-body quantum system on ~ 70 qubits. (c) Thermalization of states with designed initial energy density profiles. (d) Analog random circuit sampling, showing that the quantum computer can perform in a few minutes a calculation that would take 100 years or more on the world's largest computing clusters.

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MS4

A Hybridizable Discontinuous Galerkin Discretization for the Coupled Navier-Stokes and Biot Equations

In this talk, I will present a numerical analysis of the coupled (Navier-)Stokes equations and Biots equations for poroelasticity in the total pressure formulation, using a hybridizable discontinuous Galerkin method. I will discuss the properties of the method, provide error estimates, and present numerical results from several computational experiments.

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MS4

Higher Order Eikonal Solvers and Their Applications

The nonlinear eikonal equation with a point-source condition arises from many applications, such as ultrasound medical imaging, traveltime tomography, geophysical migration, high-frequency wave simulation, and computer graphics. One essential difficulty for solving the first-order nonlinear equation is how to initialize higher order schemes at the source point. On the one hand, we will review our works on developing high-order factorization based high-order eikonal solvers; on the other hand, we will demonstrate the capabilities of high-order eikonal solvers on tackling some challenging computational issues from high-frequency wave propagation and traveltime tomography.

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MS4

Advances in Numerical Analysis of Coupled Mixed-Dimensional Problems

Mixed-Dimensional coupled problems are characterized by coupled partial differential equations defined over domains of different dimensions. These problems arise in several applications ranging from geosciences to biomedicine, where the domains are porous media with embedded inclusions. These models are computationally efficient thanks to the dimension reduction of the physical problem valid in the inclusions. This talk presents recent advances for the numerical analysis of mixed-dimensional PDEs with co-dimension equal to two. The convergence of a discontinuous Galerkin scheme of arbitrary order is obtained via the derivation of a priori error bounds. The analysis is non-standard because of the low regularity of the weak solution. Numerical examples of flow in an organ and its vasculature are shown.

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MS5

Faster Low-Rank Approximation and Kernel Ridge Regression via the Block-Nystrom Method

The Nystrom method is a popular low-rank approximation technique for large matrices that arise in kernel methods and convex optimization. Yet, when the data exhibits heavy-tailed spectral decay, the effective dimension of the problem often becomes so large that even the Nystrom method may be outside of our computational budget. To address this, we propose Block-Nystrom, an algorithm that injects a block-diagonal structure into the Nystrom method, thereby significantly reducing its computational cost while recovering strong approximation guarantees. We show that Block-Nystrom improves the computational complexity of kernel ridge regression for statistical learning over Hilbert spaces, and it can be used to construct more efficient preconditioners for second-order optimization. Our key technical insight is that, within the same computational budget, combining several smaller Nystrom approximations leads to stronger tail estimates of the input spectrum than using one larger approximation. Along the way, we provide a novel recursive preconditioning scheme for efficiently inverting the Block-Nystrom matrix, and provide new statistical learning bounds for a broad class of approximate kernel ridge regression solvers.

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MS5

Structured Matrix Recovery Via Matrix-Vector Products

In this talk, I will give an overview of recent progress on the problem of structured matrix recovery from matrix-vector products. Given a target matrix A that can only be accessed through a limited number of (possibly adaptively chosen) matrix-vector products, we seek to find a near-optimal approximation to A from some structured matrix class – e.g., a low-rank approximation, a hierarchical low-rank approximation, a sparse or diagonal approximation, etc. This general problem arises across the computational sciences and data science, both in algorithmic applications and, more recently, in scientific machine learning, where it abstracts the problem of operator learning. I will describe recent work, in which we give optimal algorithms for approximating A with a matrix with a fixed sparsity pattern (e.g. a diagonal or block-diagonal matrix), and where we give some of the first algorithms with relative error

bounds for the important problem of hierarchical low-rank approximation from matrix-vector products. Our results are achieved using variants of the well-studied 'peeling' method for hierarchical matrix approximation, and help significantly extend existing understanding of the robustness of this approach.

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MS5

Randomized Kaczmarz Methods with Beyond-Krylov Convergence

I will discuss Kaczmarz++ and CD++, two accelerated randomized block Kaczmarz algorithms for arbitrary (under-, over-determined or square positive semidefinite linear systems) that capture large outlying singular values more efficiently than popular Krylov methods. As a result, these Kaczmarz-based methods achieve fast Krylov-style convergence, successfully competing with the standard methods, especially in the moderate target error regime that naturally arises in a variety of applications, including machine learning applications. These solvers unify the Kaczmarz/sketch-and-project framework and its recently developed sharp rate analysis, with classical numerical analysis approaches – such as adaptive momentum acceleration, Tikhonov-regularized projections, and a memoization scheme – to handle both generic and positive semi-definite systems efficiently. One of my goals is to illustrate how diverse ideas in modern randomized numerical linear algebra can be effectively combined with established techniques to create new effective approaches for realistic large-scale problems.

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MS6

Data-Sparse and Unsupervised Linear and Nonlinear Model Order Reduction Via Gpt-Pinn and Its Derivatives

This work introduces data-sparse and unsupervised model order reduction (MOR) methods for both linear and nonlinear parameterized partial differential equations (PDEs) using Generative Pre-Trained Physics-Informed Neural Networks (GPT-PINNs). We present three novel approaches: Transformed GPT-PINN (TGPT-PINN), Viscosity-Enhanced GPT-PINN (VGPT-PINN), and SGPT-PINN, each advancing traditional model reduction techniques. TGPT-PINN extends the GPT-PINN framework for nonlinear MOR in transport-dominated PDEs by incorporating a shock-capturing loss function and a parameter-dependent transform layer, enabling efficient reduction even in the presence of discontinuities. VGPT-PINN further enhances this by introducing adaptive meta-networks and viscosity-enhancement strategies to solve nonlinear conservation laws, demonstrating robust performance with minimal data. Lastly, SGPT-PINN achieves efficient model reduction with a compact architecture, utilizing knowledge distillation and data downsampling to solve parameterized PDEs with fewer parameters and reduced computational cost. Together, these methods provide a unified, efficient framework for nonlinear model reduction and shock-capturing in parameterized systems, significantly improving computational efficiency for complex scientific and engineering applications.

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MS6

ML-Enhanced Reduced-Order Models for Multiphysics and Digital Twins

This talk provides an overview of how machine learning (ML) enhances reduced-order modeling to accelerate simulations and predictions for multiphysics applications, ultimately contributing to the development of digital twins. As examples, we will discuss with more details two reduced-order models constructed by integrating data, physics, and ML techniques. The first one is a graph neural network (GNN)-based surrogate modeling that enables fast and scalable simulations for particulate suspensions. It offers an efficient computational tool for predicting the dynamic behaviors of particles in suspensions subject to hydrodynamic interaction and external forces, relevant to broad applications such as materials design, additive manufacturing, and environmental science. The second concerns statistical microstructure reduced order modeling for metal materials. This model predicts the time evolution of the joint probability density distribution of key variables characterizing the primary damage mechanisms of metal materials. This not only facilitates efficient macroscale damage modeling but also aids in the design of new materials, such

as rolled homogeneous armor steel.

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MS6

Hybridizable Neural Operators: Arbitrary Accuracy, Arbitrarily Long Rollouts

Recent works have focused on building data driven simulators using autoregressive transformer architectures, employing a physics agnostic interpolation process which instead exploits the approximation power of attention and large datasets. In this work, we introduce a hybridizable finite element which recasts autoregressive forecasting as a finite element exterior calculus problem where bilinear forms are prescribed by a transformer rather than discretizing a pde. The resulting hybrid architecture maintains the desirable approximation properties of transformers while guaranteeing geometric structure, allowing us to probably conserve hamiltonians under arbitrarily long rollouts. We demonstrate benchmarks where we drastically outperform state of the art architectures like neural odes, particularly for chaotic systems, and illustrate how the framework can be used to construct ROMs of multi physics systems. Additionally, we show that the scheme can be used as a black box regressor in a supervised learning context, regressing continuous functions to arbitrary accuracy.

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MS7

Introduction to the Geometry of Nanostructures

Nanostructures consist of atoms, which can form small molecules, big proteins or macroscopic objects such as solid crystalline materials. In all cases, a basic representation of a nanostructure is a list of atomic coordinates. However, this representation depends on a choice of a coordinate system. If we rigidly move a nanostructure by a translation or rotation, all coordinates change but the underlying structure has the same properties as before within the same ambient environment. Even if the underlying object is flexible, its different rigid conformation can differ by properties, e.g. proteins of different shapes differently interact with drug molecules. Hence rigid motion is the most practical equivalence. The fact that atomic coordinates have real (non-discrete) values implies that rigid classes of nanostructures form continuous spaces. Under almost any noise or atomic vibration, a rigid structure becomes slightly different, not rigidly equivalent to the original one, so we should distinguish all slight perturbations in terms of a distance satisfying all metric axioms. The mapping problem: design a complete invariant that uniquely identity any structure (under a given equivalence such as rigid motion) and allows a continuous distance that can be computable in a polynomial time of the input size. This problem was recently solved for protein backbones, unordered point clouds and crystals, see https://kurlin.org/research-papers.php#Geometric-Data-Science

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MS7

Using GNN Property Predictors As Molecule Generators

Graph neural networks (GNNs) have emerged as powerful tools to accurately predict materials and molecular properties in computational and automated discovery pipelines. In this work, we exploit the invertible nature of these neural networks to directly generate molecular structures with desired electronic properties. Starting from a random graph or an existing molecule, we perform a gradient ascent while holding the GNN weights fixed in order to optimize its input, the molecular graph, towards the target property. Valence rules are enforced strictly through a judicious graph construction. The method relies entirely on the property predictor; no additional training is required on molecular structures. We demonstrate the application of this method by generating molecules with specific DFT-verified energy gaps and octanol-water partition coefficients (logP). Our approach hits target properties with rates comparable to or better than state-of-the-art generative models while consistently generating more diverse molecules.

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MS7

Engineering Porous Crystals to Do Different Things

In 1988, John Maddox, then the editor of Nature, asserted that it was a scandal that crystal structures could not be predicted from a knowledge of their chemical composition. Things soon changed as crystal engineers started to build coordination networks of designed topology by learning how to link metal complexes (nodes) with organic molecules (linkers), thereby generating repeating patterns in 2D and 3D that resulted in crystals by design. Why does all of this matter? There are three main reasons: - Control over structure means exquisite control over the pore size and pore chemistry of porous materials. - The right pore size and pore chemistry brings unprecedented properties. - Direct air capture of CO2 and efficient atmospheric water harvesting are now within reach at a time when we need them. This presentation will detail this journey from 1989 (basic design principles using topology as blueprints resulted in the emergence of crystal engineering) to today (a new generation of porous materials with exceptional properties are poised to address global challenges such as carbon capture and water harvesting).

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MS8

Subsonic and Transonic Crack Propagation in a Power-Law Graded Material

Steady-state problems are solved of an interfacial crack moving along the interface between two power-law graded

half-planes under conditions of anti-plane and plane strain. Both problems are governed by Navier equations with variable coefficients. The anti-plane problem is solved explicitly. The plane problems of subsonic and transonic crack propagation in a power-law graded bimaterial require solving associated Carleman problems with two shifts of two meromorphic functions in a strip. The similarities and differences between the Carleman problems in the subsonic and transonic regimes are discussed. The Carleman problems are recast to systems of singular integral equations with a fixed singularity and solved numerically. It is shown that the plane subsonic and transonic model problems are equivalent to vector Riemann-Hilbert (RH) problems for two functions with a piece-wise constant matrix coefficient whose entries are expressed through the solution of the corresponding Carleman problem. Exact solutions of the RH problems are determined. Asymptotics of the displacements jumps and the stresses at the crack tip are recovered. For mode I, II, and III cracks propagating at subsonic speed a Griffith-type criterion of crack propagation is proposed.

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MS8

Bloch Waves in High-Contrast Photonic Crystals

We consider high-contrast photonic crystals in two and three dimensions. We will discuss previous and new success representing the Bloch eigenvalues of these photonic crystals as an analytic power series expansion in terms of the material parameter of the "host" phase, both for unitary and non-unitary material parameters in the "inclusion" phase. We will discuss how these power series expansions, together with a radius of convergence, can be used to open band gaps in the frequency spectrum for two-dimensional photonic crystals, and, time permitting, we will also discuss applications to high-frequency homogenization.

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MS8

Modeling of Composites with Thin Nano-Reinforcements

A problem for a nano-sized material surface reinforcement on the interface between two elastic isotropic semi-planes is studied. The material surface is modeled using the Steigmann-Ogden form of surface energy. The study of stationary points of the total elastic energy functional produces a boundary-value problem with non-classical boundary conditions. This problem is solved by using complex analysis methods. With the help of Cauchy-type integral representations of stresses and displacements, the problem can be reduced to either a system of two singular integral equations or a single singular integral equation. The numerical solution of the system of singular integral equations is obtained by expanding each unknown function into a series based on Chebyshev polynomials. The accuracy of the numerical procedure is studied, and various numerical examples for different values of the surface energy parameters are considered.

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MS9

Ito Calculus Approach to Understand Intrinsically Disordered Proteins in Immunity and Cell Mechanics

Proteins in cells are some of the most complex molecules known. They play vital roles, from driving immune responses to aiding cell division. These roles demand interactions and responses to various stimuli, like force or charge modifications, in complex and nonlinear ways. On the other hand, the classical freely-jointed chain from polymer physics is an extremely simple model to define: rigid segments linked together that can rotate freely through all angles. Here, I will show examples where the freely-jointed chain (1) gives complex and nonlinear behavior, and (2) can explain and predict the behaviors of a protein subset known as intrinsically disordered proteins. Examples include the T Cell receptor, which plays a role in immunological decision-making, and formin, an assembler of cellular mechanical structures (F-actin). More precise computational models exist for these proteins; the freely-jointed chain is inferior in every way except that its simplicity allows for cheap, large exploratory simulations, and mathematical analysis such as using Ito calculus. We argue that these two advantages give this 100-year-old model continued relevance in answering open questions in biology

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MS9

Meiotic Spindle Modelling: Gap Time for Dynamic Poisson Processes

Cellular division occurs by separation of genetic material via long structures called microtubules. One way that division can fail is when there are multiple centers of microtubule attachment at one or both ends; this is known as multipolarity. We study a simple model in which attachment points appear uniformly at random along an interval at a constant rate and disappear at a per-capita rate of one. We declare that multipolarity occurs when there is a large gap between attachment points and compute the time until this happens, when the gap is larger than typical, in the limit of large arrival rate. To do so we develop a new theory for computing the hitting time of a rare set in a Markov chain, purely in terms of its stationary distribution, which for this model is a Poisson point process. The method is quite general and only requires certain asymptotic estimates.

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MS9

Formulating a Model for Cell-free DNA Dynamics Using Data From Healthy Individuals and Early-stage Cancer Patients

The DNA not bound to cells detected in blood circulation is called cell-free DNA (cfDNA). Since cfDNA levels are often elevated in cancer patients, cfDNA constitutes a promising biomarker for cancer detection. However, the mechanisms by which cfDNA is shed into, and subsequently cleared from, the circulation are still poorly understood, especially for early-stage cancer patients. In the present work, we employ two previously published datasets of cfDNA from healthy individuals and early-stage cancer patients, in order to formulate a model for cfDNA dynamics in circulation. First, we find that early-stage cancer results in a multiplicative, cancer type-specific increase in cfDNA concentration that originates from healthy tissue and not the tumor. In order to determine the mechanism responsible for the increased cfDNA concentration from healthy tissue in the presence of early-stage cancer, we analyze an additional dataset reporting the tissue of origin for cell-free DNA in healthy individuals and early-stage cancer patients. We deduce that the multiplicative cfDNA increase in cancer is unlikely to originate from a proportional increase in cfDNA shedding from healthy tissue. Rather, the data are consistent with the presence of a saturation mechanism in cfDNA clearance, under which smaller increases in cfDNA shedding due to cancer lead to a large decrease in the cfDNA clearance rate.

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MS9

Modeling and Inference of Subcellular Spatial Heterogeneities in Stochastic Gene Expression

Gene expression in cells is shaped by both spatial heterogeneities from organizing structures like nucleoli and nuclear speckles, and temporal heterogeneities from processes like transcriptional bursting. Understanding how these multi-scale features interact with underlying molecular randomness requires new mathematical approaches. This talk presents a framework for inferring gene expression dynamics from static spatial patterns of mRNA molecules, combining spatial point process models with solutions to stochastic partial differential equations. I will discuss our methods for handling these spatial and temporal complexities and show how this enables new biological insights from challenging datasets.

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MS10

PAQR: Pivoting Avoiding QR Factorization

The solution of linear least-squares problems is at the heart of many scientific and engineering applications. While any method able to minimize the backward error of such problems is considered numerically stable, the theory states that the forward error depends on the condition number of the matrix in the system of equations. On the one hand, the QR factorization is an efficient method to solve such problems, but the solutions it produces may have large forward errors when the matrix is rank-deficient. On the other hand, rank-revealing QR (RRQR) is able to produce smaller forward errors for rank deficient matrices, but its cost is prohibitive compared to QR due to memory-inefficient operations. The aim of this paper is to propose PAQR (Pivoting Avoiding QR) for the solution of rank-deficient linear least-squares problems as an alternative solution method. It has the same (or smaller) cost as QR and is as accurate as QR with column pivoting in many practical scenarios. In addition to presenting the algorithm and its implementations on different hardware architectures, we compare its accuracy and performance results on a variety of application-derived problems.

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MS11

Spectral Properties of Non-Reciprocal Topological Metamaterials

The skin effect is the phenomenon whereby the bulk eigenmodes of a non-Hermitian system are all localized at one edge of an open system. We present the mathematical theory of the non-Hermitian skin effect in systems of finitely many subwavelength resonators with a non-Hermitian imaginary gauge potential and analyze their resonance behavior in the deep subwavelength regime. We will focus on 4 points: i) the mathematical nature linked to Toeplitz theory; ii) differences and similarities between one-dimensional and three-dimensional systems; iii) the stability with respect to impurities; and iv) convergence properties as the size of the system grows.

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MS11

Edge Modes in Topological Photonic Crystals

In this talk, I will discuss the mathematical methods developed to study the edge modes in topological photonic crystals (TPCs), wherein the medium coefficient attains sharp discontinuity across the interface. The edge modes in 1D TPCs can be characterized via the transfer matrix and the SturmLiouville theory. For 2D TPCs, we develop the integral equation method to characterize the edge modes.

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MS12

Preconditioning Strategies for a Nested PrimalDual Method with Application to Image Deblurring

Proximal-gradient methods are widely used in imaging and can be accelerated by adopting variable metrics and/or extrapolation steps. However, one crucial issue is the inexact computation of the proximal operator, often implemented through a nested primal-dual solver. This represents the main computational bottleneck, especially when higher accuracy is required. In this talk, we present preconditioning strategies for a nested primal-dual method aimed at efficiently solving regularized convex optimization problems. For our preconditioner inspired to the Iterated Tikhonov method, we prove the convergence of the iterates sequence towards a solution of the problem. Numerical results confirm that our preconditioned nested primal-dual method effectively accelerates iterations towards the solution of the problem, with reduced computational cost per iteration, especially in image deblurring problems with total variation regularization.

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MS12

Autoencoders for Inverse Problems

In this work, we describe a new data-driven approach for inverse problems that exploits technologies from machine learning, in particular autoencoder network structures. We consider a paired autoencoder framework, where two autoencoders are used to efficiently represent the input and target spaces separately and optimal mappings are learned between latent spaces, thus enabling forward and inverse surrogate mappings. We focus on interpretations using Bayes risk and empirical Bayes risk minimization, and we provide various theoretical results and connections to existing works on low-rank matrix approximations. Similar to end-to-end approaches, our paired approach creates a surrogate model for forward propagation and regularized inversion. However, our approach outperforms existing approaches in scenarios where training data for unsupervised learning are readily available but training pairs for supervised learning are scarce. Furthermore, we show that cheaply computable evaluation metrics are available through this framework and can be used to predict whether the solution for a new sample should be predicted well.

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MS12

A Control-Oriented Approach to Optimal Sensor Placement

We propose a control-oriented optimal experimental design (cOED) approach for linear PDE-constrained Bayesian in-

verse problems. In particular, we consider optimal control problems with uncertain parameters that need to be estimated by solving an inverse problem, which in turn requires measurement data. Specifically, we consider the case where data is collected at a set of sensors. While classical Bayesian OED techniques provide experimental designs (sensor placements) that minimize the posterior uncertainty in the inversion parameter, these designs are not tailored to the demands of the optimal control problem. In the present control-oriented setting, we prioritize the designs that minimize the uncertainty in the state variable being controlled or the control objective. We propose a mathematical framework for uncertainty quantification and cOED for parameterized PDE-constrained optimal control problems with linear dependence to the control variable and the inversion parameter. We also present scalable computational methods for computing control-oriented sensor placements and for quantifying the uncertainty in the control objective. Additionally, we present illustrative numerical results in the context of a model problem motivated by heat transfer applications.

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MS13

Close Evaluation of Layer Potentials for Stokes Equations

To understand the fluid dynamics of complex biological and environmental phenomena, fluid-structure interaction problems must be solved. Challenges exist in developing numerical techniques to solve these flow problems in the environment with boundary conditions at fluid-structure interfaces. I will present details of a novel method that is being developed to address these challenges for the Stokes equations. We are looking at accurate evaluation of layer potentials near interfaces and boundaries. I will present how classical numerical methods are problematic for evaluations close to boundaries and how newly developed numerical methods based on asymptotics can be used to improve accuracy.

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MS13

Data Assimilation in Weather Forecasting with Balanced and Unbalanced Moisture

The notion of balance has played an important role in data assimilation for weather forecasting. However, the traditional ideas of balance have been based on dry atmospheric dynamics, without moisture. Given the longstanding difficulties with data assimilation and forecasting of precipitation, it is possible that balanced versus unbalanced moisture may play a significant role in these difficulties, among many challenging aspects of moisture and precipitation. The goal of this talk is to investigate data assimilation strategies with moisture using a recently-developed formulation of balanced moisture. The impact of accounting for the balanced and unbalanced components of moisture will be explored using a simple fluid-dynamical model consisting of linear, moist, shallow-water equations to illustrate the main ideas. The results show that any erroneous aspect of the prior covariance matrix may introduce relative errors in recovered moisture of up to 15% or more. These errors are most significant on smaller spatial scales, where inertia-gravity wave variance is larger, and in cases with larger observational noise. The impact of other parameters—such as background moisture gradient and the frequency of observations—on the results will also be explored.

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MS13

Modeling of Drag through Vegetation for Wildfires

This talk will cover the problems linked to horizontal and vertical flows due to wind and buoyancy that happen through forest canopies and vegetation elements in the context of wildland fires. Experimental and modeling approaches were developed to characterize those different flow types. The modeling work was conducted mainly with the Fire Dynamics Simulator (FDS), a LES-based open-source fire modeling platform from the National Institute of Standard and Technology (NIST) that allows describing fire plumes and fire spread. FDS operates mainly at the fire front scale and allows for detailed modeling of the flame front. The first type of work was conducted to make sure that FDS was able to represent a wind flow through a forest canopy and through vegetation elements such as trees and to understand the limitation of the sub-modeling of drag. Then, another approach was developed to simulate buoyant plumes through tree canopies and assess the capacity of the model to represent those flows. The first step was to simulate a free buoyant plume by reproducing experiments in a laboratory setting with and without cross wind. Then, the second step was to conduct field experiments with pool fires in a forested parcel and measure the wind and plume characteristics. The talk will end by discussing the limitations and needs of the modeling of drag in FDS but also how to do it with other simulation tools that can simulate fire spread at different scales.

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MS14

Towards Controllable and Observable Reduced-Order Models for Digital Twins

Reduced-order models (ROMs) provide a viable avenue to enable (near) real-time decision-making and control with a digital twin, due to their rigorous mathematical derivation and fast simulation. However, not all ROM techniques are fit-for-purpose to serve as a digital twin, as decision-making and control require special properties of ROMs. In this

talk, we focus on the system-theoretic aspects of controllability and observability, and describe ways to derive nonlinear ROMs that preserve those properties. In particular, we focus on nonlinear balanced truncation ROMs as initializations of the digital twin before the physical-to-digital data stream starts. Since nonlinear balanced truncation has only been applied to systems with a handful of degrees of freedom, this talk presents several Taylor-series-based techniques to produce scalable algorithms to enable nonlinear balanced truncation for models with 1,000s of state variables. Numerical results illustrate the performance of the ROMs on several medium-to-high dimensional dynamical systems.

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MS14

Better Training Through Structure and Second-Order Information

Deep neural networks (DNNs) have achieved inarguable success as high-dimensional function approximators in countless applications, including numerous scientific applications such as surrogate modeling, operator learning, and model discovery. However, this success comes at a significant hidden cost, notably a long training time. In this talk, we will to make training easier by exploiting commonly-used network structures and incorporating second-order information. Specifically, we will use Gauss-Newton-like techniques and will demonstrate the computational advantages of our approach over traditional stochastic optimizers on several benchmark deep learning tasks.

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MS15

A Class of Variational Problems for Machine Learning Solutions of PDEs

Solving partial differential equations (PDE) using machine learning often relies on the construction of a neural network loss function based on reformulating an underlying PDE and the boundary conditions into a constraint-free variational problem of minimizing a penalized energy functional. In this talk, I will discuss general properties of such variational problems with an emphasis on the Poisson-Boltzmann (PB) free-energy functionals that have been commonly used for modeling electrostatics. In particular, I will show the convergence of the penalized functionals to the PB energy-functional in terms of their minimizers and minimum values.

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MS15

Repulsive-Attractive Interaction in a Growth-Inhibition System

A geometric variational problem is defined on subsets of a prescribed measure in the entire plane. The functional of the problem consists of two terms: the perimeter of the input subset and an interaction integral with a kernel that is the sum of a logarithmic function and a quadratic function. This kernel is bounded below and tends to infinity at zero and infinity. A single disc is always a stationary point of the functional but its stability depends on the parameters of the problem. When the parameters are in a suitable range there exist assemblies of multiple perturbed discs that are stable stationary points. This is joint work with C. Wang and J. Wei.

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MS15

On The Eigenframe Discontinuities of The Q-Tensor Model

In this talk, I will describe some work on the structure of defect set of minimizer of a Landau-de Gennes energy functional in three-dimensional domains, subject to constraint $|Q| = 1$. The set of defects is identified by discontinuities in both the eigenframe and the leading eigenvector. Through a blow- up analysis, we prove that the defect set is 1-rectifiable and classify the asymptotic profile of the leading eigenvector near singularities. This generalizes some previous results on the structure of ring disclinations in the Q-tensor model. This is a joint work with Zhiyuan Geng (Purdue University).

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MS15

Ferroelectric Smectic-A Phases of Bent-core Liquid Crystals with Weak Surface Anchoring

The ferroelectric SmA phase (SmAPF) made of bent-core molecules has been discovered in 2011 and has drawn a lot of interest in the physics community over the last twenty years. We study a continuum phenomenological model to discuss the effect of DC bias field on the structure of the SmAPF phase in thin planar cells with weak surface anchoring conditions. We will present rigorous proof of some properties of the polar director as a function of polar an-

choring strength, the bias field, cell thickness and ratio between the bend and splay elastic constants. Joint work with Alec Wendland.

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MS16

Data-Driven Stabilisation of Unstable Periodic Orbits of the Three Body Problem

Many different models of the physical world exhibit chaotic dynamics, from fluids flows and chemical reactions to celestial mechanics. The study of three body problem (3BP) and the many families of unstable periodic orbits (UPOs) within it have provided fundamental insight into chaotic dynamics as far back as the 19th century. In this talk we present a novel and interpretable data-driven approach for the state-dependent control of UPOs of the 3BP, through leveraging the inherent sensitivity of chaos. The 3BP is inherently challenging to sample due to the volume-preservation property of conservative systems which we overcome by utilising prior knowledge of UPOs and a novel augmentation strategy. This enables sample-efficient discovery of a verifiable and accurate Poincaré map in as few as 55 data points. To stabilise the UPOs we apply small thrusts once each revolution, determined by solving a convex problem formed from the linearised map and a system of linear matrix inequalities. We constrain the norm of the decision variables in this problem, resulting in thrusts directed along the local stable manifold. Critically, this locally optimal behaviour is achieved in a computationally efficient manner, without the need for an optimisation problem using many expensive simulations. We demonstrate this sample-efficient, low-energy method across several orbit families in the 3BP, with potential applications ranging from robotics and spacecraft control to fluid dynamics.

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MS16

Multiscale Partial Differential Equation Dynamics with Neural Network Operators

Neural ordinary differential equations (NODEs) enable efficient modeling of subgrid-scale effects in PDEs through a hybrid framework that synthesizes traditional numerical methods with data-driven approaches. By integrating NODEs directly into PDE formulations via the method of lines and incorporating conservation laws, we establish a rigorous methodology for capturing fine-scale dynamics without the computational burden of high-resolution simulations. We validate the framework through comprehensive experiments on three canonical systems: the two-scale Lorenz 96 equation, convection-diffusion equation, and compressible Navier-Stokes equations. This work advances operator learning techniques at the intersection of numerical analysis and machine learning, demonstrating robust capabilities for scientific and engineering applications.

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MS16

Bridging Deep Learning and Numerical Methods Through Differentiable Solvers: Balancing Speed, Accuracy, and Scalability

Machine learning (ML) is increasingly playing a pivotal role in spatiotemporal modeling. A number of open questions remain on the best learning strategies to maximize the utility of machine learning while ensuring the validity of such predictions at test time (i.e., "deployment"). This talk will focus on machine learning methods for neural PDE solvers, with an emphasis on broad learning strategies that are applicable across a wide variety of systems and neural network architectures. Some topics I will discuss include: developing expressive neural network architectures that can be trained at scale on large-scale 3D problems such as turbulent fluid flow, using self-supervised learning to change the basis of learning with spectral methods to solve fluid dynamics and transport PDE problems, and simulation-in-the-loop approaches via incorporating PDE-constrained optimization as a layer in neural networks. In these settings, I will discuss both strategies for scalable training and deployment, while balancing speed and accuracy.

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MS16

Signature of Glassy Dynamics in Dynamic Modes Decompositions

Glasses are traditionally characterized by their rugged landscape of disordered low-energy states and their slow relaxation towards thermodynamic equilibrium. Far from equilibrium, dynamical forms of glassy behavior with anomalous algebraic relaxation have also been noted, e.g., in networks of coupled oscillators. Due to their disordered and high-dimensional nature, such systems have been difficult to study analytically in the past. Here, we show that the gap between oscillatory and decaying modes in the Koopman spectrum vanishes in systems exhibiting algebraic relaxation. The dynamic mode decomposition, which is a data-driven spectral computation that approximates the Koopman spectrum, thus provides a model-agnostic signature for detecting and analyzing glassy dynamics. We demonstrate the utility of our approach through both a minimal example of one-dimensional ODEs and a high-dimensional example of coupled oscillators.

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MS17

Discrete-Time Hedging, Basis Risk, and Covariance-Dependent Pricing Kernels

Basis risk arises when hedging a financial derivative with an instrument different from its underlying asset. This risk can significantly impair hedging effectiveness and must therefore be properly managed. This article develops a discrete-time hedging framework for European-style derivatives that explicitly accounts for basis risk while incorporating key empirical properties of asset re-

turns, including time-varying volatilities, leverage effects, and a flexible dependence structure between assets. Using a covariance-dependent pricing kernel, we derive semi-closed-form solutions for the optimal risk-minimizing hedge ratio. Empirical analyses using S&P 500 index data, its futures contracts, and the VIX demonstrate that our proposed strategy consistently outperforms conventional benchmarks across various maturities and moneyness levels, providing an effective approach to managing basis risk in derivative hedging.

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MS17

Enhanced Deep Hedging with Implied Volatility Surface-Informed Decisions and Multiple Hedging Instruments for Portfolios of Options

We propose an enhanced deep hedging framework to hedge portfolios of options, which integrates implied volatility surface-informed decisions with multiple hedging instruments. Our methodology integrates no-trade regions to optimize portfolio rebalancing frequency and improve decision-making. By leveraging information from the evolving implied volatility surfaces, our approach consistently outperforms traditional delta and delta-gamma hedging approaches across diverse market conditions from 1996 to 2020. The inclusion of no-trade regions drives optimal practitioner delta-gamma solutions towards minimal rebalancing frequencies, similar to static hedging. In contrast, deep hedging strategies show superior adaptability, delivering enhanced performance in both simulated environments and backtesting.Input your abstract, including TeX commands, here.

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MS17

Harnessing Time Series Models for Accurate Option Price Prediction

We use initial state dispersion on all model parameters in an option pricing model allowing us to calibrate even non affine models a lot easier and much faster. We empirically calibrate the model very frequently and observe the variation in model parameters which we model using standard time series models. The changes in model parameters result in changes to the physical dynamics of the underlying asset and to the estimated volatility in particular. Assuming that option markets are forward-looking these we examine if this would allow a traditional volatility forecast methodology to now be able to forecast volatility increases beyond the long-term average.

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MS17

Exploring Parameter Fluctuations in Option Pricing Models: A Time Series Analysis

We use initial state dispersion on all model parameters in an option pricing model allowing us to calibrate even non affine models a lot easier and much faster. We empirically calibrate the model very frequently and observe the variation in model parameters which we model using standard time series models. We then use the forecasted model parameters for pricing future options by simply evaluating the polynomial so this way we can forecast future option prices. Not only can we price options by simply evaluating the polynomial we can also get the partial derivatives which gives which gives us the Greeks. By forecasting the Greeks, we propose enhanced hedging strategies of our option portfolios.

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MS18

Modeling Human Erythropoietic Adaptation to Altitude

Upon ascent to high altitude, the human body activates several physiological mechanisms to adapt to hypoxia and restore arterial oxygen saturation. One of the primary immediate responses is a reduction in plasma volume. We propose a mathematical model of erythropoiesis, incorporating a hypoxia factor and accounting for plasma volume reductions at higher elevations. The model consists of a system of three delay differential equations with distributed delay: the first describes the dynamics of circulating erythrocytes, the second tracks changes in EPO concentration, the primary hormone regulating erythropoiesis, and the third characterizes changes in plasma volume. We establish important mathematical properties of the model, proving the positivity of solutions, which is essential for physiological systems, as well as the existence and uniqueness of the steady state. Additionally, we show that the

homeostatic steady state at sea level is locally asymptotically stable. The model is then applied to study scenarios that are experimentally challenging or lack sufficient published data. For example, we conduct numerical simulations of multi-year sojourns at altitude. Furthermore, we estimate the timing of peak oxygen-carrying capacity following altitude exposure, a key factor in optimizing athlete training programs. In this talk, I will highlight the key features of our model and demonstrate how it can be applied to design optimal altitude training strategies for athletes.

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MS18

Analysis and Dynamics of Threshold Delays

Threshold delays arise naturally in a wide variety of dynamical systems, including maturation and transport processes, and can be found in models of hematopoiesis, cell biology and immunology to name just a few examples. When the speed of the process depends on the state of the system the delay is state-dependent and distributed, and standard off the shelf numerical methods for discrete delays cannot be applied directly. Hal Smith showed that when the (maturation) speed is strictly positive, a time rescaling reduces the equation to a constant delay problem. Perhaps for this reason, these equations have not received much attention, however the time rescaling does not result in a constant delay when there are multiple delays, and even with a single delay the resulting equation may not have a discrete delay. Since threshold delays are ubiquitous in biological problems, we will discuss the analysis and numerical treatment of these problems, and illustrate the novel dynamics that may arise in an operon model. We will also show how to linearize these models around steady states (avoiding discussion of Banach spaces), and show how some approximations lead to inaccurate stability results.

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MS18

Dynamics of Delay Maps: Transverse Connecting Orbits and Chaos

Computer-assisted proofs (CAPs) have become an essential tool for rigorously validating mathematical results, particularly in fields where pen-and-paper analytical approaches alone prove challenging. In this talk, we will discuss a posteriori validation methods; that is, CAP techniques designed to certify a solution in an explicit neighbourhood of a numerical approximation. We will explore their application to the Poincaré scenario for delay differential equations (DDEs) of the form $y'(t) = \alpha y(t) + g(y(t-\tau))$, that is the transverse intersection of the stable and unstable manifolds of a periodic orbit. We introduce an implicit discrete dynamical system that inherently reflects the dynamics of the original DDE. Within this new framework, we develop a shooting method from the unstable manifold to the stable one. By applying a Newton-Kantorovich type theorem, we demonstrate the conditions under which a transverse intersection of these manifolds occurs.

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MS18

Impact of Interhemispheric Conduction Delays on Synchronization

We present a mathematical model of a bihemispheric thalamocortical network to investigate how interhemispheric communication, mediated by myelination, affects network synchronization and seizure-like activity. Conduction velocitywhich determines the communication delay between hemispheresis directly tied to the degree of myelination along the corpus callosum. Our analysis demonstrates that variations in conduction velocity can either suppress or promote oscillatory activity, thereby influencing the likelihood of seizure-like events. Specifically, the stability of steady states depends on the distribution of interhemispheric delays, with shorter delays leading to instability. In addition, the inherent time delays in the system give rise to multistabilitya property commonly observed in delay differential equation modelswhich allows noise-driven perturbations to trigger sudden episodes of high-amplitude rhythmic oscillations. These findings suggest that alterations in myelination, and the resulting changes in conduction velocity, may significantly affect interhemispheric synchronization and contribute to the emergence of seizure-like behavior.

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MS19

Tv Flow Denoising and a Hybrid Algorithm for Inpainting Noisy Grain Orientation Maps

In this talk, we present the utility of weighted vectorized TV flow for denoising grain orientations obtained using Electron Backscatter Diffraction, a critical tool for analyzing the microstructures of polycrystalline materials. We

will also introduce a novel hybrid algorithm for addressing missing orientation values in Traditional inpainting techniques, including exemplar-based methods and machine-learning approaches designed for natural images, which often fall short when applied to EBSD data due to the unique characteristics of grain geometries and orientation datasets. To tackle this, we adapted a classical exemplar-based inpainting algorithm and a partial convolutional neural network method to better suit the demands of EBSD data. However, each approach has its limitations. Our proposed solutiona hybrid algorithmcombines the strengths of these methods. It starts with a deep learning model to provide an initial estimate of missing regions, followed by refinement using an adapted exemplar-based method to preserve grain boundaries and structural integrity. Using synthetic EBSD images generated with DREAM.3D, we demonstrate that our hybrid approach achieves better accuracy and visual coherence than standalone techniques. This method enhances EBSD map reconstruction and shows promise for broader applications in orientation-based datasets.

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MS19

Variational Algorithms for Image Registration and Segmentation

In this work, we build on the seminal work of Chan-Vese for two-phase image segmentation, and propose an efficient segmentation model, in which the computations are restricted to the region boundaries, and do not require integrals or inversions on the domains. Moreover, incorporating higher order statistics measures, we are able to segment images with more complicated pixel statistics. We show that our model can handle challenging scenarios of segmentation and registration.

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MS19

Metrics for Contrastive Image Segmentation

Imaging is a fundamental measurement modality which offers rich insights to scientists and engineers spanning a multitude of disciplines including: biology, ecology, materials science, climate science, and medicine. Coherent structures in images manifest as curves or shapes informed by level sets of some combination of pixel intensities. Methods of image segmentation work to simultaneously de-noise and extract these meaningful level-curves to inform subsequent statistics of the extracted shapes. However, the choice and composition of algorithms informing an image segmentation remain highly ambiguous and, traditionally, hand-picked. Modern advancements utilizing AI, trained on manually segmented data, have produced subjectively compelling results. But how can we quantify the efficacy of segmented objects which informa subsequent statistical analysis of shapes in an image? Are low-cost classical methods, despite small errors, capable of producing image segmentation which replicate meaningful statistics? We introduce formalisms for studying these questions in a variety of applications with the intent to drive down costs of modern state-of-the-art models used for image segmentation.

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MS19

Genus-0 Surface Parameterization using Spherical Beltrami Differentials

Spherical surface parametrization underpins key tasks in geometry, graphics, and medical imaginge.g., brain morphometry and anatomical comparisonbut existing numerical and learning methods falter on large distortions or bijectivity. In this talk, I will present a novel manifold-aware optimization frameworkLSQCNet (Least Square Quasiconformal Network)for general genus-0 surface mapping. This approach leverages the theory of least square quasiconformal energy in conjunction with a neural solver capable of learning free-boundary, non-overlapping mappings. Our neural architecture integrates multi-scale message passing and a mesh spectral layer to ensure both local and global geometric fidelity. Key to the optimization framework is the division of the sphere into hemispheres, their stereographic projection and nonlinear distortion in 2D, followed by seamless gluing in 3D, all under a principled variational framework, which is the first time to strictly achieve optimization over Beltrami differentials. In experiments on cortical surface registration, area-preserving mapping, and landmarkintensity alignment, LSQCNet delivers bijectivity, low conformal error, and robustness to anatomical variability. It also supports area uniformization and high-quality remeshing for downstream analysis This work bridges classic quasiconformal geometry with modern deep learning, opening new directions for flexible, high-fidelity surface mapping in geometric analysis and beyond.

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MS20

$O(k)$-Equivariant Dimensionality Reduction on Stiefel Manifolds

Many real-world datasets live on high-dimensional Stiefel and Grassmannian manifolds, $V_k(\mathbb{R}^N)$ and $Gr(k, \mathbb{R}^N)$ respectively, and benefit from projection onto lower-dimensional Stiefel and Grassmannian manifolds. In this work, we propose an algorithm called Principal Stiefel Coordinates (PSC) to reduce data dimensionality from $V_k(\mathbb{R}^N)$ to $V_k(\mathbb{R}^n)$ in an $O(k)$-equivariant manner ($k \leq n \ll N$). We begin by observing that each element $\alpha \in V_n(\mathbb{R}^N)$ defines an isometric embedding of $V_k(\mathbb{R}^n)$ into $V_k(\mathbb{R}^N)$. Next, we describe two ways of finding a suitable embedding map α: one via an extension of principal component analysis (α_{PCA}), and one that further minimizes data fit error using gradient descent (α_{GD}). Then, we define a continuous and $O(k)$-equivariant map π_α that acts as a "closest point operator" to project the data onto the image of $V_k(\mathbb{R}^n)$ in $V_k(\mathbb{R}^N)$ under the embedding determined by α, while minimizing distortion. Because this dimensionality reduction is $O(k)$-equivariant, these results

extend to Grassmannian manifolds as well. Multiple numerical experiments using synthetic and real-world data are performed.

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MS20

Active Query Synthesis for Preference Learning

Learning user preferences efficiently is crucial for recommendation systems and other decision making models. Traditional methods require a lot of labeled data, which can be expensive to obtain. Active learning can help reduce labeling costs by selecting informative queries. However, standard approaches often evaluate all unlabeled data points, making them computationally expensive. In this work, we propose an active query synthesis framework to generate optimal queries directly using a mutual information based objective function. This is used to synthesize paired comparison queries of the form 'Which of items A and B do you prefer?', and user preferences are estimated using responses to these queries. In addition to informativeness, the reliability of the responses is also considered, since humans are most confident in answering queries where items are neither too similar nor too distinct. Further, the synthesis framework allows for optimization in a continuous space, leading to better query generation. For problems constrained by a fixed dataset, we propose an approximation scheme to find existing points that best preserve the pairwise relationship of the synthesized pair. Instead of naively selecting the nearest neighbors, we perform a k-NN search individually and evaluate all candidate pairs for optimality. This provides a computationally efficient alternative to standard active learning while maintaining query effectiveness.

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MS20

Randomized Kaczmarz Methods for T-Product Tensor Linear Systems with Factorized Operators

Randomized iterative algorithms, such as the randomized Kaczmarz method, have gained considerable popularity due to their efficacy in solving matrix-vector and matrix-matrix regression problems. Our present work leverages insights from studying such algorithms to develop regression methods for tensors, which are the natural setting for many application problems, e.g., image deblurring. In particular, we extend the randomized Kaczmarz method to solve a t-product tensor system where the measurement tensor is given in factorized form, and we develop variants in both the consistent and inconsistent regimes. We provide theoretical guarantees of the exponential convergence rate of our algorithms, accompanied by illustrative numerical simulations. Author names: A. Castillo, J. Haddock, I. Hartsock, P. Hoyos, L. Kassab, A. Kryshchenko, K. Larripa, D. Needell, S. Suryanarayanan, K. Yacoubou-Djima

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MS21

Topological Data Analysis of Xylem Patterns

Xylem is the vascular tissue in plants that provides structure and delivers its nutrients. In this project we have developed tools using image processing and topological data analysis, more specifically persistent homology, to quantify patterns within images of healthy and mutant xylem tissue. We first process the images of xylem tissue, converting grayscale images to binary images and extracting coordinate points associated with xylem patterns. Using persistent homology, we then take that set of points and slowly increase their radii. As these points increase in size, they will begin to merge with one another and form connected components, or clusters, as well as holes or loops. We are focusing on quantifying the holes and connected components to differentiate between various types of xylem patterns.

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MS21

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MS21

Evaluation of Data Augmentation for Tabular Data

This project aimed to determine whether current data augmentation methods effectively enhance tabular data while preserving the original patterns of the data. Data augmentation is the creation of new data from pre-existing data to improve the performance of machine learning (ML) models while tabular data refers to data organized into rows and columns. Prior research in this field has mainly focused on the creation of methods for data augmentation, whereas we establish a framework that measures if patterns are kept throughout the data augmentation process. By maintaining data patterns, one ensures that the patterns in the augmented data are not false or misrepresented. We measured three types of relationships: feature-to-label dependency,

feature-to-feature dependency, and feature distributions. To do so, we utilized Chi-Squared tests, correlation matrices, sub-categorical proportions, and the Mann-Whitney U test. For all of these tests, we used the Support Vector Machines (SVM) classifier. Our augmentation methods included modified +/- one (modPMOne), random swap (randSwap), and the histogram augmentation technique (HAT). We found that these three augmentation methods were able to sufficiently maintain patterns throughout the augmentation process, though the results varied with each test we conducted with HAT generally performing the best.

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MS21

Detecting Cancer Utilizing the Randomized SVD

Our project focused on developing Python-based algorithms for efficiently analyzing large datasets using the randomized singular value decomposition (SVD). The Randomized SVD is a dimensionality reduction technique that enables scalable approximation of large matrices, making it well-suited for applications in areas such as cancer detection, music recommendation, and facial recognition. Our work explored both the theoretical underpinnings and practical implementations of these methods to improve computational efficiency, data interpretability, and possible preparation for field use.

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MS21

Modeling Quasicrystal Viral Capsids: Self assembly of Hats, Turtles, and Einstein Tiles

Mathematical research on viral architecture has aided in the medical advancements of antidotes as well as the knowledge of virus proteins. An aperiodic tessellation of a three dimensional structure is referred to as a quasicrystal. Some viral capsids are arranged in a quasicrystal array. After 50 years of searching by the mathematical community, David Smith (2022) finally discovered unitiles that could aperiodically tessellate the plane. As virus proteins self-assemble in nature, we aim to discover whether einstein tiles replicate this spherical self-assembly with 3D printed tiles and magnets. While our lab has successfully self-assembled Caspar-Klug models of protein viral capsids, so far no self-assembly of quasicrystal arrays of viral capsids has been reported. The reason that we aim to use einstein tiles is to help create an even more accurate representation of virus architecture using their relations to the shape of quasicrystals. In order to achieve our goal we have collected data from experimenting with 2D and 3D einstein, hat, and turtle tiles. This data shows us where certain vertices and edges connect to each other within most einstein tile tessellations, allowing for insight on spherical tessellations in order to model self-assembly of a polyhedron. We analyzed the tessellations of einstein tiles with several graph theoretic measures. For example, we identified which vertices and edges of each tile interacted with one another in their respective arrangements. We classified the interactions of vertices as X, Y, and T configurations. We constructed nearest neighboring networks of the corona of tiles around an individual einstein tile. The significance of our research is to aid in the research of quasicrystals and medical nanocapsules involved in drug delivery.

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MS22

Toward Early Fault-Tolerant Quantum Simulation: An End-to-End Perspective

With recent advancements in quantum hardware and the implementation of quantum error correction codes, the prospect of developing an early fault-tolerant quantum computer within the next decade has become increasingly realistic. The potential applications of such a quantum computer, particularly in solving complex problems in quantum chemistry and quantum many-body systems, are attracting significant attention. In this talk, we aim to provide an introduction to quantum simulation from an end-to-end perspective. We will begin with an introduction to quantum computers and quantum simulation, spanning multiple scales from hardware to scientific applications. In particular, we will highlight recent advancements in block encoding for quantum many-body systems.

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MS22

An exponential advantage in quantum computer-assisted sensing

Recent results in quantum learning theory have established exponential separations (in sample complexity) for learning properties of quantum states with and without a quantum computer. I will present recent work where we have translated these abstract results to a concrete quantum sensing setting. We establish that access to a quantum computer can provide an exponential advantage for many quantum sensing tasks. In practice, this advantage translates to needing exponentially less signal (e.g., light intensity) to make inferences about the world with access to a quantum computer.

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MS22

Signal Subspace Expansion with Quantum Real-Time Evolution

Quantum algorithms exploiting real-time evolution under a target Hamiltonian have demonstrated remarkable efficiency in extracting key spectral information. In this work, we introduce the framework of multi-observable dynamic mode decomposition (MODMD), which combines the observable dynamic mode decomposition, a measurement-driven eigensolver tailored for near-term implementation, with classical shadow tomography. MODMD leverages random scrambling in the classical shadow technique to construct, with exponentially reduced resource requirements, a signal subspace that encodes rich spectral information. Notably, we replace typical Hadamard-test circuits with a protocol designed to predict low-rank observables, thus marking a new application of classical shadow tomography for predicting many low-rank observables. We establish theoretical guarantees on the spectral approximation from MODMD, taking into account distinct sources of error. In the ideal case, we prove that the spectral error scales as exp(-dE*tmax), where dE is the Hamiltonian spectral gap and tmax is the maximal simulation time. This analysis provides a rigorous justification of the rapid convergence observed across simulations. To demonstrate the utility of our framework, we consider its application to fundamental tasks, such as determining the low-lying, i.e. ground or excited, energies of many-body systems.

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MS23

Structure-Preserving and Energy-Stable Algorithms for Hyperbolic and Related Pde-Based Models with Uncertainty

In this talk, we will discuss the design of structure-preserving numerical methods for hyperbolic and related nonlinear PDE-based models with uncertainty. As a primary example, shallow water systems with uncertainty will be considered, but the developed ideas can be extended to a wider class of models, including different models of conservation and balance laws. Shallow water equations are widely used in many scientific and engineering applications related to the modeling of water flows in rivers, lakes, and coastal areas. Therefore, stable and accurate numerical methods for shallow water systems are needed. Although some algorithms are well-studied for deterministic shallow water models, more effort should be devoted to handling such systems with uncertainty. We will show that the structure-preserving numerical algorithms that we developed deliver high resolution and satisfy important stability conditions. We will illustrate the performance of the designed algorithms on a number of challenging numerical tests. Current and future research will be discussed as well.

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MS23

Coupled Snow and Soil Models: Detailed Numerical PDE Model Or Data Driven Approach?

We present our recent work on modeling coupled processes in the sub- and near surface of the Arctic. These involve thermal energy, mass balance, and mechanical deformation, and feature multiple spatial scales (from pore- to Darcy to landscape scale) and multiple time scales (hours to days to years). We provide rigorous explanations to connect these scales in a comprehensive model which uses data generated by subgrid parametrizations. The model compares well to those used in geophysics and geotechnical community based on empirical data. Still, the complexity of the system is considerable especially that it is strongly dependent on atmospheric conditions. We consider therefore additional strategies to develop data driven surrogate and hybrid models, and study their sensitivity. This is joint work with many students and collaborators to be named in the talk.

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MS23

Robustness of Nonlinear Solvers for Permafrost Problems

We study the nonlinear heat equation with phase change between liquid and ice where the energy to change phase is given by the enthalpy-temperature relationship, $\alpha(\theta)$. For Stefan problems, $\alpha(\theta)$ is usually a multivalued graph where the phase transition resembles a shifted Heaviside function. For permafrost problems, $\alpha(\theta)$ is continuous but its inverse requires a nonlinear solver. For soil with trapped air and large pores, we propose a model denoted (P^*) where $\alpha(\theta)$ is a multivalued graph with piecewise continuous properties. We show how to extend analytical solutions for the Stefan problem to (P^*). Also, the robustness of our numerical algorithm will be shown, where we use various local nonlinear solvers such as Newton-Anderson, to study the performance and convergence of our solver. We also describe progress towards a coupled Salinity model.

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MS23

Partitioned and Multirate Integration for Multiscale Multiphysics

In multiscale and multiphysics simulation, a predominant challenge is the accurate coupling of physics of different scales, stiffnesses, and dimensionalities. The underlying problems are usually time dependent, making the time integration scheme a fundamental component of the accuracy. Remarkably, most large-scale multiscale or multiphysics codes use a first-order operator split or (semi-)implicit integration scheme. Such approaches often yield poor accuracy, and can also have poor computational efficiency. Recently there has been significant interest in multirate integration schemes for problems with multiple scales. Here I will first discuss when and why one would use multirate integrators in practice from both a theoretical and practical perspective. There are also other technical reasons that more advanced and higher order time integration schemes have not been adopted. One challenge that arises is the nonlinear coupling of different scales or stiffnesses. I will then present a new class of nonlinearly partitioned Runge-Kutta (NPRK) methods that facilitate high-order integration of arbitrary nonlinear partitions of ODEs, including multirate variations, and with adaptive error estimators. Methods and analysis are demonstrated on realistic and challenging problems in thermal radiation transport, radiation hydrodynamics, and magnetohydrodynamics.

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MS24

Subspace-constrained Sketch-and-project Solvers for Linear Systems with Low-rank Structure

The sketch-and-project method is a unifying framework for many popular iterative solvers for linear systems, including the randomized Kaczmarz and coordinate descent algorithms. In this talk, I will describe a framework in which the dynamics of the algorithm are constrained within a particular affine subspace, such as the solution space of a chosen subsystem, and show that the convergence can be significantly improved given a good choice of subspace. I will describe a concrete application for solving large-scale positive semidefinite linear systems with rapid spectral decay using a subspace-constrained randomized coordinate descent (SC-RCD) algorithm where the subspace corresponds to a low-rank Nystrm approximation computed by the recently analyzed RPCholesky algorithm.

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MS24

Learning Rates, Momentum, and Randomized Kaczmarz

In this talk, we consider learning rates and momentum in the context of the randomized Kaczmarz algorithm, which is an instance of stochastic gradient descent for a linear least squares loss function. First, we consider the problem of determining an optimal learning rate schedule for the Kaczmarz algorithm for noisy linear systems. Second, we consider how momentum effects how the randomized Kaczmarz algorithm converges in the direction of singular vectors of the matrix defining the linear loss function.

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MS24

Small Sketches for Big Matrix Approximations

Low-rank approximations have become foundational to the improved computational efficiency of techniques like clustering, machine learning, and optimization. Practitioners typically compute such approximations using the singular value decomposition (SVD). However, the poor computational scaling of SVD has led to increased interest in alternative approaches. One approach is the CUR decomposition, which approximates a matrix using direct subsets of its row and column indices. By using direct subsets of a matrix's rows and columns, CUR is often better than SVD at preserving native matrix structures like sparsity and nonnegativity. Despite these benefits, most approaches to forming CUR decompositions require impractical apriori knowledge of the matrix's rank. This talk will present IterativeCUR, a scalable, rank-adaptive approach that produces CUR approximations using only one small sketch of the matrix. Additionally, rigorous experiments will demonstrate that IterativeCUR outperforms state-of-the-art CUR approaches without losing accuracy.

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MS24

Randomly Sparsified Richardson Iteration: A Dimension-Independent Sparse Linear Solver

Recently, a class of algorithms combining classical fixed point iterations with repeated random sparsification of approximate solution vectors has been successfully applied to eigenproblems with matrices as large as $10^{108} \times 10^{108}$. So far, a complete mathematical explanation for their success has proven elusive. This family of methods has not yet been extended to the important case of linear system solves. In this paper we propose a new scheme based on repeated random sparsification that is capable of solving linear systems in extremely high dimensions. We provide a complete mathematical analysis of this new algorithm. Our analysis establishes a faster-than-Monte Carlo convergence rate and justifies use of the scheme even when the solution vector itself is too large to store.

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MS25

Detection of Combustion Instabilities by Integrating Machine Learning with Chaotic Analysis

We present work on detecting thermoacoustic phenomena in combustion systems by integrating nonlinear dynamics with modern machine learning techniques. We introduce a framework that addresses two critical challenges: flashback prevention and thermoacoustic oscillation characterization. Our approach combines chaotic analysis with deep learning networks to enhance flashback event detection. We analyze thermoacoustic time series data from a digital twin of an industrial combustor. Our approach reconstructs phase spaces from unsteady thermoacoustic data and extracts nonlinear features using recurrence matrices. These features are then used to train Residual Networks for flashback prediction. Additionally, we identify precursor signatures through data-driven clustering techniques, further refining the predictive framework. Furthermore, this work explores how thermoacoustic oscillations in a combustor can be detected and characterized using imaging and model decompositions. Three cases with distinct flame morphologies are investigated. We show that when strong thermoacoustic oscillations appear in the power spectral densities of pressure and heat release, model techniques effectively characterizes the instabilities. We discuss progress towards linking these shifts with instability detection and existings theory, and discuss the connection between deep learning-based flashback prediction and thermoacoustic analysis.

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MS25

Reduced-Order Models for Filtering Probability Distributions of Multiscale Systems

The capability of using imperfect stochastic and statistical reduced-order models to capture key statistical features in multiscale nonlinear dynamical systems is investigated. A new efficient ensemble forecast algorithm is developed dealing with the nonlinear multiscale coupling mechanism as a characteristic feature in high-dimensional turbulent systems. To address challenges associated with closely coupled spatio-temporal scales in turbulent states and expensive large ensemble simulation for high-dimensional complex systems, we introduce efficient computational strategies using the so-called random batch method. 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 of the flow field with distinct statistical structures. Finally, the proposed model is applied for a wide range of problems in uncertainty quantification, data assimilation, and control.

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MS25

CGKN: A Deep Learning Framework for Modeling Complex Dynamical Systems and Efficient Data Assimilation

A discrete-time conditional Gaussian Koopman network (CGKN) is developed to learn surrogate models that enable efficient state forecasting and data assimilation (DA) in high-dimensional, complex dynamical systems. Focusing on nonlinear partially observed systems common in engineering and geoscience applications, CGKN exploits Koopman embedding to uncover a latent representation of the unobserved states, such that the dynamics of the latent states are conditional linear, i.e., linear given the observed states. This transforms the combined system of observed and latent variables into a conditional Gaussian system, allowing for efficient evaluation of the latent state posterior via analytical formulae. The analytical DA formulae are incorporated directly into the model learning process, leading to a framework that unifies scientific machine learning (SciML) and DA. The performance of discrete-time CGKN is demonstrated on canonical problems governed by nonlinear PDEs with intermittency and turbulent features, where the discrete-time CGKN achieves comparable performance to the state-of-the-art SciML methods in state forecast and provides efficient and accurate DA results. The discrete-time CGKN framework also serves as an example of unifying the development of SciML models and other outer-loop applications such as design optimization, inverse problems, and optimal control.

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MS25

Model Discovery for Nonautonomous Translation-Invariant Problems

Discovery of mathematical descriptors of physical phenomena from observational and simulated data, rather than from the first principles, is a rapidly evolving research area. Two factors, time-dependence of the inputs and hidden translation invariance, are known to complicate this task. To ameliorate these challenges, we combine Lagrangian dynamic mode decomposition with a locally time-invariant approximation of the Koopman operator. The former component of our method yields an optimal low-rank linear surrogate model of a system's dynamics in the least squares sense, while the latter addresses the system's nonlinearity and non-autonomous behavior. We provide theoretical bounds of the method's interpolation accuracy and perturbation error with respect to the numerical rank and sampling frequency of training data. The accuracy and numerical stability are demonstrated on two problems, fluid flow past a solid cylinder (incompressible Navier-Stokes equations) and transport of a passive scalar (advection-diffusion equation), through comparisons with the stan-

dard and Lagrangian-based dynamic mode decompositions.

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MS26

A Complete and Bi-Continuous Invariant of Protein Backbones

Proteins are large biomolecules that regulate all living organisms and consist of one or several chains. The primary structure of a protein chain is a sequence of amino acid residues whose three main atoms (alpha-carbon, nitrogen, and carbonyl carbon) form a protein backbone. The tertiary (geometric) structure is the rigid shape of a protein chain represented by atomic positions in a 3-dimensional space. Because different geometric structures often have distinct functional properties, it is important to continuously quantify differences in rigid shapes of protein backbones. Unfortunately, many widely used similarities of proteins fail axioms of a distance metric and discontinuously change under tiny perturbations of atoms. We introduce a complete invariant that identifies any protein backbone in space, uniquely under rigid motion. This invariant is Lipschitz bi-continuous in the sense that it changes up to a constant multiple of any perturbation of atoms, and vice versa. The new invariant has been used to detect thousands of (near-)duplicates in the Protein Data Bank, whose presence inevitably skews machine learning predictions. The resulting invariant space allows low-dimensional maps with analytically defined coordinates that reveal substantial variability in the protein universe. The talk is based on the 34-page paper at https://arxiv.org/abs/2410.08203, to appear in the journal MATCH Communications in Mathematical and in Computer Chemistry.

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MS26

A Tile Model of Circuit Topology for Self-Entangled Biopolymers

It has been established that knots, slipknots, and other complex topologies exist in cellular proteins and have been conserved throughout evolution. Yet the global topology of a chain only provides a limited view of its topological entanglement. In particular, even if the chain is unknotted, there can be tangling of sites which may be distant on the amino acid sequence but are twisted together and held in place by molecular forces. We model this type of entanglement by starting with a collection of 1-string and 2-string tiles that are based on local entanglements that have been observed in protein chains. We then combine our tiles according to a well defined set of operations. Using the algebra of tiles and operations we symbolically represent all entanglements that can be built up in this way, and determine which knot types can occur.

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MS26

Programming Dna Self-Assembly by Geometry

We describe mathematical methods for design and assemble crystallographic structures by DNA. These methods model and analyzes structures obtained as bottom-up assembly, as well as the process of self-assembly itself. We show several methods based on periodic graphs and topological graph theory that enable designs of various crystals with different tertiary chiralities.

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MS26

Symmetry-preserving Crystal Generation with Diffusion Models

Diffusion modelsa generative method that iteratively turn noise into structured samplesare emerging as powerful tools for crystal structure generation, offering a route to propose candidate materials for batteries, electronics, catalysis, and more. Their appeal is the ability to explore vast combinatorial design spaces while retaining atomic-scale realism. Yet a central defining feature of crystalstheir space-group symmetryremains elusive: existing diffusion approaches either ignore symmetry (yielding invalid or low-quality structures) or implicitly copy common patterns from data, limiting novelty and underrepresenting rare symmetries. We present SymmCD, a diffusion framework that builds symmetry into generation. It factors a crystal into (i) an asymmetric unit (minimal atomic motif) and (ii) the symmetry operations that replicate it. By learning a joint distribution over these two components in an interpretable representation, SymmCD produces diverse, chemically plausible crystals while automatically enforcing realistic space-group organization, including for sparsely observed groups.

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MS27

Optimal Multimaterial Composites: the Structure of Fields, Bounds, Laminates, and Rank-One Envelope

The problem of the best periodic composite structure is formulated as a problem of the quasiconvex envelope for a multiwell Lagrangian. Since we compare all structures, the minimizers - gradient fields or stresses in an optimal structure - are independent of the geometry and are determined by a few parameters: moduli of the mixed materials, their volume fractions, and the applied field; therefore the problem can be reduced to finite-dimensional optimization problem. The problem describes the sets of variations of fields in materials in the optimal structures. The suggested pointwise inequalities constraints on the fields complement the translation bounds for multicomponent composites. The description of exact bounds is accompanied by the optimal laminates that realize them. The paper defines these laminates as paths of the Rank-One-Convex envelope

that join the found sets of the optimal fields in materials. The Rank-One-Convex envelopes structure mimics a composite cells optimal geometry.

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MS27

Dispersion, Clusters, and Gaps in Periodic Media

We study the propagation of time-harmonic waves in an infinite medium containing a periodic array of small inclusions of arbitrary shape with the Dirichlet or transmission conditions on their interfaces. The inclusion size is much smaller than the array period while the wavelength is fixed. We derive dispersion relations and show that there are exceptional frequencies for which the solution is a cluster of waves propagating in different directions with different frequencies. The approach is based on reducing the problem to the study of the condition for the existence of a zero eigenvalue of a specially constructed Dirichlet-to-Neumann operator. This allows us to use the regular perturbation techniques and obtain exact asymptotic results for the cutoff frequency in the case of homogeneous Dirichlet boundary conditions. We show that global gaps do not exist if the size of inclusion is small enough. The notion of local gaps depending on the choice of the wave vector **k**, is introduced and studied.

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MS27

Mathematics of Frozen Seas and Other Multiscale Composites

Analyzing and modeling the dynamics and thermodynamics of Earths sea ice covers involves problems ranging in scale from millimeters to hundreds of kilometers. From tiny brine inclusions to surface melt ponds on massive ice floes, sea ice is a composite material with a hierarchy of complex microstructures, most of which display some form of fractal geometry. In large scale climate and ecosystem models the parameters often involve the effective properties of sea ice on various scales. In this talk well consider problems of finding these effective properties using methods of homogenization and statistical physics. In particular, well discuss Stieltjes integral representations for effective parameters of two-phase composites, polycrystalline media, advection diffusion processes, and surface wave propagation and localization in the ice pack. Finally, well also consider applications to other areas of materials science such as twistronics.

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MS28

Regulating MRNA Targeting to Mitochondria with Genetics, Geometry, and Transport

Many mitochondrial genes are encoded in the nucleus, translated in the cytosol, and the proteins imported into mitochondria. The mRNA for many of these nuclear-encoded mitochondrial genes associate with the mitochondria surface, tethered by a nascent polypeptide attached to a translating ribosome on the mRNA and a mitochondrial import complex. Experiments have shown that the degree of mRNA association varies between genes and with mitochondrial volume, and is altered by perturbations to intracellular transport. We use quantitative modeling to show how translation kinetics controls the ability of mRNA to associate with mitochondria, while mitochondrial volume affects how frequently an mRNA will encounter mitochondria, together determining mitochondrial mRNA association. In larger cells mitochondria are nonuniformly distributed, and mitochondrial transport to and from regions of elevated mitochondrial concentration, and perturbation of this transport, also impacts association of mRNA with mitochondria. This work describes how translation kinetics and intracellular transport combine with mitochondrial size and distribution to regulate mRNA targeting to mitochondria.

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MS28

Stochastic Dynamics of Translation and Cotranslation Folding

Translation of proteins define a stochastic process that is heterogeneous across organisms and genes. Using experimental data from high throughput sequencing and structural biology, we investigated the determinants of such heterogeneity. Our analysis relies on the properties of the Totally asymmetric simple exclusion process (TASEP), that we used to model the traffic of ribosome on a mRNA sequence to infer their local dynamics and derive first principles of translation regulation. As variations in translation speed can also affect the folding of the nascent polypeptide, we further derive a coarse grained representation of the ribosome 3D structure and its exit tunnel from cryo-EM structures, that allows to study the dynamics of the polypeptide ribosome complex and investigate various biological processes associated with cotranslational folding and translational arrest.

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MS28

Mathematical Analysis of the Formation of Traplining in Bees

Many foraging animals, including bees, develop near-optimal movement patterns based on memory. While models have simulated how bees establish deterministic traplines, formal mathematical proofs of their behavior remain scarce. We address this gap by adapting and simplify-

ing the Dubois et al. (2024) model to enable mathematical analysis. We prove that simulated bees will always eventually converge to a single deterministic route. Additionally, we propose conjectures about the distribution of routes to which simulated bees may converge. Future work could explore inference methods for learned behavior based on this model. These findings have implications beyond biology, providing insights into reinforced random walks and reinforcement learning.

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MS28

Stochastic Models for Local Regulation of Biological Species

Motivated by recent explorations in theoretical ecology on the role of dispersal traits in range expansion, we consider stochastic models of populations in locally regulated spatial populations which incorporate Allee effects. We discuss the deterministic models described by integro-differential equations obtained as one scaling limit of these models, and some observations describing the trade-off between the capacity constraint, Allee threshold and the speed of range expansion. We then consider the stochastic limits obtained as a different scaling limit of the individual based model in the form of stochastic differential equations and stochastic partial differential equations. We posit the dependence of the population extinction or of its survival on the dispersal trait, constraint, and Allee threshold.

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MS29

Modellig Solid Tumour Phenotypic Plasticity As a Driver of Resistance to Targeted Therapies

Intra-tumour heterogeneity, either the product of genetic mutations or phenotypic adaptation, is a leading cause of treatment failure and disease progression in cancer. Accordingly, there is increased interest in the development of mathematical approaches that capture this heterogeneity and its role in the development of treatment resistance. Here, I'll discuss some recent work focused on developing mathematical approaches to understand the emergence of treatment resistance in preclinical experiments of treatments for solid cancers.

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MS29

Optimizing Clonal Reduction Strategies Targeting Perturbed Stem Cell Kinetics in Acute Myeloid Leukemia

Acute myeloid leukemia (AML) arises from mutations in hematopoietic stem cells, causing them to convert to leukemic stem cells (LSCs) and blocking the downstream differentiation of myeloblasts. Standard AML therapies use cytotoxic chemotherapies to debulk these undifferentiated myeloblasts but they do not target the LSCs sustaining the disease, leading to relapse. This explains why the overall survival of older patients diagnosed with AML has not significantly increased. Thus, targeting LSCs is key to acute myeloid leukemia cure. In vitro drug repurposing screens by our collaborators identified specific cardiac glycosides and glucocorticoids that preferentially target LSC-enriched CD34+ cells, induing their death or differentiation. To identify which of these drugs holds the most promise for ongoing clinical development, we constructed a stochastic mathematical model of the stem cell pool during AML and integrated pharmacokinetic and pharmacodynamic models of five drugs of interest. Our results show that despite their potency, cardiac glycosides are too toxic for safe use in humans. Conversely, our model predicted that mometasone could prevent relapse through its ability to drastically reduce the LSC population. Hence, this work highlights the prospect of glucocorticoids for anti-LSC strategies and underlines the use of quantitative approaches to preclinical drug translation in AML.

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MS29

Strategies for Optimizing the Efficacy of Oncolytic VirusImmune System Interactions

Oncolytic virotherapy (OVT) is an innovative cancer treatment in which oncolytic viruses are introduced into a patient to selectively target and destroy tumor cells. In the absence of these viruses, tumors are known to create an immunosuppressive environment. However, upon administration of oncolytic viruses and initiation of virotherapy, the immune system is activated, leading to a robust anti-tumor response. Despite this, oncolytic viruses alone have rarely been shown to induce complete and sustained regression of established tumors in vivo. In this talk, I will discuss key strategies for enhancing the efficacy of oncolytic virotherapy. These include the integration of immunotherapy approaches with virotherapy to amplify anti-tumor immune responses, as well as optimizing the timing, dosage, and sequencing of viral administrations to maximize therapeutic benefits. By refining these strategies, we aim to improve treatment outcomes and potentially enhance the therapeutic impact of oncolytic virotherapy.

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MS30

Solving the Transmission Problem for Open Waveguides

We introduce a class of computationally tractable scattering problems in unbounded domains, which we call *decomposable problems.* In these decomposable problems, the computational domain can be split into a finite collection of subdomains in which the scatterer has a "simple" structure. A subdomain is simple if the domain Green's function for this subdomain is either available analytically or can be computed numerically with arbitrary accuracy by a tractable method. These domain Green's functions are

then used to reformulate the scattering problem as a system of boundary integral equations on the union of the subdomain boundaries. This reformulation gives a practical numerical method, as the resulting integral equations can then be solved, to any desired degree of accuracy, by using coordinate complexification over a *finite* interval, and standard discretization techniques.

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MS30

Homogenized Graphs with Spectrally Embedded Defect States

By homogenizing high-contrast periodic metric graphs, we create continuous media that admit bound states produced by local defects at energies embedded in the continuous spectrum. This is achieved by embedding two coupled copies of a three-dimensional lattice graph simultaneously into space. Convergence of the metric graphs to a continuous dispersive medium with spectrally embedded defect states is obtained through operator-norm convergence of resolvents. This is joint work with Kirill Cherednichenko.

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MS30

Topological Many-Body Ground States in Magic Angle Twisted Bilayer Graphene

Over the past few years, magic angle twisted bilayer graphene (MATBG) has drawn immense interest due to the experimental observation of superconductivity and other exotic phases of matter in this material. The electronic properties of MATBG are dominated by electron-electron effects which require many-body theory to describe. In this talk, I will discuss our recent characterization of the entire many-body ground state manifold of MATBG in a simplified limit. Remarkably, while the single particle model for MATBG is Chern trivial, after adding electron-electron interactions the many-body ground states spontaneously develop a non-trivial Chern index. This result suggests that some of the properties of ground states of MATBG in the simplified limit may be topologically protected when moving to the physically realistic regime.

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MS31

Quantizaton and Reordering for Lp-Lq Regularization

Linear discrete ill-posed problems arise in many areas of science and engineering. Examples of this kind of problems are computed tomography and image restoration. Theirs solution is very sensitive to perturbations in the data. To reduce the sensitivity to the perturbation, the original problem is often replaced by a minimization problem with a fidelity term and a regularization term that depends on a regularization matrix L applied to the desired solution. We present an extension of the method proposed in [A. Buccini, et al. On the choice of regularization matrix for an $\ell_2 - \ell_q$ minimization method for image restoration. *Appl. Numer. Math.*, 164 (2021)] for choosing a matrix L that performs a reordering of the entries of the solution after applying a quantization. If we are able to choose the exact reordering, quantization has the effect of including the exact solution in its null space. We also allow the norm of the fidelity term to be different than 2 for adapting the method in case of non-Gaussian error and we investigate the choice of other differential operator than the first order finite difference bidiagonal matrix.

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MS31

Reconstruction of Extended Regions in EIT with a Generalized Robin Transmission Condition

In this talk, we will discuss an application of the Regularized Factorization Method (RegFM) to a problem coming from Electrical Impedance Tomography (EIT) with a second-order Robin condition. This method falls under the category of qualitative methods for inverse problems. Qualitative methods are used in non-destructive testing where physical measurements on the surface of an object are used to infer the interior structure. The Robin condition on this boundary asymptotically models delamination. We assume that the Dirichlet-to-Neumann (DtN) mapping is given on the exterior boundary and will be used to recover an unknown, extended region. Using Cauchy data as physical measurements, we can determine if all of the coefficients from the Robin condition are real- or complex-valued. We study these two cases separately and show how RegFM can be used to detect whether delamination has occurred and recover the damaged subregion. Numerical examples will be presented for both cases in two dimensions in the unit circle.

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MS31

Efficient Methods for Dynamic Image Reconstruction with Motion Estimation

Large-scale dynamic inverse problems are typically ill-posed and suffer from complexity of the model constraints

and large dimensionality of the parameters. A common approach to overcome ill-posedness is through regularization that aims to add constraints on the desired parameters in both space and temporal dimensions. In this work, we propose an efficient method that incorporates a model for the temporal dimension by estimating the motion of the objects alongside solving the regularized problems. In particular, we consider the optical flow model as part of the regularization that simultaneously estimates the motion and provides an approximation for the desired image. To overcome high computational cost when processing massive scale problems, we combine our approach with a generalized Krylov subspace method that efficiently solves the problem on relatively small subspaces. The effectiveness of the prescribed approach is illustrated through numerical experiments arising in dynamic computerized tomography and image deblurring applications.

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MS32

Modeling Flying Formations as Flow-mediated Matter

Collective locomotion of flying animals is fascinating in terms of individual-level fluid mechanics and group-level structure and dynamics. In this talk, I will introduce a model of formation flight that views the collective as a material whose properties arise from the flow-mediated interactions among its members. It builds on an aerodynamic model that describes how flapping flyers produce vortex wakes and how they are influenced by others' wakes. Long in-line arrays show that the group behaves as a soft, excitable "crystal" with regularly ordered member "atoms" whose positioning is susceptible to deformations and dynamical instabilities. Perturbing a member produces longitudinal waves that pass down the group while growing in amplitude; with these amplifications even causing collisions. The model explains the aerodynamic origin of the spacing between the flyers, the springiness of the interactions, and the tendency for disturbances to resonantly amplify. Our findings suggest analogies with material systems that could be generally useful in the analysis of animal groups.

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MS32

Reversals of the Large-scale Circulation in Thermal Convection

The large-scale circulation (LSC) associated with thermal convection is known to spontaneously reverse direction. In the atmosphere, reversals can result in a sudden change in wind direction, while in the liquid core, reversals may play a role in magnetic dipole shifts. We examine LSC reversals within the context of thermal convection in an annular domain. Through comparison with direct numerical simulations, we show that a low-dimensional dynamical system derived systematically from Galerkin truncation of the governing equations accurately describes a sequence of parameter bifurcations, including the onset of circulatory flow, the appearance of chaotic LSC reversals, and finally a high-Rayleigh-number state of periodic LSC reversals with small-scale turbulence. When cast in terms of the fluids angular momentum and center of mass, the model reveals equivalence to a pendulum system with driving term that raises the center of mass above the fulcrum. It is the competition between driving, restoring, and damping that leads to the range of convective states. This physical picture yields accurate predictions for the frequency of regular LSC reversals in the high Rayleigh-number limit and offers a transparent mechanism for reversals.

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MS32

Predictive Models for Experimental Measurements of Dissolving Particles in Environmentally Applicable Water Flows

The transport dynamics of non-spherical particles in turbulent flowsparticularly within the inertial subrangeremain an open and complex problem in fluid mechanics. This study quantitatively characterizes particle kinematics, including tumbling and spinning motions, and evaluates associated enstrophy for both fixed-size and dissolving particles in environmental flow regimes. We develop and assess dynamic panel data (DPD) models that estimate the evolution of particle size and density based on current and lagged values of key dynamic variables. An important feature of the DPD approach is that we can model the flux transition from one observation to the next using generalized method of moment statistical techniques. These models are applied to experimental datasets featuring particles of varying aspect ratios and initial sizes, within both homogeneous isotropic turbulence and stratified flows. Results from (i) neutrally buoyant particles suspended in homogeneous isotropic turbulence and (ii) negatively buoyant particles settling through a two-layer stratified fluid indicate that the last periods observed mass is the dominant predictor of this periods observed mass. Particle density and surface-area-to-volume ratio serve as dominant predictors in modeling mass flux. The DPD approach has significant implications for empirical modeling of particle-fluid inter-

actions in environmental and industrial contexts.

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MS32

Low-order Reaction-diffusion System Approximates Heat Transfer and Flow Structure in Annular Convection

The heat transfer of fluid can be greatly enhanced by natural convection, leading to the famous Nu-Ra scaling that has been a focus of modern fluid dynamics. Our work explores natural convection in an annular domain, where the annular geometry reinforces the large-scale circulation (LSC) and leads to an altered Nu-Ra scaling. To understand the heat transfer and flow pattern in this novel geometry, we derive a reduced model from the Navier-Stokes-Boussinesq equations where the equations of flow and heat are transformed to a system of low-order reaction diffusion equations. As we increase the Rayleigh number, this reduced model recovers the three states seen in the direct numerical simulation (DNS): the motionless conductive state, the circulating state with a steady LSC, and the reversal state where the LSC reverses direction spontaneously. Moreover, the reaction diffusion equations preserve the same boundary layer structures seen in the DNS, allowing us to directly measure the Nusselt and Reynolds numbers. By matching the solutions inside and outside the boundary layer, we recover the Nu-Ra and Re-Ra scaling law of the DNS, further demonstrating the accuracy of this reduced model. Our results also provide a systematic way of analyzing thermal convection in an annular domain, which brings us one step closer to understanding the origin of LSC and the mechanism of convective heat transfer.

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MS33

Future Grids Need Flexibility: How AI and Digital Twins Can Enable Real-Time Decision Making for Low-Carbon Power Grids

Power grids are rapidly decarbonizing to address climate challenges and expanding to meet increasing loads from electrification and AI growth. However, integrating increasing quantities of renewable generation presents a challenge to how we operate power grids: power grids rely on fine control of generation resources. Renewable resources are uncontrollable and intermittent, reducing decision-making timescales from days to minutes. As these systems rapidly change, digital twins become increasingly necessary to provide real-time visibility and control. By layering AI applications on top of real-time monitoring, we can achieve real-time decision making and operational flexibility throughout the grid. This talk will focus on increasing grid efficiency using network reconfiguration. The specialized use of physics-informed machine learning for fast and accurate decision making will be introduced. Our results show how integrated intelligent systems can adapt existing systems to realize next generation grid operations, and exemplify the use of digital twins for critical infrastructure.

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MS33

A Noninvasive Method for Determining Elastic Properties of Valve Tissue

Valvular heart disease is a leading contributor to cardiovascular morbidity and mortality, affecting nearly 19 million people globally and accounting for 20% of cardiac surgeries in the United States. Despite the prevalence of this condition, selecting the optimal repair strategy for individual patients remains a significant challenge. While computer simulations of virtual interventions hold potential for guiding valve repair, computational models simulated using mechanical parameters derived from ex vivo experiments often differ from in vivo observations. This mismatch reduces clinical applicability of in silico valve repair for achieving optimal surgical outcomes. To address this, we introduce ADEPT, a noninvasive framework that determines in vivo elastic parameters of heart valve tissues from clinical 3D echocardiograms (3DE). ADEPT combines image-derived valve displacements from 3DE time sequences with physics-informed neural networks to estimate the complex nonlinear mechanical properties of valve tissue. Finite element simulation of a heart valve using elastic properties derived from ADEPT showed excellent alignment with the reference image segmentation data, demonstrating less than 1 mm variation in the systolic frame. This noninvasive, image-derived approach to estimating mechanical properties from readily available clinical data presents substantial translational potential for advancing patient-specific heart valve modeling and treatment strategies.

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MS34

Splay Nematic Equilibrium Structures

We consider a free energy functional to study the splay nematic phase in bent-core liquid crystals. We numerically investigate the behavior of the solutions as a physical parameter related to temperature varies, with the goal of identifying the regime of stability for the so-called single splay and double splay states. This is joint work with Carlos Garca-Cervera and Sookyung Joo.

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MS34

Formation of Chiral Structures in Nematic Liquid Crystals

The formation of chiral structures from both chiral molecules and achiral liquid crystal systems is considered in one dimension. We first examine cholesteric liquid crystals, determining their minimizers when the intrinsic pitch conflicts with the twist imposed by boundary conditions. Nematic liquid crystals composed of achiral bent-core molecules, which exhibit periodically modulated structures, have been observed relatively recently and have since been extensively investigated in the field of liquid crystals. One such phase is the twist-bend nematic phase, in which the molecules arrange in a heliconical structure with a nanoscale pitch. We characterize heliconical formation within a certain material parameter range and identify the parameter regimes that ensure the stability of strong local minimizers in the nematic and cholesteric phases. Numerical simulations based on constrained minimization illustrate the predictions of our analysis. This is a joint work with C. Garcia-Cervera, T. Giorgi, and Z. Li.

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MS34

Particle Approximation of Nonlocal Energies

We consider particle interaction energies defined via a pairwise interaction kernel. These energies are directly related to, and can be considered as, discrete versions of continuous interaction energies defined over probability measures. In their discrete or continuum form, such pairwise interaction energies appear in many biological or physical applications, ranging from swarming models to models of molecular structure. Under rather general assumption on the interaction kernel we prove that the discrete energies admit minimizers for sufficiently large number of particles, they converge to their continuum counterpart in the weak-* topology of probability measures, and minimizer of discrete energies converge to the minimizer of the continuum energy. This is a joint work with Davide Carazzato and Aldo Pratelli.

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MS34

Maximizing Problem for Convex Mean p-Stress

This talk will demonstrate that if u is the nonnegative solution/stress of the classic torsion problem on an n-dimensional bounded convex domain B with positive volume $|B|$ then such a maximizing problem for the convex mean p-stress: $\sup_B \int_B (u/|B|^{\frac{1}{p}+\frac{2}{n}})^p$, is not only achievable but also the boundary ∂B_* of the induced maximizer B_* is C^1-smooth - consequently - if the gradient of the stress of B_* is constant on ∂B_* then B_* must be a ball.

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MS35

Operator Learning Via Non-Smooth Dynamics

Neural nets are often used both to learn operators and also to identify data sets. A typical architecture for doing this is a ResNET, which in turn can be thought of as a discretisation of a neural ODE. We can then pose the question of what sort of operators, or data set labelling, can be learned through such an architecture. If classical smooth ODEs are used to describe the neural ODE then there are restrictions on what is possible. However, in practice, the activation functions used in a ResNET are non-smooth and the resulting neural ODEs are also non-smooth. This allows them to have much greater expressivity, and this expressivity can be explored by using the theory of non-smooth dynamical systems. In this talk I will describe some of this theory, and will show not only how it explains some of the great expressivity possible in a ResNET, but also indicates what might be appropriate architectures and training meshanisms for them to approximate complex operators.

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MS35

Compositional Physics-Informed Neural Flows

Physics-Informed Neural Networks (PINN) have recently been applied to solve many forward and inverse problems. For time-dependent problems, PINN is trained by minimizing a residual loss function sampled on a fixed spatial domain and time interval, which can result in poor generalizability beyond its training time interval. Instead, we propose Compositional Physics-Informed Neural Flow (CPINF) to learn flow maps of dynamical systems, while preserving its compositional structure and enabling rigorous error estimation on its prediction beyond the training time interval. Specifically, for dynamical systems with a compact positively invariant set, we show that the error of CPINF on future time intervals can be bounded by the training error on its initial training time interval and the sampling error of the residual.

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MS35

Symplectic Neural Flows

The Hamiltonian formalism provides a powerful framework for describing several dynamical systems with conserved energy. The flow of a Hamiltonian system preserves a volume form, a symplectic form, and the Hamiltonian energy.

This talk focuses on canonical Hamiltonian systems on Euclidean spaces. We introduce a symplectic neural network designed to approximate the flow map of a given Hamiltonian system. Our architecture demonstrates improved long-term behaviour compared to unconstrained alternatives, even when both approaches perform similarly over short intervals. We also apply the proposed method to data-driven tasks, showing its effectiveness in approximating the flow map of unknown Hamiltonian systems.

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MS35

Diffeomorphic Neural Operator Learning

This talk introduces an operator-valued approximation technique for the data-driven reconstruction of a class of evolution operators. The core idea is to approximate the solution operator as a map into the space of composition operators. We draw parallels between this technique and shape analysis via landmark matching in an infinite-dimensional setting and propose a computationally tractable algorithm using neural operators (NOs). Our formulation exhibits novel resolution properties which complement, yet are distinct from, the discretization invariance exhibited by NOs. We characterize these properties analytically and illustrate them numerically for the data-driven forecasting of a turbulent fluid flow. This geometric operator learning approach indicates a clear performance benefit by embedding known infinite-dimensional geometric structure into the learning problem as a hard constraint.

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MS36

Optimal Switching of Investment Between Emergency, Target Date, and Retirement Savings Accounts

People are advised to save money for emergencies, for another known expense arriving at different timescale (e.g. future university education expenses for children), and for retirement. The emergency account should likely be very liquid and be kept in zero risk cash or a near cash equivalent; the other accounts will have different risk-return characteristics. The consequences to not having an emergency account large enough to meet a pressing emergency may be quite expensive, but a too large emergency account will not generate much in the way of investment return. Money is not fully fungible between other various government sponsored accounts. How then should a household allocate a stream of savings to these different accounts? I will present a stylized, analytically tractable, model of the situation and discuss how the regulatory and practical complexities might alter the optimal solutions obtained with this model.

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MS36

Rethinking Dollar Cost Averaging: A New Perspective on Retirement Contributions

Dollar Cost Averaging (DCA) is a widely used investment strategy in which an investor divides a total investment across periodic purchases of an asset to reduce the impact of volatility. This approach contrasts with the lump sum (LS) strategy, where the entire investment is deployed at once. Traditional finance literature often positions DCA as a risk mitigation tool, emphasizing its role in reducing market timing risks. However, empirical studies suggest that LS tends to outperform DCA in most scenarios, given the general upward trend of markets over time. In this study, we challenge the conventional view of DCA by examining how real-world investor behavior influences investment outcomes. While LS may offer higher expected returns in a purely mathematical sense, it does not account for practical factors such as cash flow constraints, investment discipline, and psychological barriers to investing large sums at once. By considering how investors make decisions in practice - including their perceptions of market fluctuations and their commitment to consistent contributions - we find that DCA can offer meaningful advantages. This perspective reframes DCA not just as a risk management tool but as a strategy that aligns with the way people actually invest.

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MS36

Approximating the Money-Weighted Rate of Return

We develop a closed-form approximation to the so-called money-weighted rate of return (MWRR), in the context of a stylized retirement savings account. The approximation is general in the sense that (i) it allows for contributions of varying sizes made at irregularly-spaced times (including both discrete and continuous contributions), (ii) it allows the composition of the underlying portfolio (as manifested through the mean and standard deviation of its instantaneous return) to vary through time and (iii) it does not make any specific assumptions on the stochastic dynamics of the underlying portfolio return. The approximation facilitates rigorous insights into a complicated object, which in turn allows us to explain and/or resolve findings elsewhere in the literature. This is joint work with R.M. Reesor, M. Lau and D. Polegato.

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MS36

Density Ratio Estimation of Trading Data During Market Shocks for Behavioural Change-point Detection

Clients choose portfolios under the advice of financial advisors, and the construction and trading behaviours in those portfolios are meant to reflect client risk tolerance levels. However, uncertainty caused by market crashes affects client choices, where groups of clients make sub-optimal de-

cisions relative to their risk tolerance and financial goals. Clustering algorithms that aim to cluster time series over large periods of time fail to capture these potential dynamic cluster memberships over time. This talk investigates the relationship between cluster structures in financial data and significant market events, specifically market crashes, using distance-based sliding window clustering for change-point detection. Using a double sliding window approach, we examine the changes in cluster structures, which represent shifts in client behaviours. We detect these shifts using nonparametric density ratio estimation (DRE), specifically the relative unconstrained least-squares importance fitting (RuLSIF) method, to estimate divergence measures between financial time series. By comparing cluster reorganizations with distributional divergences, we establish changes in group choices for pre- and post-crash periods. By linking cluster dynamics to divergence metrics, this approach bridges the gap between DRE-based change-point detection and clustering methodologies, offering a two-fold perspective on both structural (cluster-based) and statistical (DRE-based).

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MS37

Global Continuation of Periodic Solution to a Coupled Delayed Algebraic-Differential Equations

We examine a coupled delayed algebraic-differential system motivated by emerging infectious disease outbreaks with population behavioural change in response to perceived risks associated with the incidence. We focus on the impact of behavioural adaptation on the global dynamics of the disease spread, and we show the occurrence of persistent periodic waves with large amplitudes.

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MS37

Understanding Immunological Memory Responses to Sars-CoV-2 Infections and Covid-19 Vaccines Through Mathematical Modeling

Durable immunity against SARS-CoV-2, generated from prior natural infection or vaccination, is critical for long term protection against severe COVID-19. However, the potency and longevity of immune responses to SARS-CoV-2 reinfections vary depending on how immune memory is established and the distinct waning dynamics of its key components, including T cells, B cells, and antibodies. To gain deeper insights into these dynamics, we developed a series of modular, mechanistic mathematical models to study immunological memory responses to SARS-CoV-2 after natural infections and mRNA COVID-19 vaccinations. Specifically, we extended an immunovirological model describing cytokine-regulated immune innate and adaptive responses to primary SARS-CoV-2 infection to include the establishment and recall of CD8+ T cell and B cell memory to study infection and reinfection. Extending this to vaccines, we characterized how mRNA vaccines initiate and enhance memory responses during both primary and subsequent vaccinations. Throughout, we investigated key factors influencing memory responses across different pathways of memory establishment. Our integrated model also allowed us to address immunological questions related to the interplay between innate, cellular, and humoral immune responses, hybrid immunity, and breakthrough infections.

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MS37

Modeling Delays in a Within-Host Infection Differential Equation Model

Simple ordinary differential equation virus dynamics models can be used to describe within-host infection time courses. These typically assumes that the immune response is constant over time and fails to account for the components of the immune response not being activated at the same time, due to many factors, including pre-existing immunity. To understand the evolution of long-term immunity and the impact of recurrent infections, we developed a delay differential equation model that explicitly accounts for both the innate and adaptive immune responses, which are broadly the first and second phases of the immune response, and the generation of immunological memory post-infection. In this talk, I will present the underlying mechanisms of the immune response, from which we derive our model. Numerical simulations of the model, under different conditions, will be presented to illustrate how this model can be used to understand immunity dynamics and study strategies that enhance immunity and minimize infection and reinfection.

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MS37

Modeling Viral Dynamics with Dual Infection Modes, Immune Response, and Intracellular Delays

Understanding viral infection dynamics is crucial for improving treatment strategies. In this talk, I will present a mathematical model that integrates two infection modesvirus-to-cell and cell-to-cell transmissionalong with the CTL immune response and distributed intracellular delays in infection, viral production, and immune cell recruitment. Our analysis identifies key threshold parameters to determine the viral dynamics. I will discuss the stability of three equilibria: the infection-free state, the immune-inactivated state, and the immune-activated state. Our results reveal that delays in CTL recruitment can induce stability switches, leading to oscillatory viral loads. Additionally, I will highlight the relative contributions of different infection modes and explore how Filippov control strategies can optimize antiretroviral therapy. Numerical simulations validate our theoretical findings and offer insights into controlling infection dynamics. This talk is

based on joint work with Drs Deng, Shu and Wang.

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MS38

Statistical Inversion for Diffuse Optical Tomography Using Ml and Level Set Methods

In this talk, we will provide an overview of the ill-posed inverse problem in Diffuse Optical Tomography (DOT). Then we present the Bayesian inversion using machine learning and level sets for image reconstruction. The results of image reconstruction will be 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 (Xian Jiaotong-Liverpool University).

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MS38

Graph-Based Active Learning for Nearly Blind Hyperspectral Unmixing

Hyperspectral unmixing (HSU) is an effective tool to ascertain the material composition of each pixel in a hyperspectral image with typically hundreds of spectral channels. This talk involves two graph-based semisupervised unmixing methods. The first one directly applies graph learning to the unmixing problem, while the second one solves an optimization problem that combines the linear unmixing model and a graph-based regularization term. Following a semisupervised framework, our methods require a very small number of training pixels that can be selected by a graph-based active learning method. Compared with other popular blind unmixing methods, our methods significantly improve performance with minimal supervision. Specifically, the experiments demonstrate that the proposed methods improve the state-of-the-art blind unmixing approaches by 50% or more using only 0.4% of training pixels.

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MS38

Texture Segmentation From a Manifold Learning Perspective

A manifold-learning approach to image segmentation is introduced that separates textures with minimal prior knowledge. The image is studied as a point cloud of patches, and ideas from density estimation and clustering are used to differentiate between patterns inherent to the image. After selecting a subset of patches that have high estimated density, the Continuous k-Nearest Neighbors (CkNN) algorithm is used to find a persistent clustering of the selected patches. Classification of the remaining patches and the pixels within are inferred in turn from the high-density patches. The method is shown to automatically detect regions of images with distinct textures in artificially generated images and representative images from materials science.

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MS38

Detecting AI Generated Images Through Texture and Frequency Analysis of Patches

The significant improvement in AI image generation in recent years poses serious threats to social security, as AI generated misinformation may infringe upon political stability, personal privacy, and digital copy rights of artists. Building an AI generated image detector that accurately identifies generated image is crucial to maintain the social security and property rights of artists. This paper introduces preprocessing pipeline that uses positional encoded azimuthal integrals for image patches to create fingerprints that encapsulate distinguishing features. We then trained a multi-head attention model with 97.5% accuracy on classification of the fingerprints. The model also achieved 80% accuracy on images generated by AI models not presented in the training dataset, demonstrating the robustness of our pipeline and the potential of broader application of our model.

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MS39

Advancing Gender Equality in Mathematics: Efforts and Initiatives of the Gender and Equity Committee of the Mexican Mathematical Society

The Gender and Equity Committee of the Mexican Mathematical Society plays a crucial role in promoting gender equality in mathematics in Mexico. Established to address the underrepresentation of women in the field, the committee works through research, advocacy, and community-building initiatives to foster a more inclusive mathematical community. In this talk, we will present a few of the activities (and their motivations) and achievements of the committee, including activities, data collection on gender disparities, mentorship programs, outreach efforts, and policy recommendations aimed at improving the participation of women in mathematics. We will also discuss ongoing challenges, emerging opportunities and potential collaborations. By sharing our experiences, we aim to contribute to a broader discussion on innovative initiatives for women in mathematics.

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MS39

Putting a Creative Touch in Our Academic Career Abstract

An academic career involves teaching, research, training of graduate students, administration and anything else you can think of. Academic mathematicians have a certain amount of freedom and creativity on how they orient their career. How do women mathematicians use this freedom? Where do they feel most comfortable? Do they do things differently from men? I will discuss these issues, and bring

a personal point of view of someone who launched the international year Mathematics of Planet Earth 2013 and spearheaded the proclamation of the International Day of Mathematics.

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MS39

Overview of the Icms Retreats for Women in Applied Mathematics in the UK- Challenges, Opportunities and Successes

The "Retreat for Women in Applied Mathematics (RWAM)" was launched as an ICMS (International Centre for Mathematical Sciences) Strategic Event in 2023, by Professor Majumdar (University of Strathclyde) and Professor Mihai (Cardiff University), primarily as a pilot event to build a strong sense of community and professional camaraderie amongst female applied mathematicians in the UK, in response to the strong sense of professional isolation created by the two-year long pandemic. RWAM has been funded three consecutive times from 2023-2025 with overwhelmingly positive feedback from junior female researchers. The main objectives of RWAM are to (i) build a sense of community amongst female applied mathematicians; (ii) to provide a holistic overview of the multi-faceted nature of academic life; (iii) to provide a safe and trusted space for issues specific to female professionals in mathematics; (iv) to discuss career journeys from being a PhD student to a full professor, including work-life balance, and (vii) most importantly, to mentor and support the next generation of junior female mathematicians. In this talk, we review the successes of the RWAM initiative in the past three years and discuss how RWAM can be used to build a strong UK network of female applied mathematicians, that will self-sustain and grow nationally and internationally with time.

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MS39

A Geometers Perspective: How to Create Opportunities for Women in Mathematics?

May 12 marks a global celebration of Women in Mathematics, honoring the legacy of Maryam Mirzakhani and inspiring young minds to follow in her footsteps. Through a couple of personal stories and insights, I will discuss how outreach initiatives like the ones taking place on May 12 encourage young women to pursue mathematics. However, attracting female students in mathematics is a half-fulfilled objective. There are many challenges that women continue to face at various stages in their careers in mathematics and for many of the female students or faculty to reach their full potential highlights the importance of mentorship and building a supportive community.

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MS40

Risk Assessment in River Flooding: Into the Water

We created a Teaching Module which walks students through the process of creating a model for river flooding, which allows us to find the 100 and 500 year flood levels by using a Weibull distribution. This talk will walk the audience through that process and demonstrate how the module can be used to repeat the research project for students in their own regions.

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MS40

Harnessing Artificial Intelligence for Sea Level Rise Risk Assessment

In the mathematics education graduate course Problem Solving for Teachers, we implemented several modules which included research using artificial intelligence. We describe a mathematical and quantitative literacy activity on finding linear regressions, as well as a technological literacy activity on using artificial intelligence to research possible strategies for climate resiliency. The information being modeled comes from the National Oceanic and Atmospheric Administrations Tides and Currents tool, which shows the amount of mean sea level change at various geographic locations across time. Sea level rise and increased flooding in the coastal regions can threaten supply chains and endanger human lives. Conducting climate analyses is now a routine part of national defense strategy, as being informed about the risks of the results of climate change and planning ahead accordingly can help us alter our actions to better prepare for disaster relief. We show middle and high school teachers analyses and feedback on the use of AI in this activity, and present quantitative survey results on the use of AI more broadly in the semester-long course.

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MS40

Risk Assessment Using Block Maximum Techniques in Statistics Through the Lens of River

Flooding

This talk will explicitly discuss the module we created, at the Reconnect 2023 workshop, particularly describing the module summary, targeted audience, prerequisites, expectations and learning outcomes. Will go through the definitions, how to use different distributions to model different situations and why the Weibull distribution is the most appropriate. Please follow the next presentation by Prof. Brian Birgen to learn more details of the applications.

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MS40

Data-Driven Risk Assessment: Undergraduate students research using Federal Emergency Management Agency's National Risk Index

In this presentation, we describe how the 2023 risk assessment educational module, Big Wind Blows the Budget, sponsored by the Center of Discrete Mathematics and Theoretical Computer Science at Rutgers University, was used as a data analytics undergraduate research project. The research compares Expected Annual Loss (EAL) information from the Federal Emergency Management Agency's National Risk index tool across several geographic regions, with a goal of analyzing price trends of disasters over time. The undergraduate researcher conducted this activity in pre-service teacher courses for middle school mathematics and secondary science and mathematics courses in Spring 2024, focusing on better understanding the reasoning behind EAL values and developing ideas for social solutions for mitigating risk of loss. We also present the results of a survey that pre-service teachers took as they reflected on their beliefs in their abilities to implement social justice mathematical lessons with future students.

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MS41

Reading Data Out of a Quantum Computer with Tensor Factorizations

For many practical applications of quantum computing, the most costly steps involve coherently accessing classical data. This is especially true for many proposed applications of quantum linear algebra. We help address this challenge by applying mass production techniques, which can reduce the cost of applying an operation multiple times in parallel. We combine these techniques with modern approaches for classical data loading based on "quantum read-only memory.' We find that we can polynomially reduce the total number of gates required for data loading, but we find no advantage in cost models that only count the number of non-Clifford gates. Furthermore, for realistic cost models and problem sizes, we find that it is possible to reduce the cost of parallel data loading by an order of magnitude or more. We present several applications of quantum mass production, including a scheme that uses parallel phase estimation to asymptotically reduce the gate complexity of state-of-the-art algorithms for estimating eigenvalues of the quantum chemical Hamiltonian. We also show that mass production can be used to reduce the cost of serial calls to the same data loading oracle.

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MS41

Explicit Quantum Circuits for Block Encodings

Block encoding is a fundamental building block in quantum linear algebra, enabling the embedding of a matrix A into a larger unitary operator U suitable for quantum computation. Despite its theoretical importance, block encoding is often treated as a black-box primitive, with limited attention given to practical, low-depth circuit implementations. In this talk, we present explicit constructions of efficient quantum circuits for block encoding practical classes of structured and sparse matrices. Numerical examples from spin systems and graph-based models will be used to illustrate the construction and performance of these block encodings, highlighting their potential for use on near-term quantum computers.

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MS41

Quadrature Rules for Efficient Quantum Rational Transformations

In classical computing, rational functions form an essential tool for developing effective algorithms for solving interior eigenvalue problems and approximating matrix functions. In quantum computing, the use of rational functions is underexplored. We propose an efficient method for computing the rational transformation of a Hamiltonian using a quantum computer. Since any rational function of a matrix can be written as a sum of resolvents, we focus on the computation of the matrix resolvent. The matrix resolvent can be represented as an integral in terms of a complex matrix exponential. Using a quadrature rule, this integral is approximated by a weighted finite sum of real-time evolutions. Classical results on quadrature rules allow us to quantify the quantum computational cost in terms of maximum and total evolution time. We propose the use of the Gauss-Legendre quadrature rule since it allows control

over the maximum evolution time and, compared to other quadrature rules, provides the smallest total evolution time required to compute a matrix resolvent. We illustrate numerically how our method can be used to accelerate the ODMD eigensolver for low lying exicted states by applying a rational filter to improve the initial state.

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MS42

Low-Dissipation Central-Upwind Schemes

The talk will be focused on central-upwind schemes, which are highly accurate and robust finite-volume methods for hyperbolic systems of conservation and balance laws. I will first briefly go over the derivation of central-upwind schemes. First, we reconstruct a piecewise polynomial interpolant out of the available cell averages. We then evolve the computed solution according to the integral form of the studied hyperbolic system. The evolution is performed using a nonsymmetric set of control volumes, whose size is proportional to the local speeds of propagation: this allow one to avoid solving any (generalized) Riemann problems. Once the solution is evolved, it must be projected back onto the original grid. The projection should be carried out in a very careful manner as the projection step may bring an excessive amount of numerical dissipation into the resulting scheme. In order to more accurately project the solution, we have recently introduced a new way of making the projection. A major novelty of the new approach is that we use a subcell resolution and reconstruct the solution at each cell interface using two linear pieces. This allows us to perform the projection in the way, which would be extremely accurate in the vicinities of linearly degenerate contact waves. This leads to the new second-order semi-discrete low-dissipation central-upwind schemes, which clearly outperform their existing counterparts as confirmed by a number of numerical experiments.

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MS42

Conformal Finite Element Methods for Nonlinear Rosenau-Burgers-Biharmonic Models

We present a novel and comparative analysis of finite element discretizations for a nonlinear RosenauBurgers model including a biharmonic term. We analyze both continuous and mixed finite element approaches, providing stability, existence, and uniqueness statements of the corresponding variational methods. We also obtain optimal error estimates of the semidiscrete scheme in corresponding Bochner spaces. Finally, we construct a fully discrete scheme through a backward Euler discretization of the time derivative, and prove well-posedness statements for this fully discrete scheme. Our findings show that the mixed approach removes some theoretical impediments to analysis and is numerically easier to implement. We provide numerical simulations for the mixed formulation approach using C^0 Taylor-Hood finite elements on several domains. Our numerical results confirm that the algorithm has optimal convergence in accordance with the observed theoretical results.

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MS42

On the Choice of Viscous Discretization for Artificial Viscosity-Based Entropy Stable Discontinuous Galerkin Methods

Recently, [J. Chan, *arXiv:2501.16529*] introduced a semi-discrete entropy stable discontinuous Galerkin method. This method utilizes an artificial viscosity approach in which the viscosity coefficients are locally computed and depend on auxiliary variables introduced in the Bassi-Rebay (BR-1) discretization, as well as a volume entropy residual corresponding to a local cell entropy inequality. In this work, we explore the local discontinuous Galerkin (LDG) method as an alternative viscous discretization. We show that the resulting method is still entropy stable but results in smaller magnitude artificial viscosity coefficients. Several numerical examples are given to compare the two methods.

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MS43

Passive Emitter Localization Via Generalized Wirtinger Flow

The localization of radio frequency (RF) emitters is important in many civilian and military applications. Passive emitter localization refers to the problem of passive imaging of a moving RF emitter in terms of position and velocity estimation using sparsely distributed receivers. We develop a novel imaging method for passive emitter localization using the Generalized Wirtinger Flow (GWF) algorithm. We assume that the emitter related information, including the transmitted waveforms and its center frequency, are unknown. We develop a passive measurement model that does not explicitly depend on the emitter related terms. The model assumes that the measurements at all receivers are due to the same source distribution. For GWF, we perform cross-correlation between receivers and use a lifted forward model which linearizes the problem of passive emitter localization. We then recover the position and velocities by solving a constrained optimization problem using computationally efficient convex solvers. We present numerical simulation results to demonstrate the performance of our method in the presence of additive noise. We also demonstrate the advantages of our method over the state-of-the-art techniques in terms of computational efficiency

and reconstruction performance.

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MS43

Data-Driven Roms for Sar Imaging in Multi-Scattering and Lossy Environments

Conventional algorithms of SAR imaging can be polluted by multiple echoes and other nonlinear artifacts. Data-driven reduced order models absorb much of the nonlinearity of the inverse problems, thus making the subsequent imaging a lot more straightforward. A set of 1D, 2D and 3D synthetic examples is presented to show efficacy of the proposed approach.

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MS43

Transionospheric Autofocus for Synthetic Aperture Radar

The performance of low-frequency orbital SAR systems is negatively affected by the dispersive propagation of radar signals though the ionospheric turbulence. Variations of the electron number density along the signal propagation path result in phase perturbations that depend on both the antenna and target coordinates. When the phase perturbations are significant, the quality of the SAR image deteriorates. The transionospheric setting is different from the case of antenna trajectory uncertainty where phase perturbations do not depend on the target coordinates. We design an optimization-based autofocusing procedure that, unlike the traditional autofocus methods (e.g., map-drift or PGA), can evaluate and compensate the phase errors in the transionospheric case. We test our method using numerical simulations where the ionosphere is modeled via an infinitesimally thin layer called the phase screen. We employ the cost function that emphasizes image sharpness, whereas the optimization variables parametrize the electron number density function on the phase screen. To evaluate the autofocus efficiency, we generate multiple imaging scenarios with different configurations of the target and phase screen. As an alternative to optimization-based autofocus, we consider a recently proposed screen projection method and compare the performance of the two. The performance of the optimization-based method is typically superior. A possible combination of these approaches is discussed.

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MS43

Rich Tomography and Volumetric Reconstruction in SAR

For many applications and imaging modalities sensor technology is becoming increasingly multidimensional, providing richer data. This is true also for radar, with polarimetric, multichannel and element-level digitisation of arrays common, and multistatics with multiple, distributed transmitters and receivers increasingly practical thanks to improvements in position, navigation and timing (PNT) solutions. This rich data brings new new information about the scene, but with this comes new mathematical challenges in efficient, multidimensional reconstruction. One motivation for multistatics is producing volumetric SAR imagery. This can reduce the need for a large number of repeat passes to capture a 2D aperture of data, instead filling the vertical aperture simultaneously with multiple receivers. However, the data may contain phase errors across the vertical aperture due to PNT inaccuracies or between a smaller number of repeat passes. Moreover, the true reflectivity of objects may vary with observation angle, contributing further phase differences. The vertical aperture may still be sparsely or unevenly covered. As such, traditional SAR image formation methods such as back-projection may perform poorly, necessitating a different reconstruction approach such as regularised inversion. In this talk well present our recent progress on 'rich tomography' reconstruction for SAR, including underpinning theory enabling regularisation of complex-valued images.

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MS44

Big Data, Small Footprint: Compressing Linear Algebra for the Modern Era

Linear algebra is fundamental to numerous applications, including graph analysis, machine learning, and scientific simulation. The ever-increasing scale of data, however, poses significant challenges to sustainability and cost. Data often contains substantial redundancy, frequently introduced for programming convenience, such as when using simple data structures. This talk addresses these challenges by introducing novel compression techniques designed to reduce the cost of both memory access and computation. These techniques focus on compressing compu-

tation patterns to minimize metadata overhead associated with compressed data structures. Furthermore, they exploit properties of underlying data types, such as floating-point representation, to compress workloads and improve memory hierarchy utilization. Critically, these methods are integrated with new automation techniques to alleviate the programmer's burden and facilitate ease of use.

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MS44

Overcoming Parallelism Challenges in Data Analytics Using Sparse Linear Algebra

The diverse and non-trivial challenges of parallelism in data analytics require computing infrastructures that go beyond the demand of traditional simulation-based sciences. The growing data volume and complexity have outpaced the processing capacity of single-node machines in these areas, making massively parallel systems an indispensable tool. However, programming on high-performance computing (HPC) systems poses significant productivity and scalability challenges. It is important to introduce an abstraction layer that provides programming flexibility and productivity while ensuring high system performance. As we enter the post-Moore's Law era, effective programming of specialized architectures is critical for improved performance in HPC. As large-scale systems become more heterogeneous, their efficient use for new, often irregular and communication-intensive data analysis computation becomes increasingly complex. In this talk, we discuss how sparse linear algebra can be used to achieve performance and scalability on extreme-scale systems while maintaining productivity for emerging data-intensive scientific challenges.

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MS44

Efficient Simulation of Quenching in Excitable Media: An Actor Model Approach

Excitable media, such as cardiac tissue, exhibit traveling wave phenomena where predicting the critical quenching amplitudethe minimum perturbation required to suppress stable excitationsis essential for applications like defibrillation. Traditional approaches rely on direct numerical simulations, which are computationally expensive, especially for high-dimensional parameter sweeps. In this talk, we present a novel actor model-based framework to parallelize and automate the search for critical quenching values. By distributing simulations across multiple actors, we efficiently evaluate parameter configurations while leveraging accelerated root-finding algorithms to refine predictions. This approach can significantly reduces simulations time, making accurate direct numerical simulations more accessible for researchers. We demonstrate the effectiveness of our framework on reaction-diffusion models, highlighting its scalability, fault tolerance, and adaptability.

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MS44

When More Communication Saves Time: Experiences with An Actor-Based Runtime for Graph Analytics

This talk summarzies two previously published performance engineering case studies that show when and why fine-grained asynchronous distributed-memory parallel algorithms can outperform bulk-synchronous ones, even at higher communication volume. The case studies come from bioinformatics (k-mer counting) and graph analytics (influence maximization), where our algorithmic techniques are designed to match a runtime for asynchronous 1-sided active messaging. This runtime, HClib, adopts the "actor model" of distributed computation. This work is joint with Souvadra Hati, Akihiro Hayashi, and Shubhendra Pal Singh at Georgia Tech.

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MS45

The Crystal Net Cataloguing Problem

With hundreds of thousands of known crystals and millions of hypothetical crystal structures, the problem of cataloging crystal structures has become severe. Focusing on covalent crystals, which may be represented by periodic graphs (aka "crystal nets'), there is an infinite (structured) ensemble of (parametrizable) spaces that together capture all possible geometric realizations of all possible crystal structures. But this ensemble is infinite, intricate, and not readily traversed. Furthermore, except for crystal nets of small molecule crystals, crystal nets are often taken to represent covalent crystals in which the vertices represent molecular building blocks rather than atoms, and edges represent ligands rather than bonds. In practice, crystallographers often reduce one crystal net to another, so we now interested in the relationships between different spaces of realizations of crystal nets. Given this ensemble, the cartographic problem becomes how to organize it in a manner that is useful for crystallographers. Mathematically, this project generalizes to the following. Given an ensemble of complete metric spaces of voltage graphs and given an assortment of properties we might expect of a few of their derived graphs, how might we organize this ensemble so that given a property we can readily find a voltage graph whose derived graph has that property?

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MS45

Cyclic Random Graphs Predicting Giant Molecules in Hydrocarbon Pyrolysis

Various structures arising in nature can be modeled using random graphs. We propose using random graphs to describe the molecular composition in the hydrocarbon pyrolysis, a complex chemical reaction system composed of two atoms, carbon and hydrogen, at extreme temperatures and pressures. We aim to design a model that accurately predicts molecule sizes. The property that neighborhoods of

nodes are almost always trees and that small loops are rare underlies many classical random graph models, including the configuration model. However, many real networks exhibit small loops with non-zero density, which are crucial for measuring emergent properties of networks. Carbons tend to form small loops peaking at the size of five. The presence of these loops reduces the size of the giant component approximately by a factor of 2 compared to the configuration model. We propose a random graph model featuring disjoint loops as an analytically tractable model for real networks with sparse loops without assortative mixing by degree. The model uses the works of M. E. J. Newmans group as building blocks. We apply the proposed model to hydrocarbon pyrolysis and demonstrate that it accurately predicts the small molecule size distribution and the size distribution of the largest molecule at the pressure of 40.5 GPa, temperature range of 3200K5000K, and H/C ratio range from 2.25 as in octane through 4 as in methane.

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MS45

Saturation and Periodic Self-Stress in Geometric Auxetics

We present an approach for obtaining auxetic designs with underlying three-dimensional periodic graphs of low valency. It starts with an initial framework with valency seven and one degree of freedom. Then we describe a saturation process, whereby edge orbits are added up to valency 16, with no alteration of the deformation path. This is reflected in a large dimension for the space of periodic self-stresses. The saturated version has higher crystallographic symmetry and allows a precise description of the deformation trajectory. Reducing saturation by adequate removal of edge orbits results in vast numbers of distinct auxetic designs which obey the same kinematics.

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MS45

Crystal Math: Rapid and Accurate Prediction of Molecular Crystal Structures and Properties Using Topological and Simple Physical Descriptors, Informatics, and Machine Learning Strategies

The different solid structures or polymorphs of atomic and molecular crystals often possess different physical and chemical properties. Structural differences between organic molecular crystal polymorphs can affect, for example, bioavailability of active pharmaceutical formulations, the lethality of contact insecticides, and diffusive behavior in host-guest systems. Such differences can also influence the behavior of smart materials, such as self-healing crystals. Crystallization conditions can influence polymorph selection, making an experimentally driven hunt for polymorphs difficult. Theory and computation can potentially play a vital role in mapping the landscape of crystal polymorphism. Traditional methods for predicting crystal structures and investigating solid-solid phase transformation behavior face their own challenges, and therefore, new approaches are needed. In this talk, I will show, by leveraging concepts from mathematics, specifically geometry and topology, in combination with simple physical principles, database processing, and machine learning strategies, including autoencoders and deep graph neural networks, that we have been able to develop a new framework, which we are calling Crystal Math that represents a new paradigms in our ability to predict molecular crystal structures and crystal properties, orders of magnitude faster and with far fewer resources than more traditional methods.

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MS46

The Effects of Internal Heat Generation and Convective Cooling on the Melting and Solidification in Phase Change Materials

We study the evolution of the interface between liquid and solid phases in materials with internal generation in planar, cylindrical, spherical, and semi-infinite geometries subject to convective boundary condition. The governing equations are derived under the assumption that the interface moves relatively slower than the temperature evolution. We obtain infinite series representations for the temperature in both phases and a nonlinear first-order differential equation for the front. We investigate the effect of the Biot number, Stefan number, and internal heat generation on the melting and solidification and consider a special case of remelting. We also use the method of catching the front into a node to compute solutions numerically and compare the results with quasi-steady solutions recently obtained by Alsulami et al. (https://doi.org/10.1016/j.applthermaleng.2022.119849).

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MS46

Quasiperiodic Composites: Homogenization and Spectral Properties

From quasicrystalline alloys to twisted bilayer graphene, materials with a quasiperiodic structure exhibit unusual properties that drastically differ from those with periodic structures. A key feature of quasicrystalline microgeometry is a long-range order in the absence of periodicity. Quasiperiodic geometries can be modeled using the cut-and-projection method that restricts or projects a periodic function in a higher dimensional space to a lower dimensional subspace cut at an irrational projection angle. Homogenized equations for the effective behavior of a quasiperiodic composite can be derived by cutting and projecting a periodic function in a higher dimensional space. Using equations for the local problem in the higher dimensional space established in the homogenization process, we develop the Stieltjes analytic representation of the effective properties of quasiperiodic materials; this representation determines the spectral characteristics of fields in quasicrystalline composites and can be used to derive bounds for the effective properties. A joint work with

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MS46

Homogenization of Gurtin-Murdoch Model

This talk is concerned with the periodic homogenization of the antiplane elasticity problem for a composite reinforced by arbitrary-shaped inclusions, periodically distributed in the matrix material. The inclusions and the matrix are joined through an imperfect interface described by the Gurtin-Murdoch model of surface elasticity. We will derive the homogenized effective response of this heterogeneous material in the limit when the size of the microstructure tends to zero.

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MS47

Modeling Co-Infection Dynamics in Sockeye Salmon: Deterministic and Stochastic Approaches

We develop a mathematical model to study the co-infection dynamics of salmon lice (Lepeophtheirus salmonis) and infectious hematopoietic necrosis virus (IHNV) in sockeye salmon (Oncorhynchus nerka). The model combines a compartmental ODE system, a continuous-time Markov chain (CTMC), and a multitype branching process to analyze disease transmission and persistence. We derive the basic reproduction number and establish conditions for infection extinction or persistence. Our results show that pathogen interactions influence transmission dynamics, that stochastic modelling allows for understanding the extinction of the infection at the beginning, and that co-infection thresholds depend on key epidemiological parameters. Moreover, when the infection starts with IHNV, it differs from when it starts with salmon lice.

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MS47

Pattern Formation and Spike Dynamics in the Presence of Noise

Noise plays a crucial role in the formation and evolution of spatial patterns in various reaction-diffusion systems in mathematical biology and ecology. In this talk, I give two examples where noise significantly influences spatial patterning. The first example describes how patterned states can provide a refuge and prevent extinction under stressed conditions. It also illustrates the importance of not only the absolute level of climate change, but also the speed with which it occurs. The second example studies the effect of noise on dynamics of a single spike pattern for the classical Gierer–Meinhardt model on a finite interval.

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MS47

Recurrent and Chaotic Outbreaks in An Sir Model

We examine several extensions to the basic SIR model, which are able to induce recurrent outbreaks (the basic SIR model by itself does not exhibit recurrent outbreaks). We first analyze how slow seasonal variations can destabilize the endemic equilibrium, leading to recurrent outbreaks. In the limit of slow immunity loss, we derive asymptotic thresholds that characterize this transition. In the outbreak regime, we use asymptotic matching to obtain a two-dimensional discrete map which describes outbreak times and strength. We then analyse the resulting map using linear stability and numerics. As the frequency of forcing is increased, the map exhibits a period-doubling route to chaos which alternates with periodic outbreaks of increasing frequency. Other extensions that can lead to recurrent outbreaks include addition of noise, state-dependent variation and fine-graining of model classes

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MS47

Consequences of Surface Receptor Organization on Ligand Discrimination: Insights from Stochastic Modelling

T cells must reliably discriminate between foreign-derived antigens that require an adaptive immune response from non-specific self-antigens that do not. This discrimination is highly specific to the affinity of the bond between ligand and T cell receptors (TCRs), as well as highly sensitive to the concentration of ligand. We examined these features of T cell mediated immunity in the context of multivalent ligand-receptor interactions between clusters of TCRs with pMHC-coated nanoparticles (NPs). Using Monte Carlo simulations of NP-T cell surface interactions, we compared the effect of TCR clustering on the dose-response profiles of various NP designs. These simulations, combined with a kinetic proofreading model of T cell activation, demonstrated a trade-off between sensitivity and specificity mediated by the clustering of receptors. In this talk, I will present an overview of these findings.

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MS48

Estimating Non-monotonic Combination Dose-responses of Cytokines for in Vitro T Cell Differentiation and Maturation

Chimeric antigen receptor (CAR)-T cell therapy is a promising approach that has already been approved to treat certain blood cancers. Unfortunately, its use is limited by the need to harvest a patients T cells, many of which are suppressed due to cytotoxic chemotherapies. In response, induced pluripotent stem cells (iPSCs) have been proposed as an alternative T cell source. The use of iPSCs requires them to be differentiated and matured into T cells in vitro using cytokines. To optimally perform this cell stimulation requires designing appropriate schedules using computational and mathematical models. However, models are limited by typical monotonic dose-response curves, which prevent them from being used for cytokine effects that are largely non-monotonic. To address this shortcoming, we developed a novel mathematical model describing non-monotonic dose-response surfaces of cytokine interactions that distinguishes synergy of efficacy and synergy of potency. We showed that our approach successfully recapitulates non-monotonic observed dose-response surfaces characterizing in vitro T cell progenitor differentiation following stimulation by combinations of cytokines. Our results further highlighted cytokine combinations that have antagonistic effects alone, but that are synergistic in combination. Together, our framework accelerates the efficient cell generation assays and extends drug interaction surfaces to a broader range of dose-responses.

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MS48

Mathematical Modelling of Aging Effects in the Immune Response to Cancer

Cancer is generally thought of as a disease of aging, with the incidence rate increasing most rapidly around age 50. But there are many counter-intuitive physiological process that occur which counteract cancer incidence and progression. In this talk, I will summarize some of the changes that occur in our immune response as we age. I will present a mathematical model that describes immune interactions with cancer, and using experimental data, use the model to explore aging effects in cancer growth. With a virtual population, I will then leverage the framework to explore the potential effects of age-related immunological alterations on cancer incidence rates. This work was done in collaboration with Marie Arbez and Carlos Delgado.

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MS49

On a Quantum Mechanical Theory for Surface Plasmons

In this talk, I will discuss formally from a PDE perspective the dispersion of waves arising from collective charge excitations near a fixed plane via one-particle Schrödinger-type dynamics in the quasi-electrostatic limit. The starting point is an effective nonlinear Hartree-type equation with a potential for binding to the plane and Coulomb pairwise interaction in three spatial dimensions. The linearization of this equation around the ground state yields a homogeneous singular integral equation for the perturbed wave function in the vertical direction. The explicit solution of this equation implies a dispersion law which is obtained in closed form. For strong binding, the classical long-wavelength formula for the surface plasmon emerges, along with higher-order terms. I will also discuss limitations and possible extensions of this approach, and its relevance to the description of realistic plasmons in 2D materials.

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MS49

Momentum Space Method for Multi-walled Incommensurate Carbon Nanotubes

Moir physics has yielded exotic many-body effects including correlated insulators and superconductivity. To understand many-body models, a thorough understanding of the single-particle picture is critical as the single-particle basis is used to construct two-body models. Here we introduce an algorithm using momentum space, to construct quasi-band structure for multi-walled carbon nanotubes and observables. Particularly, we focus on the case where the chirality of the nanotubes results in moir patterns.

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MS49

Subwavelength Localisation in Aperiodic Block Resonator Systems

We elucidate wave localisation in the high-contrast subwavelength regime in one-dimensional resonator arrays consisting of aperiodically arranged blocks. Adopting the capacitance and propagation matrix formalisms, we analyse localisation via adapted localisation criteria, investigate the robustness of spectral band gaps in disordered configurations and relate the whole-system spectral characteristics to those of the constituent blocks. In particular, we dissect the integrated density of states, uncovering three distinct spectral regimes: spectral gaps with complete eigenmode suppression, smooth distributions within pass-bands, and novel fractal-like spectra arising from constrained eigenmode hybridisation. Exploiting the limited interaction underlying this fractal behaviour, we introduce an efficient meta-atom approach that enables rapid and accurate spectral characterisation.

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MS50

Generalized Golub-Kahan Methods for Large-Scale Hierarchical Bayesian Inverse Problems

Uncertainty quantification for large-scale inverse problems remains a challenging task. For linear inverse problems with additive Gaussian noise and Gaussian priors, the posterior is Gaussian but sampling can be challenging, especially for problems with a very large number of unknown parameters (e.g., dynamic inverse problems) and for problems where computation of the square root and inverse of the prior covariance matrix are not feasible. Moreover, for hierarchical problems where several hyperparameters that define the prior and the noise model must be estimated from the data, the posterior distribution may no longer be Gaussian, even if the forward operator is linear. Performing large-scale uncertainty quantification for these hierarchical settings requires new computational techniques. In this work, we consider a hierarchical Bayesian framework where both the noise and prior variance are modeled as hyperparameters. Our approach uses Metropolis-Hastings independence sampling within Gibbs where the proposal distribution is based on generalized Golub-Kahan based methods. We consider two proposal samplers, one that uses a low rank approximation to the conditional covariance matrix and another that uses a preconditioned Lanczos method. Numerical examples from seismic imaging, dynamic photoacoustic tomography, and atmospheric inverse modeling demonstrate the effectiveness of the described approaches.

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MS50

Autoencoder Solvers for L1-regularized Inverse Problems

Inverse problems are ubiquitous in many applications including medical imaging, data compression and other data analysis. In this presentation, we present novel generative approaches to inverse problem solving, leveraging variational auto-encoders and demonstrate use cases for solving generalized LASSO problems as well as applications in data assimilation.

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MS50

Low Rank Tensor Completion for X-Ray Spectromicroscopy

X-ray spectromicroscopy is a powerful tool for studying material distributions, which is extracted from the data using a combination of PCA and cluster analysis. However, the traditional data collection setting has some significant weaknesses (e.g., long scanning times and material degradation due to x-ray radiation). It has been demonstrated [O Townsend, Undersampling Raster Scans in Spectromicrsocopy for reduced dose and faster measurements, 2022] that iterative methods based on low-rank matrix completion are well suited for recovery of near identical results from sparse undersampled data, greatly reducing the experimental time. However, the data sets formed through spectromicroscopy experiments are naturally 3D tensors, allowing for further improvement in data recovery if we can avoid the first step of flattening the data into matrices. In this talk, we present a novel iterative algorithm for low rank tensor completion, recovering the missing entries in the datas native space. The new method allows the selection of robust sampling patterns, tensor multi-rank and undersampling ratio, while minimising the impact of undersampling on the cluster analysis. Results obtained on real data will be illustrated.

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MS50

Long-Time Accuracy of Ensemble Kalman Filters for Chaotic and Machine-Learned Dynamical Systems

Filtering is concerned with online estimation of the state of a dynamical system from partial and noisy observations. In applications where the state is high dimensional, ensemble Kalman filters are often the method of choice. This work establishes long-time accuracy of ensemble Kalman filters. We introduce conditions on the dynamics and the observations under which the estimation error remains small in the long-time horizon. Our theory covers a wide class of partially-observed chaotic dynamical systems, which includes the Navier-Stokes equations and Lorenz models. In addition, we prove long-time accuracy of ensemble Kalman filters with surrogate dynamics, thus validating the use of machine-learned forecast models in ensemble data assimilation.

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MS51

Coupling Between Moving Solids and Convective Flows

The mantle of Earth is known to convect on a geophysical time scale, and its motion drives the plate tectonics and leads to natural disasters such as earthquakes and tsunamis. Understanding the dynamical coupling between the moving continents and the convecting fluid is thus significant, and we will discuss a fluid-structure interaction investigation in this talk. Combining numerical simulations and laboratory experiments, we show how a freely-floating plates motion is affected by its thermal and mechanical coupling to the fluid beneath it. We further model and analyze the dynamics and the interactions between multiple moving plates, and demonstrate how the thermal blanket effect influences the formation and stability of supercontinents.

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MS51

Mean Field Control of Coherent Structures in Nonlinear Fluids

This talk focuses on the Hamilton-Jacobi method and computations for stochastic dynamic systems arising from mean-field control of coherent structures in nonlinear fluid system. We will derive the Hamilton-Jacobi equation (coupled with the Fokker-Planck forward equation) for the mean-field control problem in nonlinear fluids system. Two models for controlling passive tracers and for controlling fluid vorticity are established, with links to functional Hamilton-Jacobi equations on probability spaces. Passive tracer mean-field control model is also served as a decoupling procedure for solving the optimal solution in the non-separable mean-field control problem. An iterative solver for the mean-field control model is proposed and tested on a prototype model modified from the viscous Burger's equation simulating the multiscale vortical advection by an incompressible flow.

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MS51

Learning Model Equations for Fire Plume Dynamics

The increasing frequency and severity of wildfires underscore the need for accurate fire and plume spread models. Traditional instrumentation often yields sparse measurements, whereas computer vision techniques enable the extraction of rich data from visual and infrared video sources. Analyzing plume imagery provides data that quantifies heat transport, turbulent statistics, and plume structurephenomena fundamental to advancing our understanding of wildland fire plume dynamics. I will present a computer vision technique developed in our group, Fire Dynamic Vision (FDV), which isolates and tracks plume behavior across a wide range of spatial and temporal scales. Once tracked, these data are passed into weak SINDy, a system identification method that recovers governing dynamical systems from observations.

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MS53

A Regularizing Property of the 2D Eikonal Equation

The 2D Eikonal equation is closely related to the variational analysis of a classical energy functional, called the Aviles-Giga functional in connection with smectic liquid crystals and thin film blisters. In the variational setting, significant effort has been devoted toward understanding solutions of the 2D Eikonal equation with low fractional Besov regularity. Notably, weak solutions under certain low regularity conditions exhibit automatic regularization. In this talk, I will present a new regularizing effect for weak solutions of the 2D Eikonal equation under a weak fractional Besov regularity. This regularity lies at the borderline between continuity and the presence of vortex singularities. This is joint work with Xavier Lamy and Andrew Lorent.

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MS53

Defects in Optimal Quantizers on Closed Surfaces

Given a compact surface $\mathcal{M}$ with metric ϱ and surface measure σ, we consider the functional $\mathcal{E}(Y) = \int_{\mathcal{M}} \varrho(x,y)^r \, d\sigma(x)$ for finite $Y \subset \mathcal{M}$ and fixed $r > 0$. The minimizers Y_n of $\mathcal{E}$ among sets of size $\leq n$ exhibit striking geometric regularity for large n. In a robust sense, most cells of the Voronoi tessellation generated by Y_n tend toward Euclidean regular hexagons but, for topological reasons, they cannot all be hexagonal. Thus, we study the number of non-hexagonal cells (defects). In this talk, I shall show that, whereas for surfaces with boundary this number is on the order of $\sqrt{n}$, it can be much lower on closed surfaces. In particular, the number of defects for the hexagonal torus is at most $O(n^{1/4})$ and admits a tighter bound related to the gaps between Löschian numbers. I will also discuss the adaptation of the method to the 2-sphere where we conjecture a similar bound holds.

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MS53

Lens Clusters in Nonlocal Ternary Systems

The functional of the variational problem combines an interface short-range interaction energy promoting micro-domain growth with a Coulomb-type long-range interaction energy which prevents micro-domains from unlimited spreading. Here we consider a scenario in which two species are dominant, and one species is vanishingly small. In this scenario two energy levels are distinguished: the zeroth-order energy encodes information on the optimal arrangement of the dominant constituents, while the first-order energy gives the shape of the vanishing constituent. This first-order energy also shows that, for any optimal configuration, the vanishing phase must lie on the boundary between the two dominant constituents and form lens clusters also known as vesica piscis. Joint work with Stanley Alama, Lia Bronsard, and Xinyang Lu.

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MS54

The Akhiezer Iteration for Matrix Functions and Sylvester Equations

We present an iterative method for solving indefinite linear systems and computing matrix functions via orthogonal polynomial expansions. We utilize orthogonal polynomials for weight functions supported on intervals that roughly correspond to the eigenvalues of the matrix in question. When two or more intervals are considered, extensions of the Chebyshev polynomials, often called the Akhiezer polynomials, are employed. The iterative method achieves a provable geometric rate of convergence and applies in settings where classical polynomial approximations behave poorly and are therefore not applicable. Applied to the matrix sign function, the method yields a fast inverse-free iteration for solving Sylvester matrix equations.

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MS54

Airy Phase Functions

It is well known that phase functions methods can be used to numerically solve a large class of oscillatory second order linear ordinary differential equations in time independent of frequency. These methods breakdown in the presence of turning points, which is unfortunate given that equations with turning points arise frequently in applications. We will describe a numerical method which generalizes the phase function approach and which allows for the extremely efficient solution of a large class of second order linear ordinary differential equations, including many satisfied by classical special functions. We will discuss applications of our method to the rapid numerical calculation of the associated Legendre functions.

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MS54

An adaptive delaminating Levin method in two dimensions

In this talk, we present an adaptive delaminating Levin method for evaluating bivariate oscillatory integrals over rectangular domains. Whereas previous analyses of Levin methods impose non-resonance conditions that exclude stationary and resonance points, we rigorously establish the existence of a slowly-varying, approximate solution to the Levin PDE across all frequency regimes, even when the non-resonance condition is violated. This allows us to derive error estimates for the numerical solution of the Levin PDE via the Chebyshev spectral collocation method, and for the evaluation of the corresponding oscillatory integrals, showing that high accuracy can be achieved regardless of whether or not stationary and resonance points are present. We then present a Levin method incorporating adaptive subdivision in both two and one dimensions, as well as delaminating Chebyshev spectral collocation, which is effective in both the presence and absence of stationary and resonance points. We demonstrate the effectiveness of our algorithm with a number of numerical experiments.

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MS54

Fast Algorithms for Sobolev Orthogonal Polynomials

Sobolev orthogonal polynomials are those polynomials orthogonal with respect to an inner product including derivatives. They have a beautiful and rich theoretical history. We propose fast algorithms for Sobolev orthogonal polynomials by careful consideration of the properties of the Sobolev–Gram matrix. We begin with a description of a matrix equation for the Sobolev–Gram matrix with a number of terms proportional to the order of the Sobolev inner product. We describe conditions on the vectorial measure that cause the Sobolev–Gram matrix to be banded, leading to linear complexity Cholesky factorization. Next, we convert the problem of including Dirac measures into that of a finite-rank perturbation of a known Cholesky factorization,

which can also be performed in linear complexity. Finally, in the case of conversion to Chebyshev polynomials, we harness the power of randomized numerical linear algebra to solve the connection problem in $\mathcal{O}(n \log^4 n)$ flops.

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MS55

A Dynamic Structural Model for Contingent Convertible Debt

This article presents a comprehensive numerical framework to analyze the design of contingent capital for depository institutions. We consider a debt portfolio composed of straight debt and contingent convertible (coco) bonds. Coco bonds are written down or converted into equity upon meeting predetermined capitalization ratio thresholds, thus providing capital loss absorption mechanisms. The quality of the design of coco bonds (parameterized by write-down/conversion factors and trigger levels) is gauged with default probabilities at various horizons, shareholders incentive for risk-shifting, and the present value of bankruptcy costs.

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MS55

A Unifying Approach for the Pricing of Debt Securities

In this study, we propose a unifying framework for the pricing of debt securities under general time-inhomogeneous short-rate diffusion processes. The pricing of bonds, bond options, callable/putable bonds, and convertible bonds (CBs) is covered. Using continuous-time Markov chain (CTMC) approximation, we obtain closed-form matrix expressions to approximate the price of bonds and bond options under general one-dimensional short-rate processes. A simple and efficient algorithm is also developed for the pricing of callable/putable debts. The availability of a closed-form expression for the price of a zero-coupon bond allows for the perfect fit of the approximated model to the current market term structure of interest rate, regardless of the complexity of the underlying diffusion process selected. We further consider the pricing of convertible bonds (CBs) under general bi-dimensional time-inhomogeneous diffusion processes to model equity and short-rate dynamics. Credit risk is also incorporated into the model. Based on a two-layer CTMC method, an efficient algorithm is developed to approximate the price of convertible bonds. When conversion is only allowed at maturity, a closed-form matrix expression is obtained. Numerical experiments show the high level of accuracy of the methods across a wide range of model parameters and short-rate models.

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MS55

Spectral Expansions for Structural Credit Risk Models with Occupation Area and Time

We analyze structural credit risk models that incorporate liquidation barriers and hazard rates based on occupation area and time. The defaults within these models are characterized according to Chapter 7 (a liquidation process) and Chapter 11 (a reorganization process) of the U.S. Bankruptcy Code. The risk-neutral default probabilities involve joint probability distributions of the underlying firms value, with a killing imposed at the liquidation barrier and its occupation time or area relative to the reorganization barrier. The spectral methodology is applicable for solvable diffusions, such as geometric Brownian motion (GBM), the Bessel-K model, and other state-dependent volatility diffusion models. We discuss and compare various approaches and present numerical results.

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MS55

Warrant Pricing with Leverage and Dilution Effects

We consider option and warrant pricing under the structural framework (both Merton and first-passage time (FPT) paradigms). We study the calibration of structural frameworks using a market implied volatility skew.

We show that the model implied volatility skew under FPT framework is more flexible than that under the Merton framework. Moreover, we extend the FPT structural framework to include warrants into the firms capital structure. Using historical market data, we show the pricing model (for both options and warrants) under the FPT framework significantly outperforms the pricing models relative to the Merton approach.

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MS56

Region Segmentation Using Heat Equation for Geodesic Distance with Respect to a CNN Generated Riemannian Metric

Leveraging geodesic distances and the geometrical information they convey is key for many data-oriented applications in image analysis. Geodesic distance computation has been used for long for image segmentation using Image based metrics. Main methods for distance map computation are fast marching and heat equation using the Varadhan formula. We introduce a new method by generating Riemannian metrics adapted to a problem using CNN and give as illustrations an example of application. We then apply this idea to the segmentation of brain tumors as unit balls for the geodesic distance computed with the metric potential output by a CNN, thus imposing geometrical and topological constraints on the output mask. In order to segment longitudinal structures like blood vessels, and vascular tree, we need to use anisotropic metric, for which computation the heat equation is more adapted. We show that geodesic distance modules work well in machine learning frameworks and can be used to achieve state-of-the-art performances while ensuring geometrical and/or topological properties.

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MS56

Deep Learning-Based Surface Reconstruction from Point Clouds

In this presentation, we introduce an advanced deep learning approach for reconstructing surfaces from unorganized point clouds. By leveraging an implicit surface representation through a level set function, our method ensures watertight results and seamlessly adapts to various topologies. We employ the p-Poisson equation to precisely learn the signed distance function (SDF), improving accuracy through a variable splitting strategy that incorporates the SDF gradient as an auxiliary variable. Additionally, we enforce a curl-free condition on the auxiliary variable to exploit the irrotational nature of conservative vector fields. Our numerical results illustrate that this strategic integration of partial differential equations and key vector field characteristics efficiently reconstructs high-quality surfaces without the need for prior surface knowledge.

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MS56

Deep Learning Approaches for Efficiently Solving Hamilton-Jacobi Equations

Hamilton-Jacobi partial differential equations (HJ PDEs) are fundamental in a wide range of applications, but obtaining viscosity solutions remains a challenging task. This talk explores deep learning approaches for solving HJ PDEs based on the method of characteristics. Unlike traditional numerical approaches that reformulate the PDE as a linear system, deep learning techniques convert the problem into an optimization task. We discuss how characteristics can be employed to design loss functions that effectively capture viscosity solutions. Additionally, we highlight how neural representations and the mesh-free nature of deep learning address the challenges of classical approaches, particularly in solving large-scale, high-dimensional problems.

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MS57

Joint Reconstruction and Segmentation in Computed Tomography

Computed tomography (CT) is a widely used noninvasive nondesctructive imaging modality, with wide ranging applications in medicine, science, and engineering. Often the next step to image reconstruction is image segmentation, in order to delineate distinct objects or regions in the image for quantitative measurements and inference. In this work, we propose a new joint model, so that the segmentation can be computed directly from CT measurements, bypassing the image reconstruction step. This reduces the efforts needed from users for computation and tuning of two separate steps, and incorporating the expectation of a segmentation helps regularize the reconstruction model.

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MS57

Interpretable Deep Learning Theory and Model Construction Based on Optimal Transport

Optimal transport studies how to map a given probability distribution to another probability distribution at the lowest cost, and it is a very hot research direction in the field of deep learning at present. In this talk, we will first introduce the basic theory and related algorithms of optimal transport, then interpret the generation and classification tasks from the perspective of optimal transport, and finally introduce some new generation models that can avoid mode collapse and long-tailed classification models based on optimal transport.

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MS57

Numerical Methods for PDE-Based Diffeomorphic Image Registration

We discuss numerical algorithms for PDE-based diffeomorphic image registration. We consider a Newton-Krylov method for numerical optimization. Our contributions are to develop effective numerical methods to evaluate the forward and adjoint operators. We propose a multigrid algorithm to precondition the reduced space Hessian and compare it to other preconditioning strategies. We report results for synthetic and real world data. We assess performance in terms of registration accuracy, rate of convergence, and time-to-solution.

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MS60

Analyzing Urban Vulnerability: Citizen Science and Soft Target Risk Assessment

Recent disasterswildfires, floods, and pandemicshave spurred ordinary citizens to take an active role in scientific efforts aimed at disaster preparedness, response, and recovery. Soft Targets-Crowded Places (ST-CPs), such as shopping malls, schools, and sports stadiums, are locations that attract large crowds but often have limited security measures, making them particularly vulnerable to threats. The risk to these venues is highest at moments of peak occupancy. In this talk, we present the Foot Traffic Project, a classroom-based citizen science initiative in which student teams systematically collect, record, and analyze foot traffic data at a designated public venue. By determining periods of maximum occupancy, students assess when the location is most susceptible to potential threats. This project engages students in identifying soft targets within their communities and applying fundamental mathematical and statistical techniques to evaluate risk and develop evacuation strategies for both natural and human-made emergencies.

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MS60

Using the National Risk Index As a Springboard for Student Research

Hazard mitigation planning reduces loss of life and property by minimizing the impact of disasters... Mitigation plans are key to breaking the cycle of disaster damage and reconstruction. (www.fema.gov). The National Risk Index summarizes estimated natural hazard loss for communities at the local and national level in a user-friendly, visually engaging interactive format that encourages exploration and further research. Understanding the risk for a particular area allows students to investigate how their communities may be impacted and what their communities can do to mitigate this risk.

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MS60

Risk Assessment & Evacuation: An Undergraduate Research Lab

This unit empowers undergrads to tackle real-world evacuation challenges through hands-on research. Students design and execute an evacuation drill, addressing FEMA special needs considerations. They then develop a multidimensional study of evacuation dynamics, visualizing data with scatter plots and trendlines. Analyzing R^2 values and residual plots, students assess model fit. Finally, they explore how venue geometry impacts evacuation safety. This project-based unit fosters critical thinking, data analysis skills, and an understanding of risk assessment, making it a valuable addition to any undergraduate curriculum.

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MS61

Near-Optimal Parameter Tuning of Level-1 QAOA for Ising Models

The Quantum Approximate Optimization Algorithm at depth one (QAOA1) encodes solutions to QUBO problems into a parameterized quantum circuit with only two angles, (?,), but its highly oscillatory cost landscapewhose oscillation frequency grows with problem size, density, and weightrenders parameter tuning challenging. We address this by analytically deriving the optimal for any ?, reducing the search to one dimension, and by establishing the maximum sampling interval required to accurately resolve the ? landscape. Building on these insights, we introduce a polynomial-time algorithm for estimating optimal parameters and prove that, for regular graphs, the global optimum ?* lies very close to zero and coincides with the first local extremum, enabling efficient gradient descent in lieu of exhaustive searches. When integrated into Recursive QAOA, our method consistently outperforms both coarsely tuned RQAOA and semidefinite-program relaxations across diverse QUBO instances.

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MS61

Optimal Placement of Bivariate Bicycle Codes on

Neutral Atom Arrays

Neutral-atom processors arrange qubits on a 2-D grid whose gate quality drops sharply with distance, turning code-vertex placement into a distance-minimizing assignment problem. For the recently proposed bivariate bicycle error-correcting codes this task becomes a highly symmetric quadratic assignment, yielding a massive search space. We recast the problem as a mixed-integer optimization model, add orbit-based symmetry-breaking constraints, and employ standard linearizations that give tight bounds to a branch-and-cut solver. GAMS/CPLEX currently struggles to optimally (or near-optimally) place instances with up to 144 vertices versus heuristic approaches. Complete models, benchmark data, and scripts will be shared to invite the optimization community to explore this physics-motivated challenge.

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MS61

Structure-Exploiting Methods for Maximization of Quantum Fisher Information

We consider the problem of maximizing quantum Fisher information (QFI) of states generated by a variational quantum circuit, given a model of decoherence and an interaction Hamiltonian. In this talk, we will more specifically discuss the successes and failures that we encountered in using various optimization models and methods within this problem setting.

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MS61

Decoded Quantum Interferometry and Max Cut

Decoded Quantum Interferometry (DQI) is a promising recently proposed quantum algorithm for approximating discrete optimization problems that could offer an exponential quantum advantage. DQI provides the currently best-known approximation guarantees for some problems; however, it requires very special problem structure. We show that for Max Cut, the instances for which DQI gives a nontrivial approximation guarantee are solvable exactly by an efficient classical algorithm. In this case the problem structure that enables good DQI approximations also renders the problem classically tractable.

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MS62

Incorporating Wastewater-Based Surveillance Data into Mathematical Models of Disease Spread

In this talk, we'll discuss opportunities and challenges for incorporating wastewater-based surveillance (WBS) data into mathematical models of disease spread. We'll illustrate this with a single strain model and extend the model to two strains with a cross-immunity delay. Furthermore, we'll investigate the role of recovered individuals who are still shedding virus into the wastewater. These models will be applied to WBS data and results will be explored.

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MS62

Mathematical Modeling of SARS-CoV-2 Reveals Immune Cell Dysfunction

In response to the impact of COVID-19 pandemic, the scientific community has focused considerable research efforts to understand the spread of the virus. Despite a tremendous volume of research, how the human immune system responds to SARS-CoV-2 has not been yet fully understood due to limited analysis of the experimental or clinical information to date. Mathematical models that account for the interaction between SARS-CoV-2 and the human immune system will improve the scientific community's ability to analyze the vast amount of data available. We have developed a mathematical model for the immune response to SARS-CoV-2 to investigate the role of various molecular pathways in successful viral clearance and the key mechanisms responsible for disease severity. Specifically, our model explicitly represents the interactions between the virus, immune cells, and selected cytokines. These interactions are formulated in a system of coupled ordinary and delayed differential equations. Using this model, we use sensitivity analysis to determine the implications of variation of parameters. Our model demonstrates key aspects of the immune response to SARS-CoV-2, specifically its sensitive pathways, which might be responsible for disease severity. These have the potential to be used to identify several therapeutic targets that would provide hypotheses to be tested clinically, thus, serving as a foundation for the development of evidence-based therapeutic strategies.

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MS62

Model Design for Bacteria Interacting with Multiple Phages

Antibiotic resistant bacteria infections result in tens of thousands of deaths each year. Although several alternative therapies are currently under investigation, bacteriophage (phage) cocktail therapy appears poised for long-term success. Recently it has been experimentally es-

tablished that multi-phage therapy is typically more effective than the application of a single phage type, but no mathematical models have been developed to fully understand the complicated dynamics. We build from our single-phage-model to have more types of phage and resistant bacteria and explore the effects of different treatment strategies (e.g. multi-phage cocktails) on bacterial density and resistance resolution. We also explore different model structures to best capture experimental data. The simplest phage predation model is based on linear phage infection modality, which assumes a well-mixed environment where phages easily encounter and infect bacteria. A better option to capture the spatial heterogeneity would be $F(P) = \tilde{\theta}P^{\gamma}$ where $\tilde{\theta}$ is the nonlinear adsorption rate and $\gamma < 1$ is the power-law exponent. Phage predation has also been modeled as a saturated process, which assumes that at high phage density multiple phage particles adsorb to a single bacterium so that phage infection follows a saturating Hill function. We also compare with a delay differential equation model for sequential phage therapy and explore treatment dynamics.

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MS63

Enabling High-Performance Coupled Multiphysics Fusion Simulations with the Parallel Coupler for Multi-Model Simulations (pcms)

Realizing a fusion powered grid will require advances in high performance mathematical software to enable whole facility models that can be used for computational design and optimization. Although tremendous progress has been made towards analysis of various components of magnetically confined fusion reactors (e.g., core plasma, edge plasma, magnetic coils, etc.), the integration of these components remains a key challenge. To address this gap, the Parallel Coupler for Multimodel Simulation (PCMS) has been developed to enable coupling of exascale multiphysics simulations. This talk will describe the design and implementation of the PCMS field transfer and parallel control modules. And will provide examples of coupled fusion simulations based on structured and unstructured meshes. Lastly, it will introduce progress towards support for complex physics based coordinate transformations and geometry aware coupling as needed for fusion digital twin applications.

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MS63

High Performance Computing Applications with the SUNDIALS Library of Time Integrators

The SUNDIALS library of time integrators and nonlinear solvers has recently increased its support for large-scale GPU-based systems through new data structures and solver package interfaces. This talk will overview the SUNDIALS packages and recently added capabilities then show results on newly deployed systems. Several applications have taken advantage of these capabilities to improve their time integration performance, and results from a selection of these, including combustion, phase field modeling, and cosmology, will be shown. Prepared by LLNL under Contract DE-AC52-07NA27344. LLNL-ABS-844590.

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MS63

The Importance of Mathematical Software for Scientific Applications

This talk is an introduction to the minisymposium with emphasis on the importance of scientific software for application codes, including scientific software ecosystems, such as the extreme-scale scientific software development kit (xSDK).

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MS63

Amrex: Software Framework for Structured Mesh Applications

AMReX is a software framework designed for developing structured mesh applications that solve systems of partial differential equations on machines from laptops to exascale supercomputers. It supports applications across a wide range of fields, including accelerator modeling, astrophysics, atmosphere and ocean modeling, biology, combustion, cosmology, epidemiology, microelectronics, microfluidics, neutrino quantum kinetics, particle-laden multiphase

flows, and solid mechanics, among others. In this talk, I will present an overview of AMReX's key features, including parallel communication, performance portability for CPUs and GPUs, adaptive mesh refinement, particle support, complex geometry, linear solvers, and integrations with other mathematical software packages such as HYPRE, PETSc and SUNDIALS. I will also highlight recent development such as Python interfaces and parallel FFT support.

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MS64

On the Influence of Boundary Conditions on Time Parallel Time Integration

Time parallel time integration has become a very active field of research over the past two decades. At first, it seems rather unusual to try to parallelize a completely sequential time stepping process in the time direction. Nevertheless, many methods have been developed that can successfully achieve this, and give substantial speedup compared to the sequential time stepping on a parallel computer. More recently, it was also understood that the nature of the problem to be solved, often partial differential equations of parabolic or hyperbolic type, has also a tremendous influence on if it is possible to solve such evolution problems in a parallel in time fashion. I will show in my presentation that in addition to the nature of the problem, the boundary conditions imposed have a very important impact on the parallelizability of evolution problems in the time direction, both for parabolic and hyperbolic problems.

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MS64

Addressing Reproducibility Challenges in HPC with Continuous Integration

The high-performance computing (HPC) community has adopted incentive structures to motivate reproducible research, with major conferences awarding badges to papers that meet reproducibility requirements. Yet many papers do not meet such requirements. The uniqueness of HPC infrastructure and software, coupled with strict access requirements, may limit opportunities for reproducibility. In instances of restricted access to resources, regular documented testing, through continuous integration (CI), coupled with complete provenance information, may be sufficient. While HPC-based CI frameworks exist, they are often limited to internal use. Here we argue that better CI solutions will improve reproducibility of HPC applications. We first present a survey of reproducibility initiatives and describe the barriers to reproducibility in HPC. We then present a GitHub Action, based on Globus Compute, to enable automated execution of tests on remote HPC resources. Finally, we evaluate our action by applying it to HPC applications and demonstrate its effectiveness in enhancing reproducibility.

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MS64

Automating Galerkin-in-Time Discretizations in Irksome

Irksome is a library based on the Unified Form Language (UFL) that enables automated generation of methods for time-stepping with finite element spatial discretizations of partial differential equations. Allowing users to express semidiscrete forms of PDEs, it generates UFL for the stage-coupled variational problems to be solved at each time step. The Firedrake package then generates efficient code for evaluating these variational problems and allows users a wide range of options to deploy efficient algebraic solvers in PETSc. In this presentation, we will discuss the recent extension to Irksome to include both continuous and discontinuous Galerkin-in-Time discretizations, and how this automates the development of structure-preserving discretizations.

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MS64

GPU Acceleration of the Summa-Sundials Land Model

The Structure for Unifying Multiple Modeling Alternatives (SUMMA) is a land model for large-scale hydrologic simulations. Efficiently obtaining accurate solutions of the partial differential equations that describe the underlying thermodynamics and hydrology over large geographic domains is nontrivial and computationally demanding. The accuracy challenge is addressed by the Suite of Nonlinear and Differential-Algebraic Equation Solvers (SUNDIALS); however, the use of SUNDIALS comes at a higher computational cost than the previous version of SUMMA, which was based on a constant-stepsize backward Euler method with no rigorous error control. High computational cost is prohibitive for operational use, where ensembles of simulations must be completed in a timely manner and often with limited computing resources. Fortunately, SUNDIALS can use GPU parallelism and increase computational throughput (often dramatically). Although written for C++ applications, we developed an SUNDIALS GPU interface to work with Fortran, which is the language in which SUMMA is programmed. GPU computing allows us to substantially reduce the time required to obtain accurate solutions with relatively modest hardware. In this presentation, we demonstrate improved accuracy and computational throughput of the SUMMA implementation that

utilizes GPU computations combined with the SUNDIALS solvers to obtain accurate solutions more efficiently than existing backward Euler and SUNDIALS-based implementations.

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MS65

Training on Group Structured Data and the Emergence of Invariance

We investigate the capacity of classical Hopfield networks for storing the isomorphism class of a graph. We observe that the orbits of many natural classes of graphs can be efficiently stored in a Hopfield network by minimizing a convex objective called the Energy Flow. Crucially, only a vanishingly small fraction of examples are required for the Hopfield network to strictly memorize the entire orbit. We analyze this phenomenon by drawing a connection to Support Vector Machines (SVMs) and provide a sample complexity analysis. We also remark that this phenomenon does not appear to hold for modern Hopfield networks, and discuss potential applications.

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MS65

A Unifying Functional Form for the Eigenstructure of Rotation-invariant Kernels on High-dimensional Datasets

Thanks to recent advances, we now have an essentially complete mathematical understanding of kernel regression with arbitrary kernels on arbitrary distributions, phrased in terms of the eigendecomposition of the kernel with respect to the data distribution. The problem's that this kernel eigenstructure is fairly abstract: it's unclear what the eigenfunctions of common kernels on realistic data distributions look like, and thus it's hard to extract further insight out of these theories. In this talk, I'll discuss work in progress in which we develop an ansatz for the eigenstructure of generic dot-product kernels w.r.t. generic Gaussian measures, then show that our ansatz actually works pretty well for e.g. CIFAR-10, (hopefully) opening up some new types of questions about the inductive bias of kernel regression.

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MS65

The Condensation Phenomenon of Deep Learning

Condensation (also known as quantization, clustering, or alignment) is a widely observed phenomenon where neurons in the same layer tend to align with one another during the nonlinear training of deep neural networks (DNNs). It is a key characteristic of the feature learning process of neural networks. In this talk, I will first introduce the condensation phenomenon observed in experiments. Then, I will discuss the global loss landscape structure underlying condensation, highlighting the prevalence of condensed critical points. Finally, I will present results on the quantification of condensation and its generalization advantage, which includes a novel estimate of sample complexity in the best-possible scenario. These results underscore the effectiveness of the phenomenological approach to understanding DNNs, paving the way for a deeper understanding of deep learning in the near future.

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MS65

Attention Sinks and Outlier Features: A Catch, Tag, and Release Mechanism for Embeddings

Large language models (LLMs) often concentrate their attention on a small set of tokensreferred to as attention sinks. Common examples include the first token, a prompt-independent sink, and punctuation tokens, which are prompt-dependent. Although these tokens often lack inherent semantic meaning, their presence is critical for model performance, particularly under model compression and KV-caching. Yet, the function, semantic role, and origin of attention sinksespecially those beyond the first tokenremain poorly understood. In this talk, Ill present a comprehensive investigation revealing that attention sinks catch a sequence of tokens, tag them with a shared perturbation, and release them back into the residual stream, where they are later retrieved based on the tags they carry. Probing experiments show that these tags encode semantically meaningful information, such as the truth of a statement. This mechanism persists in models with query-key normalizationwhere prompt-dependent, non-BOS sinks have become more commonand DeepSeek-distilled models, where it spans more heads and accounts for greater variance in the embeddings. To support future theoretical work, we introduce a minimal task that is solvable via the catch, tag, release mechanism, and in which the mechanism naturally emerges through training.

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MS66

From Exact Relations for Composites to Weakly Stable Differential Inclusions

Many nonlinear PDEs can be reformulated as differential inclusions of the form $\nabla u \subset K$, where K is a subset in a finite dimensional vector space. Of special interest are weakly stable differential inclusions whereby all weak limits of solutions are also solutions. Many examples of such inclusions come from sets K that have no rank-one connections and whose geometry guarantees that any weakly convergent sequence of solutions converges strongly. In this talk I will present a procedure that converts any exact relation for composite materials into a weakly stable differential inclusion. The corresponding sets K will be subsets of algebraic varieties and have plenty of rank-one connections; their weak stability being a consequence of their exact relation provenance. In some examples the algebraic varieties themselves will be obviously weakly stable, being given in terms of null-Lagrangians. This raises the question whether or not this should be true in general.

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MS66

Bounds and Limitations on Quasi-Static Cloaking

Consider the following challenging question: is it possible to use a passive cloak to make invisible a dielectric inclusion on a finite frequency interval in the quasistatic regime of Maxwells equations for an observer close to the object? In this talk we discuss our proof that, due to the passivity of the cloaking device, the answer to this question is negative even when the observer is near the cloak. Furthermore, based on the properties of a class of analytic functions (namely, Herglotz functions) that model passive devices, we give bounds on the Dirichlet-to-Neumann (DtN) map and show how they impose fundamental limits on passive cloaking device over a finite frequency interval. To do this we exploit some deep connections between Herglotz functions and the theory of composites. Our work also builds on the previous work [M. Cassier and G. W. Milton, Bounds on Herglotz functions and fundamental limits of broadband passive quasi-static cloaking, J. Math. Phys., 58, 071504 (2017)] which treats the far-field (as opposed to the near-field) cloaking problem, providing inequalities on the polarizability tensor (as opposed to the DtN map) associated with the cloaking device. This is joint work with Maxence Cassier (Institut Fresnel) and Graeme W. Milton (Univ. of Utah).

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MS67

Mathematical Modeling of Contact Lenses: From Drug Delivery to Ocular Reshaping

Contact lenses are used by 140 million of people worldwide to correct vision and have been recently proposed as devices to treat ocular diseases such myopia (nearsightedness) and glaucoma. In this talk I will propose mathematical models to study the potential of contact lenses as novel drug delivery systems and to study the biomechanical interactions between the eye and contact lenses. To investigate the effect of lens and drug properties on the drug release from contact lenses in-vitro, we will present a mathematically enhanced analysis of experimental data, based on mathematical modeling, parameter estimation and statistical tools. To study the mechanical interactions between the eye and the lens, we will present a coupled mathematical model of the lens and eye biomechanics. In the model, the eye and the contact lens are coupled via the non-linear suction pressure under the lens.

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MS67

Investigation of Hair Growth Duration in Normal Vs. Alopecic Conditions Using Uncertainty Quantification and Sensitivity Analysis

Hair follicles constantly cycle through phases of growth, regression and rest, and hair loss disorders disrupt the cycle making the growth phase very short. In androgenetic alopecia (AGA) hair loss occurs due to high sensitivity to androgens, and in alopecia areata (AA) hair loss occurs due to an autoimmune reaction that kills hair-producing cells, called matrix keratinocytes (MKs). We performed parameter screening, uncertainty quantification and global sensitivity analysis of a mathematical model for the human hair cycle, which we informed with experimental data for the lengths of hair cycle phases from male control subjects and subjects with AGA, as well as of a mathematical model for AA that we connected with estimates for the duration of hair cycle phases from the literature. This talk will present the analysis procedures and comparison of the results within and between the control and AGA subject groups as well as among AA, control and AGA conditions. Our findings indicate, for example, that in AA, lower proliferation of MKs and weaker communication of the dermal papilla with MKs via signaling molecules could be expected than in control and AGA conditions, and in AA stronger inhibition of MK proliferation by regulatory molecules could be expected than in AGA.

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MS67

Investigating Chromatin Organization Using Topological Data Analysis

We developed an analytical method using topological data analysis (TDA) to identify chromatin loop features in live cells via single particle tracking. Unlike traditional time series analysis, which struggles with complex spatial patterns, TDA analyzes particle trajectories as continuous paths in 3D/4D space (x, y, z, time) using persistent homology to characterize data shape. We tested the methods accuracy with polymer bead spring models, simulating chromatin segments under varying conditions (chain persistence, tethering, cross-linking). A sliding window approach measured persistence amplitude to detect loops when amplitudes exceeded a threshold. Simulations accurately identified loops in tethered chains, with quantitative analyses defining detection limits for small, short-lived loops. Tracking results from lacO-LacI-GFP arrays suggest TDA is a valuable tool for studying chromatin dynamics in live cells.

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MS67

Topologically-based Parameter Inference for Agent-based Model Selection from Spatiotemporal Cellular Data

Fibroblasts in a confluent monolayer are known to adopt morphologies that differ from those of isolated cells. Moreover, confluent fibroblasts, though completely surrounded by neighboring cells, are known to be motile. Previous studies involving time lapse microscopy showed that confluent fibroblast cells spontaneously arrange themselves into a nematic order. We previously collected and analyzed new time lapse microscopy data to show that the movement of neighboring cells in confluent monolayers are oriented parallel to each other and often moving in opposite directions in a collective motion phenomenon we refer to as fluidization of the cell population. Here, we performed an in-silico model selection study to show that topological data analysis could be used to distinguish between biophysical mechanisms that generate distinct fluidization patterns in an agent-based model of cell motility. We have added a new mechanism to represent cell alignment to the existing DOrsogna model. We have compared this model to the DOrsogna model using Bayesian Information Criteria.

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MS68

Structured Light in Natural Convective Turbulence: Rayleigh-Bnard Experiments

We pose the following question: What is necessary to predict the impact of optical turbulence on propagated structured light? This problem is explored from three perspectives: (1) characterizing the complex medium volumetrically through numerical simulations, (2) designing experiments to image received light in physically generated optical turbulence using Rayleigh-Bnard convection, and (3) constructing structured light that remains resilient on propagation. Each approach provides crucial insights for developing effective adaptive optical systems. Different optical components are used to capture various light properties: a lens produces the Fourier transform, a log-polar prism transforms circular phase distortions into a linear representation in the mode sorter, and a microlens array in the phase sensor records spatial focal displacements that map wavefront variations. The objective of this experimental research is to measure different light modalities to extract as much information as possible about turbulence dynamics, ultimately enabling the prediction of light behavior under varying turbulence conditions. Could we mathematically formulate problem that uses measured light modalities to inform the predictive algorithms?

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MS68

Reduced Order Modeling for First Order Hyperbolic Systems with Application to Inverse Wave Scattering

Waveform inversion seeks to estimate an inaccessible heterogeneous medium by using sensors to probe the medium with signals and measure the generated waves. It is an inverse problem for a hyperbolic system of equations, with the sensor excitation modeled as a forcing term and the heterogeneous medium described by unknown, variable coefficients. The traditional formulation of the inverse problem, called full waveform inversion (FWI), estimates the unknown coefficients via nonlinear least squares data fitting. For typical band limited and high frequency data, the data fitting objective function has spurious local minima near and far from the true coefficients. This is why FWI implemented with gradient based optimization can fail, even for good initial guesses. We propose a different approach to waveform inversion: First, use the data to "learn a good algebraic model, called a reduced order model (ROM), of how the waves propagate in the unknown medium. Second, use the ROM to obtain a good approximation of the wave field inside the medium. Third, use this approximation to solve the inverse problem. I will give a derivation of such a ROM for a general first order hyperbolic system satisfied by all linear waves in lossless media (sound, electromagnetic or elastic). I will describe the properties of the ROM and will use it to solve the inverse problem for sound waves.

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MS68

Statistics of Waves in the Branched Flow Regime

Waves propagating through weakly disordered smooth media undergo a universal phenomenon called branched flow when the correlation length of the medium is larger than the wavelength. In this process, the waves split, creating channels (or branches) of enhanced intensity that further divide as they propagate, creating tree-like branching patterns. By considering the paraxial wave equation as a representative model, we elaborate a multiscale, stochastic theory of branched flows. We consider coherent and partially coherent initial wave fields. We derive closed-form equations that give the evolutions of the field and intensity correlation functions, and we determine the value and the propagation distance of the maximum of the scintillation index (the relative variance of the intensity), which characterize the dynamical formation of incoherent branched flows.

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MS68

Generalized Snell Laws for Rough Interfaces

In this talk, we revisit the problem of reflection and transmission of waves through a rapidly oscillating rough interface with general mixing properties. Under the paraxial (parabolic) scaling, the specular and speckle (diffusive)

components of the reflected and transmitted waves can be precisely characterized. The scenario of a critically scaled interface will be presented, where the amplitudes of the interface fluctuations and the central wavelength are of the same order. When the correlation length of the interface fluctuations is smaller than the beam width, homogenization phenomena occur, and we will illustrate how the rough interface can be approximated as an effective flat interface, leading to deterministic specular cones. However, this scenario also results in the formation of broader cones (speckle cones) containing speckle patterns. We will present two-point correlation functions for these speckle patterns and a central limit type theorem, demonstrating that these patterns can be modeled as Gaussian random fields. This framework allows us to identify generalized Snells laws for refraction and transmission, influenced by an effective scattering operator at the interface.

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MS69

Low Frequency Extrapolation to Aid Solution of Seismic Inverse Problems

The cycle skipping problem that plagues seismic inversion could be resolved if receivers recorded low-frequency data which captures the kinematics of wave propagation, in conjunction with a reasonable initial velocity model. However, seismic sources and receivers are band-limited and cannot record seismic signals down to 0 Hz. To improve solution of the seismic inverse problem one can synthesize this missing low-frequency content by solving a regression problem using machine learning (ML). The recorded high-frequency (HF) seismic data is the input and the ML models are trained to predict the missing low-frequency (LF) seismic data. Deep learning models utilizing convolutional neural networks (CNNs) and generative adversarial networks (GANs) demonstrate important capabilities for LF extrapolation. However, such models require powerful hardware and careful training. We explore the feasibility of using less costly ML models such as a random forest, Gaussian process surrogates, and gradient boosting as alternatives to computationally expensive deep learning models.

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MS69

Iterative Refinement and Flexible Iteratively Reweighed Solvers for Linear Inverse Problems with Sparse Solutions

This talk presents a new algorithmic framework for computing sparse solutions to large-scale linear discrete ill-posed problems. The approach is motivated by recent perspectives on iteratively reweighted norm schemes, viewed through the lens of iterative refinement. This framework leverages the efficiency and fast convergence of flexible Krylov methods while achieving higher accuracy through suitable restarts. Additionally, we demonstrate that the proposed methods outperform other flexible Krylov approaches in memory-limited scenarios. The performance of the proposed algorithms is illustrated through a range of numerical examples, including image deblurring and computed tomography.

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MS69

Recovering Sparse DFT from Missing Signals Via Interior Point Method on GPU

We propose a method to recover the sparse discrete Fourier transform (DFT) of a signal that is both noisy and potentially incomplete, with missing values. The problem is formulated as a penalized least-squares minimization based on the inverse discrete Fourier transform (IDFT) with an -penalty term, reformulated to be solvable using a primal-dual interior point method (IPM). Although Krylov methods are not typically used to solve Karush-Kuhn-Tucker (KKT) systems arising in IPMs due to their ill-conditioning, we employ a tailored preconditioner and establish new asymptotic bounds on the condition number of preconditioned KKT matrices. Thanks to this dedicated preconditioner – and the fact that FFT and IFFT operate as linear operators without requiring explicit matrix materialization – KKT systems can be solved efficiently at large scales in a matrix-free manner. Numerical results from a Julia implementation leveraging GPU-accelerated interior point methods, Krylov methods, and FFT toolkits demonstrate the scalability of our approach on problems with hundreds of millions of variables, inclusive of real data obtained from the diffuse scattering from a slightly disordered Molybdenum Vanadium Dioxide crystal.

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MS69

Inference in the Presence of Model Misspecification: Implications and Approaches

Computational model predictions provide critical information to inform high-consequence decisions for real-world engineering applications in regimes where observational data is unavailable. The extrapolative nature of such predictions makes accurate uncertainty quantification essential to assess their credibility/trustworthiness. While Bayesian inference provides a unifying framework for extrapolating uncertainties, practical and theoretical issues arise when applying such approaches to real-world problems where model-form uncertainties are prevalent. Standard Bayesian frameworks rely on the implicit assumption the model exactly represents the observed quantity of interest; as a result, model uncertainty collapses in the limit of infinite data, even for misspecified models, potentially leading to an underestimation of prediction uncertainty. Even with existing approaches to model enrichment, discrepancies between the assumed model and observational data make uncertainty quantification capable of extrapolating to new scenarios/regimes challenging. Recent works explore how to address these issues through hierarchical approaches or by relaxing the assumption that the model perfectly represents an observed quantity. However, to date, there has been limited focus on the efficacy/accuracy of these approaches for propagation to extrapolative predictions. This work compares such approaches, highlighting the practical

implications and challenges associated therein.

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MS70

High-Order Finite Element Methods for Multicomponent Compressible Flows

We derive and analyze a broad class of finite element methods for simulating the stationary, low Reynolds number flow of concentrated mixtures of several distinct chemical species in a common thermodynamic phase. In particular, we discretize the Stokes–Onsager–Stefan–Maxwell (SOSM) equations, which model bulk momentum transport and multicomponent diffusion within ideal and nonideal mixtures. Unlike previous approaches, the methods are straightforward to implement in two and three spatial dimensions, and allow for high-order finite element spaces to be employed. We accomplish this by reformulating the SOSM equations in terms of the species mass fluxes and chemical potentials, and discretize these unknown fields using stable $H(\mathrm{div})$-L^2 finite element pairs. We prove that the methods are convergent and yield a symmetric linear system for a Picard linearization of the SOSM equations. We also discuss how the proposed approach can be extended to the Newton linearization of the SOSM equations, which requires the simultaneous solution of mole fractions, chemical potentials, and other variables. Our theoretical results are supported by numerical experiments and we present an example of a physical application involving the microfluidic non-ideal mixing of hydrocarbons.

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MS70

Stabilization, Robustness and Accuracy of Numerical Simulations of Fluids From Thin Films to Global Scales

In this introductory presentation, we would like to present different approaches for the numerical solutions of PDEs for applications arising mainly in Computational Fluid Dynamics (CFD) at different scales. Starting from problems emerging in the context of viscoelastic thin films (long waves), we are going to end with examples in global scale, non-hydrostatic, atmospheric modeling for numerical weather and climate predictions. First, we show a numerical investigation of the nonlinear interfacial dynamics of dewetting/wetting thin layers/droplets of non-Newtonian (viscoelastic) fluids of Jeffreys type in different settings. The effects of viscoelasticity and the substrate slippage on the dynamics of thin viscoelastic films and the coalescence of droplets are investigated. Finally, we present some recent work in the Climate Modeling Alliance (CliMA), a consortium project developing a new Earth System Model (ESM), with a focus on ClimaCore.jl, the new open-source dynamical core (dycore) library for the land and atmosphere components of the ESM. We will include explorations and developments in the integration of stabilization methods, such as flux-limiters and flux-corrected transport, as a means of improving robustness and positivity preservation, enabling the model to achieve a given numerical accuracy even in the presence of moist processes and to conserve energy, mass, and water without resorting to the ad hoc fixers common in some atmosphere models.

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MS70

Some Techniques for Stable Hypersonic Cfd Simulations

Simulating hypersonic flows presents significant numerical challenges due to unique characteristics such as strong shocks, thin boundary layers, high-temperature regions post-shock, and complex nonequilibrium thermochemistry. Achieving stable simulations requires a careful balance of various numerical techniques. In the simulation of hypersonic blunt bodies, numerical anomalies known as carbuncles, an abnormal growth of the bow shock along the stagnation line, can occur and disrupt the prediction of critical flow quantities, such as wall heat transfer. Common remedies involve introducing numerical dissipation in shock-capturing schemes, but these often compromise boundary layer resolution, which is crucial for modeling dynamic viscous interactions. More advanced approaches utilize different numerical schemes to address various aspects of flow physics; for instance, a dissipative method may effectively capture strong shocks, while a less-dissipative scheme can be applied outside the shock region. Despite the adoption of hybridized numerical methods in hypersonic flow simulations, challenges remain regarding robustness across diverse flow conditions. In this presentation, we will discuss techniques for achieving stable hypersonic CFD simulations, focusing on the hybridization of numerical schemes through a shock sensor based on flow attributes. Additionally, we will introduce a novel approach to controlling numerical dissipation based on entropy stability.

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MS70

Stabilisation of Subsonic to Transonic Flows for Industrial Turbomachinery Applications

Due to continued advancements in code and hardware, higher-fidelity Computational Fluid Dynamics modelling-such as implicit Large Eddy Simulation and Direct Numerical Simulation has become increasingly feasible. These simulations are generally performed using high-order solvers, which offer reduced computational costs compared to second-order methods. In the turbomachinery industry, Reynolds-Averaged Navier-Stokes simulations are routinely employed to assess the performance of various engine components. While these have been widely successful, they are limited in capturing unsteady phenomena, introducing approximation errors. Consequently, the gradual adoption of high-order methodologies within the turbomachinery community is enabling the study of complex unsteady effects, such as boundary layer transition or in-

flow disturbances. This provides designers with higher-fidelity information for design improvement. This talk will showcase successful applications of Nektar++s compressible flow solver for preliminary design, such as flat plates and then high-pressure turbines with and w/o shocks. A detailed discussion will cover the entire workflowfrom preprocessing (CAD and grid generation) to achieving a converged solutionhighlighting key challenges and techniques used to address them. Additionally, different stabilization strategies will be examined, with a comparative analysis of three methodologies in terms of their effects on flow behaviour and solver efficiency.

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MS71

Population Dynamics In Networks of Adapting Integrate-and-Fire Neurons with Global Delayed Coupling

We investigate the collective dynamics of a network of heterogeneous integrate-and-fire neurons with adaptation and global constant-delay coupling. Using a mean-field approximation we study the interplay between, heterogeneity in the applied current, strength of the adaptation and magnitude of the time delay. Perturbation and bifurcation analysis reveal interesting transitions in the behavior in the limits of weak heterogeneity and coupling strength. Our analysis shows that synaptic delays have little impact little impact on the generation of collective oscillations in networks with weak connectivity or weak adaptation. In other parameter regimes, delays primarily function as an excitatory drive, promoting the emergence of oscillations and even inducing new macroscopic dynamics. In particular, torus bifurcations may occur in a single population of neurons without an external drive, serving as an important mechanism for the emergence of population bursting with two nested frequencies.

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MS71

Effects of Disorder on Neural Network Dynamics and Computations

Structural disorder has been reported to promote ordered network dynamics in various complex systems (Zhang et al. 2021 PNAS). In neuroscience, technological developments have led to massive data sets for cell-type-resolved brain structure. These data sets revealed a previously underappreciated level of neural heterogeneity, suggestive of high levels of structural disorder at the level of nodes in neural networks (Scala et al. 2021 Nature). In this work, I will discuss recent advances in treating heterogeneous, adaptive spiking neural networks via the Ott-Antonsen ansatz. Recently, we derived a set of mean-field equations which allows us to relate the heterogeneity of spike thresholds across neurons directly to the macroscopic network dynamics (Gast et al. 2023 PRE). We show via the mean-field equations that the heterogeneity of inhibitory interneurons plays a crucial role in shaping the dynamic regimes of neural circuits: heterogeneous inhibitory interneuron populations preserve the dynamic repertoire of local excitatory populations, whereas homogeneous interneurons overwrite excitatory dynamic repertoires and facilitates synchronized dynamics (Gast et al. 2024 PNAS). Furthermore, we find that neural heterogeneity directly controls the encoding and function generation capacity as well as the dimensionality of spiking neural networks. Together, our results suggest that neural heterogeneity is an important control variable for computational states in neural networks.

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MS71

Ballistic Codes Implemented in Firing Rate Fluctuations Caused by Initial Voltage Distributions

Firing rate fluctuations are observed experimentally over multiple time scales in both single neuron's and across populations. However, to the extent that these fluctuations can be used to potentially encode information remains an open problem. Here, we analytically derive the fluctuations in the firing rate as a function of the initial voltage distribution for networks of uncoupled integrate-and-fire models, and as a closed form approximation for coupled networks through explicitly solving the Fokker-Planck system for said networks as a wave equation. We explicitly derive the firing rate fluctuations as the time-varying flux in the Fokker-Planck system. This solution was numerically validated in coupled and uncoupled networks of multiple integrate-and-fire neuronal types, with and without coupling, and with/without time-varying input currents. Finally, as the firing rate fluctuations are dependent on the initial voltage distribution, this relation-

ship can be inverted and used as a coding scheme. For a desired time-dependent fluctuation, a given initial voltage distribution can be determined which leads to a ballistic code scheme where trajectories of dynamical systems can be easily stored as initial voltage distributions in presynaptic connections.

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MS71

A Constructive Approach to Neural Field Theories

The neuronal dynamics governing sensory, motor, and cognitive function are commonly understood through field theories for neural population activity. Classic neural field theories are integro-differential equations and have inspired a range of dynamical systems analyses. They are, however, derived strong and restrictive assumptions on the underlying biophysical dynamics. Here, we will discuss recent and ongoing work in a constructive approach to neural field theories that allows directly incorporating biophysically motivated nonlinearities and uncovering their impact on macroscopic, coordinated, and patterned activity in neuronal networks.

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MS73

Particular Cases of Sobolev-Type Zernike Orthogonal Polynomials

We consider various Sobolev-type inner products found in the literature and examine the special case of the Zernike polynomials. We developed the basis, succeeding in writing them as linear combinations of the radial part of the unperturbed Zernike polynomials. We show several examples of polynomials in this context and graph the first polynomials, writing them explicitly.

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MS73

Applications of Quadratic Decomposition for Bivariate Orthogonal Polynomials

In this seminar, we present bivariate polynomial sequences that are orthogonal to a symmetric weight function, expressed in terms of several bivariate polynomial sequences orthogonal with respect to Christoffel transformations of the initial weight under a quadratic transformation. We examine the construction of a symmetric bivariate orthogonal polynomial sequence derived from a given one that is orthogonal to a weight function defined on the positive plane. A key aspect of this analysis is the role of Bcklund-type matrix transformations in the three-term matrix coefficients involved. As a case study, we explore the relationships between symmetric orthogonal polynomials defined on the ball and those on the simplex.

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MS73

On Symmetric Multivariate Orthogonal Polynomials

We consider symmetric orthogonal polynomials in n real variables that are obtained from applying the Gram-Schmidt orthogonalization process to the Schur polynomials. We investigate basic properties such as a three-term recurrence relation, as well as the localization of their zeros.

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MS75

Neo-Galerkin: Neural Operator Refinement via Neural Galerkin Schemes for Parameterized PDEs

Solving parameterized partial differential equations (PDEs) efficiently and accurately remains a fundamental challenge in computational science and engineering. Traditional numerical methods achieve high accuracy but incur significant computational costs, whereas neural operators offer rapid predictions at the expense of precision. We propose Neo-Galerkin, a novel framework that integrates neural operators with a lightweight Neural Galerkin refinement step to enhance both computational efficiency and high accuracy. Neo-Galerkin consists of two key components: (1) a neural operator that provides high-quality initial approximations and (2) a refinement step that improves these approximations with minimal additional computation. We establish rigorous theoretical guarantees on Neo-Galerkin's accuracy and efficiency across multiple PDE classes, demonstrating its advantages over standard Neural Galerkin methods. Neo-Galerkin generalizes well beyond the training domain, making it a promising approach for solving parameterized PDEs.

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MS75

On Finite Sample Bounds for Learning PDEs with Kernel Methods

In this talk, we will explore explicit connections between specific operator learning problems and kernel methods. We will examine kernel constructions that are both precisely aligned with the target operator and capable of yielding meaningful and interpretable finite-sample rates. While our primary focus is on problems related to elliptic operators, we will also discuss other relevant examples. Additionally, we will present empirical evidence to support our findings.

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MS75

Iterative Algorithms to Partitioned Neural Networks with Applications to PDEs

Iterative algorithms are presented for partitioned neural network approximation to partial differential equations. The partitioned neural network approximation has an advantage over a single large neural network approximation in that it can deal with the model complexity, such as discontinuous coefficients, multi-physics properties, and large problem domain, more effectively by introducing a suitable subdomain partition and corresponding local neural networks. On the other hand, the corresponding loss function for training parameters in the partitioned neural networks needs a special care on the interface of the subdomains and the success of this approach highly depends on the loss function formulation. In our work, an iterative algorithm based on the interface solution value is proposed by using well-established domain decomposition methods and it is further extended to train the partitioned neural networks. In addition, to enhance the scalability of the iterative algorithm, preconditioning methods are developed and numerical results will be presented to show promising features of the proposed schemes.

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MS75

Application of Neural Network Solvers for Inferring Dynamical Systems

System inference for nonlinear dynamic models represented by Ordinary Differential Equations (ODEs) remains a significant challenge in many fields, particularly when the observed data is imperfect. Such data is often derived from repeated cross-sectional observations or involves unobservable components. To address these challenges, we propose a deep generative model-based approach to reconstruct a complete and accurate dataset. This method not only accurately quantifies system parameters in ODEs but also infers unobserved system components. We validate its effectiveness through examples based on realistic experiments, showcasing its potential for broad applicability across various domains, from scientific research to engineered systems, enabling the discovery of full system dynamics.

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MS76

Securing Controller Area Networks with Graph Neural Networks: CAN We Detect the Undetectable?

Automotive vehicles are an integral part of our critical infrastructure. Vehicles are involved in countless aspects of our daily lives. They drive us to work every day, transport all kinds of products, starting with food and house-hold items, to gas and nuclear waste. Securing them from malicious attacks should be a top priority, as they directly impact our safety and day-to-day activities. Modern day vehicles have multiple sensors and actuators that are connected throughout the vehicle. These include components such as the Anti-lock Braking System (ABS), Engine Control Unit (ECU), and various sensors for monitoring engine performance or temperature, which communicate with one another via Controller Area Networks (CAN). Controller Area Networks were designed with efficiency and speed in mind, but not security. A lot of work has been done to enhance their security. However, detecting masquerade attacks has been challenging due to their ability to hide in plain sight. In this talk, we will explore the ability of Graph Neural Networks to effectively detect such attacks.

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MS76

Improving Network Robustness of Machine Learning-Based Autonomous Systems

Novel cyberattacks can disrupt network functionality and remain undetected for extended periods of time this challenge can be particularly devastating for autonomous systems. Machine learning-based approaches which form the foundation for many of these systems are also susceptible to adversarial perturbations and effects. In this talk, I explore whether advances in topological data analysis (TDA) and adversarial machine learning approaches can help address these network security problems for autonomous systems. In addition, I examine whether these approaches provide insights into how to improve the robustness of network intrusion detection systems.

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MS76

Improving Research Methods in Cybersecurity Us-

ing Tools from Applied Mathematics and Data Science

Cybersecurity is a broad field that aims to secure our digital ecosystem. However, much of the current research focuses on specific domains and contexts, often lacking rigorous mathematical validation and strong empirical support. As a result, cybersecurity practices rely heavily on heuristic methods and informal models of adversary behavior. This raises concerns about whether traditional research methods in cybersecurity consistently produce reliable outcomes. Modern approaches in the philosophy of science, supported by applied mathematics and data science, offer tools to address these challenges and advance cybersecurity as a scientific discipline. As cyber systems grow more complex and adversaries become more sophisticated, applied mathematicians and data scientists have a significant opportunity to contribute. By using research methods such as statistical analysis, machine learning, and data visualization, these disciplines can help address key challenges in building a science of cybersecurity. This minisymposium will begin by outlining obstacles to developing a scientific foundation for cybersecurity. It will then demonstrate how methods from applied mathematics and data science can address these challenges. Subsequent talks will showcase contributions to cybersecurity from areas such as computational mathematics, network science, machine learning, and topology.

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MS76

A Topological View of Cyber Networks

Cyber networks are incredibly complex systems. To study their operation and understand their current state we must be able to analyze the many data streams that are captured by logging services. These include (but are definitely not limited to!) network flow, host, process, and authentication logs. There has been significant work in analyzing these data using graph models, machine learning, and natural language processing (NLP) inspired methods. While these approaches have shown significant value they also have some drawbacks. Graph models may miss some of the complex interactions present between network entities like hosts, users, processes, and protocols that show up in the log metadata. Machine learning can infer and extrapolate from very complex patterns but their reasoning can be difficult to communicate to an analyst user. And while NLP is very good at analyzing sequences of tokens, such as those in cyber logs, they may not take advantage of the structure in the logs themselves. To address some of these drawbacks I will provide examples where hypergraphs and a topological perspective have been able to derive valuable insight and situational awareness for cyber networks. Hypergraphs can capture the kinds of multi-way relationships among behaviors within cyber networks and topology can capture high order structural properties that graph methods cannot. The results from hypergraph and topological analytics can be more interpretable for analysts as a consequence.

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MS77

Computational Modelling of Resistance to Hormone-Mediated Remission in Childhood Absence Epilepsy

Childhood absence epilepsy (CAE) is a pediatric generalized epilepsy disorder characterized by brief episodes of impaired consciousness and distinctive 2.5-5 Hz spike-wave discharges (SWDs) on electroencephalography. While CAE often remits during adolescence, the mechanisms driving remission are poorly understood. Progesterone and its neuroactive metabolite allopregnanolone (ALLO) have been linked to modulating absence seizure activity. Using a thalamocortical model, we previously showed that ALLO enhances GABAa receptor-mediated inhibition, resolving SWDs and suggesting that pubertal hormonal shifts may facilitate remission. However, not all patients experience remission despite similar hormonal changes. To investigate resistance mechanisms, we developed an enhanced thalamocortical model with a layered cortical structure to examine cortical heterogeneity and frontocortical connectivity. Our findings suggest that non-resolving CAE may result from increased frontocortical connectivity and the underlying cellular composition of the network. Specifically, a higher proportion of bursting-type neurons may prevent ALLO's therapeutic effects. This work highlights the role of network-level properties in disease outcomes and demonstrates the utility of computational modeling in exploring divergent disease trajectories where empirical models remain limited.

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MS77

An Overview of Mathematical Approaches to Advancing Women's Health

In this talk we provide an introduction to the two-part minisymposium focusing on research related to diseases, disorders, and conditions that are unique to women, affect women differently, or disproportionately affect women. The minisymposium will include work related to breast cancer, osteoporosis, the menstrual cycle, lyme disease, estrogen, and neurosteroids. We will also discuss approaches to incorporate projects related to womens health into a greater research program and provide some examples from our own work in mathematical modeling of circadian rhythms, metabolism, and blood coagulation. We will conclude with a brief overview of the outlook for the field and opportunities for future work.

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MS77

Dynamics of the Menstrual Cycle

The menstrual cycle is governed by the complex interplay of hormones, including estrogen and progesterone, regulated by the hypothalamic-pituitary-ovarian axis. A large percentage of the global population menstruates, yet the menstrual cycle and its role in health remain largely understudied. This talk will provide an overview of how mathematical models can be used to help understand menstrual cycle dynamics, including inter-individual variation, effects of oral contraceptives, and interplay with other aspects of physiology. I will additionally share some recent results on oral contraceptive dosing and how missed doses influence the menstrual cycle.

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MS77

Mathematical Models of Kisspeptin Signaling and Ovulation

This work analyzes and expands upon existing mathematical models of ovulation as preliminary steps towards modeling the effects of stress on ovulation. Methods include a model expansion to include kisspeptin and gonadotropin-releasing hormone (GnRH). The resulting model will allow us to investigate underlying mechanisms in the relationship between GnRH, stress hormones, and ovulation. We will present preliminary results for parameter fitting of the modified model to data and discuss biological implications.

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MS78

The ACM-ASA-MAA-SIAM-ADSA Task Force to Define Knowledge, Skills and Abilities for Undergraduate Data Science Programs and Credentials

Recently, a taskforce with representatives from the ACM, ASA, MAA, and SIAM was formed and tasked to extend the ACM Computing Competencies for Undergraduate Data Science Curricula by producing a multidisciplinary set of competencies for data science. The overarching goal is to identify and describe the knowledge areas relevant to data science, and to outline a data science model curriculum. This session will present out their initial work in these efforts and to seek feedback from the members of SIAM. This work, and gathering community input on it, is extremely important as more and more educational institutions are developing data science curricular programs, and the field of data science grows in influence.

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MS78

California Learning Labs Data Science Grand Challenge

The California Learning Labs Data Science Grand Challenge fosters coordination and collaboration among institutions across the UC, Cal State, and Community College systems, advancing data science education through strategic partnerships, professional development, and capacity building. By bringing together educators and researchers through a mix of in-person and online panels, the initiative supports the development of new courses, enhances faculty training, and strengthens institutional alignment. This collaborative framework has catalyzed new initiatives in data science education and has positioned many interdisciplinary teams to successfully secure funding from the California Learning Lab, NSF, and other agencies, ensuring sustained innovation and growth across the states higher education segments. Over a multiple year process the stakeholders have been educating members about the intersegmental articulation process, built a UC Transfer Pathway, and are currently working on a Transfer Model Curriculum.

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MS79

Prevalence Estimation for Infectious-Disease Surveillance

Gathering observational data for infectious-disease surveillance often involves uncertainties arising from both type I (false positive) and type II (false negative) errors. In this talk, I will present a statistical model to improve infectious-disease surveillance by aggregating results from repeated and combined tests. This approach is especially valuable in situations requiring rapid and cost-effective testing methods, as seen during the SARS-CoV-2 pandemic. Our model enables the development of testing protocols with an arbitrary number of tests, which can be customized to meet requirements for type I and type II errors. This allows us to adjust sensitivity and specificity according to application-specific needs. Additionally, we derive generalized RoganGladen estimates of disease prevalence that account for an arbitrary number of tests with potentially different type I and type II errors. I will also briefly discuss a few clinical applications where combined testing is useful beyond infectious-disease surveillance.

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MS79

The Two-Cave Problem: Connecting Unsupervised Learning and Attacks on Machine-Learning Models via Corrupted Training Data

Disease ecology raises unique mathematical questions in sampling, machine learning (ML), and probability theory. In this talk, we consider a prototypical but foundational example that we refer to as the two-cave problem. The goal in solving this problem is to determine which animals in two distinct populations have been infected by a disease and thereby estimate its prevalence. Motivated by real-world applications of detecting pathogens in bats, we only consider settings in which we are given impure training data (whose underlying classes are unknown) for constructing classifiers. Critically, however, we assume that the prevalence of the disease in the two populations is different. The goal of this talk is to demonstrate how the two-

cave problem unifies aspects of both unsupervised learning and analysis of poisoned ML models. In particular, we use a recently-developed level-set theory of ML to show that the two-cave problem can be reduced to solving a system of quadratic equations, and, in some instances, these reduce to a corresponding linear system. We also show how this result generalizes to the M-Cave problem, i.e. the multiclass version of the two-cave problem. Critically, our results provide not only rigorous routes to undoing the effects of poisoned training data, but also practical methods for solving problems in disease ecology. Throughout, real-world data is used to motivate and explain mean ideas.

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MS79

Relative Entropy Methods for Computing Committor Functions

Motivated by challenges arising in molecular simulation, we devise new means of characterizing and sampling rare transitions between stable states in dynamical systems driven by noise. Our main technical advance is a new loss function that measures the accuracy of approximations to the committor associated with a given chemical reaction or other rare transition event. Our loss admits a simple interpretation in terms of the distribution of reactive trajectories, and it can be computed in practice to compare the accuracies of different approximations of the committor, including reduced or coarse-grained approximations. We also derive a method of calculating committors by direct minimization of the loss via stochastic gradient descent.

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MS80

Orthogonal Polynomials and Perfect State Transfer

A tridiagonal (Jacobi) matrix can be interpreted in various ways by mathematicians. For instance, those in the field of orthogonal polynomials might see the Jacobi matrix as a recurrence relation that generates a sequence of orthogonal polynomials, while those in mathematical physics may view it as the Hamiltonian governing a quantum spin chain. Given these different interpretations, it is natural to apply the theory of orthogonal polynomials to study quantum walks on graphs. In this talk, we will discuss some applications of orthogonal polynomials in quantum information processing, focusing on the associated Jacobi operators and how these can be used to detect perfect state transfer. We also will explore how orthogonal polynomials have been used to give results which are analogous to those given by Karlin and McGregor when studying classical birth and death processes. Finally, we show how these ideas have been extended to quantum walks with more than nearest neighbor interactions using exceptional orthogonal polynomials.

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MS80

Currents in Non-equilibrium Steady States of Open Inhomogeneous XX-spin Chains

Spin chains enabling perfect state transfer (PST) have attracted significant interest as a means of implementing quantum communication protocols without requiring active intervention. These systems allow for the end-to-end transport of a qubit with perfect fidelity, achieved through precise engineering of the internal couplings between neighboring spins. The transfer of excitation between the two ends of the chain suggests a connection between PST and efficient spin transport across the system, and leads to the following question: Do spin chains exhibiting PST inherently facilitate spin and heat transport when interacting with thermal baths at different temperatures? In this presentation, we will discuss our recent investigations addressing this question, including the connections to orthogonal polynomials and the symmetries of Jacobi matrices.

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MS80

Distance Measures for Quantum States and Channels: Properties and Applications

Discriminating between quantum states and channels is an important task in the field of quantum computation and quantum information theory. Metrics and statistical distances form the tools for various approaches proposed for this task. We analyze existing results to compare properties, main purpose, computability, and advantages and disadvantages of each approach.

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MS80

A Dynamical Algebra of Protocol-induced Transformations on Dicke States

Quantum n-qubit states that are totally symmetric under the permutation of qubits are essential ingredients of important algorithms and applications in quantum information. Consequently, there is significant interest in developing methods to prepare and manipulate Dicke states,

which form a basis for the subspace of fully symmetric states. Two simple protocols for transforming Dicke states are considered. An algebraic characterization of the operations that these protocols induce is obtained in terms of the Weyl algebra $W(2)$ and $\mathfrak{su}(2)$. Fixed points under the application of the combination of both protocols are explicitly determined. Connections with the binary Hamming scheme, the Hadamard transform, and Krawtchouk polynomials are highlighted.

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MS81

High-Performance Computing for Complex Simulations Through the Deal-II Open Source Software

The deal.II library aims at providing building blocks that can be leveraged by research groups to design high-performance software for complex simulations. Although it is over 20 years old, the deal.II library has been constantly evolving to adopt new paradigms that adequately use modern high-performance computing ressources. This comes off as a challenge since the library needs to remain as flexible as possible to adapt to the needs of all of its user while ensuring high computational efficiency in very large-scale computations. In this work, we present some of the development within the deal.II library that target high-performance application. We first present the matrix-free architecture within deal.II and how it has been leveraged by multiple users in various application to design highly performant and scalable software. Then, we focus on the drastically different particle architecture which large-scale particle simulations ranging from granular flow to geophysics. We conclude by discussing some of the lessons we have learned developing a large community-driven open-source software for finite element simulations.

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MS81

Advances in Linear System and Least Squares Solvers for GPU-Accelerated Distributed Memory Machines

We present recent advances in the solution of linear systems and linear least squares problems for modern GPU-accelerated distributed-memory machines. The focus is on minimizing communication using advanced algorithms such as Communication Avoiding LU and QR (CALU, CAQR), the Random Butterfly Transform (RBT), and GPU-native implementations. Our implementations in the SLATE library are portable across GPU vendors (CUDA, ROCm, and SYCL), as well as CPU-only machines.

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MS81

Hypre: High-Performance Preconditioners and Solvers

This talk will give an overview of the hypre software library of linear solvers and preconditioners developed at Lawrence Livermore National Lab. hypre is well-known for providing scalable multigrid preconditioners that may be accessed through a variety of conceptual interfaces. We will discuss the high-level design and strategies of these solvers and interfaces before presenting recent results on exascale machines and highlighting ongoing work on the project.

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MS81

Supporting the Geometry and Meshing Requirements of Fusion System Simulation Codes

The accurate simulation of the systems being design by the fusion energy industry requires inclusion of geometrically accurate models of components such as RF antenna, divertors, limiters, etc. This presentation will first present FASTMath efforts on the development of tools for the manipulating of CAD design and manufacturing models, definition of plasma physics geometry (e.g., flux surfaces) and their combination to produce geometrically accurate simulation geometries. Consideration will then be given to overviewing tools (i) to automatically mesh these geometries, including curved element meshes for high-order simulations, (ii) support parallel mesh adaptation and (iii) support of mesh-based particle simulations including PIC

plasma codes and neutronics codes. The integration and use of these tools in fusion energy system simulation workflows will be demonstrated.

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MS82

New Insights into Nonlinear Reduced Basis Methods

The Reduced Basis (RB) method is a powerful computational tool that enables efficient evaluation of functional outputs associated with parametrized partial differential equations. The method constructs a linear space that spans pre-computed finite element solution snapshots taken at optimally selected parameter values through a greedy algorithm. In cases where the field variable changes smoothly with respect to the parameters, the linear RB method can achieve high accuracy with a small number of snapshots. When assuming affine parameter dependence, both the RB approximation and its corresponding error bounds can be computed efficiently using offline-online procedures. However, in cases where the parameter domain is large or where the solution exhibits significant nonlinear behavior, such as in transport equations, we need high dimensional linear RB space, resulting in a high computational cost during the online phase. This motivates the need for nonlinear model reduction techniques such as nonlinear RB methods. Although the concept of nonlinear model reduction has been explored in the literature, existing nonlinear RB methods often lack rigor and completeness. In this research, we introduce a novel algorithm based on partitioning the parameter domain and provide theoretical results that rigorously characterize the convergence of the nonlinear RB method. Specifically, we establish results regarding the number of parameter subdomains required to achieve a desired accuracy.

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MS82

Comparison of Different Error Representations in Goal-Oriented Adaptive Algorithms

In Finite Element analysis, goal-oriented error estimation focuses on estimating the approximation error of a specific quantity of interest. This talk presents several globally equivalent error representations that are used to drive goal-oriented adaptive algorithms. It borrows previously developed error representations and draws a comparison of their efficiency and accuracy with newly introduced representations. The error representations are defined in the context of an abstract problem, using duality techniques and Galerkin orthogonality properties. They are then applied within h-adaptive algorithms, considering a 1D boundary-layer problem and the 2D Poisson problem on an L-shaped domain. The algorithms are tested with different marking strategies and quantities of interest. Numerical results demonstrate how the error representations vary locally, and how the choice of the representation affects the performance of the adaptive algorithms. The results are then used to determine a ranking of the various error representations.

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MS82

A Pod-Enhanced Finite Element Scheme for Mass Transfer

We are interested in the numerical simulation of the dynamic of a temperature distribution driven by the motion of an unsteady fluid. In the broad spectrum of approaches to model multiphysic flow and the capture of its behaviour, Galerkin methods, such as the finite element method, give high fidelity approximation of the solution (i.e. of controlled accuracy). However, these methods exhibit a relatively low computational efficiency. This is mainly due to the nonlinear (advection) and saddle-point (incompressibility) nature of the Navier-Stokes model driving the unsteady fluid and the coupling effect of the other physical quantities (here the temperature). A reduced order model (ROM) based on the initial system could be considered; however, due to the complexity of the model, the gain in efficiency would be at the expense of precision. In this presentation, we propose to take advantage of the effectiveness of the coupled projection method, which lessen the complexity of the model and frees us of the saddle point obstacle, and combine it to the ROM approach (here a POD) to increase the performance of the discrete model. Tackling only part of the model with a ROM, we will show that the high pre-

cision nature of the initial discrete model is maintained, producing effectively an *accelerated* finite element scheme for a Navier-Stokes and heat equation system.

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MS83

Adaptive Kernel Predictors From Feature-learning Infinite Limits of Neural Networks

Previous influential work showed that infinite width limits of neural networks in the lazy training regime are described by kernel machines. Here, we show that neural networks trained in the rich, feature learning infinite-width regime in two different settings are also described by kernel machines, but with data-dependent kernels. For both cases, we provide explicit expressions for the kernel predictors and prescriptions to numerically calculate them. To derive the first predictor, we study the large-width limit of feature-learning Bayesian networks, showing how feature learning leads to task-relevant adaptation of layer kernels and preactivation densities. The saddle point equations governing this limit result in a min-max optimization problem that defines the kernel predictor. To derive the second predictor, we study gradient flow training of randomly initialized networks trained with weight decay in the infinite-width limit using dynamical mean field theory (DMFT). The fixed point equations of the arising DMFT defines the task-adapted internal representations and the kernel predictor. We compare our kernel predictors to kernels derived from lazy regime and demonstrate that our adaptive kernels achieve lower test loss on benchmark datasets.

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MS83

The Computational Advantage of Depth: Learning High-Dimensional Hierarchical Functions with Gradient Descent

Understanding the advantages of deep neural networks trained by gradient descent (GD) compared to shallow models remains an open theoretical challenge. In this work, we introduce a class of target functions (single and multi-index Gaussian hierarchical targets) that incorporate a hierarchy of latent subspace dimensionalities. This framework enables us to analytically study the learning dynamics and generalization performance of deep networks compared to shallow ones in the high-dimensional limit. Specifically, our main theorem shows that feature learning with GD successively reduces the effective dimensionality, transforming a high-dimensional problem into a sequence of lower-dimensional ones. This enables learning the target function with drastically less samples than with shallow networks. While the results are proven in a controlled training setting, we also discuss more common training procedures and argue that they learn through the same mechanisms.

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MS83

Fixed Point Structure in Multi-Index Models: Implications for Dynamics, Interpretability, and Distillation

Training dynamics in deep learning can exhibit complex behavior, even under gradient flow in the vanishing learning rate regime. In this talk, I will present insights gained from analyzing multi-index models in two distinct regimes: the over-parameterized regime relevant to deep learning and the under-parameterized regime relevant to large language models. Specifically, I will introduce a novel characterization of fixed points that emerge from the partitioning and linear combination of index vectors. I will also describe a sharp threshold for a saddle-to-minimum transition, which occurs when the dot product between index vectors exceeds a critical value. These findings have notable implications for training dynamics. Fixed points resulting from index vector partitioning and combination create plateaus in the MSE loss curve. Meanwhile, when index vectors become highly correlated (under correlation loss), the resulting local minimum hinders the networks ability to learn them individually. I will conclude by discussing the broader implications of these fixed-point families for mechanistic interpretability and knowledge distillation.

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MS83

Learning Dynamics of Overparameterized Neural Networks

Understanding how the dynamics of gradient-based methods help overparameterized neural networks learn useful features for classification is a central question in modern deep learning theory. In this talk, we analyze the learning dynamics of gradient flow for three network architectures. For overparameterized linear networks, we show that the weights converge at a linear rate that depends on the imbalance between input and output weights (which is fixed at initialization) and the margin of the initial solution. For overparameterized ReLU networks, we show that the dynamics undergo a feature learning phase, where neurons collapse to one of the class centers, followed by a classifier learning phase, where the loss converges to zero at a rate of 1/t. Finally, for data drawn from an orthogonal mixture of Gaussians, we show that overparameterized ReLU networks learn a classifier that is not robust to adversarial perturbations, while pReLU networks provably learn a robust classifier.

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MS84

An Incommensurate Lattice Problem: the Elec-

tronic Properties of Twisted Trilayer Graphene

Although recent experimental results seem to indicate the existence of flat bands for twisted trilayer graphene (TTG), at present there is no convergent algorithm for approximating the density of states (or other desirable observables). We attempt to address this by using kernel polynomial approximation with an ab initio momentum-space tight-binding model. The unique challenge in the case of TTG is the lack of a periodic moiré supercell. This is addressed by modifying the truncation to account for more complex Umklapp scattering.

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MS84

Reconstruction of Spectral Measure from Noisy Measurements with a Certificate of Optimality

In this talk, I will discuss the problem of noisy data fitting and spectral measure recovery in the classes Stieltjes and Completely monotone functions. The analytical setting is non-negative least squares over the conical hull of a curve in $\mathbb{R}^n$. While the non-negative least squares problem receives much attention, no method exists to analyze convergence of approximate data to the optimal data nor approximated spectral measure to the optimal spectral measure, and popular numerical algorithms come with very few guarantees. I will introduce a simple theory of minimization over convex cones, by which we can convert the non-negative constraints to convex ones. In this context, convergence analysis is well understood. Algorithms for the convex problem along with this theory provide means to compute a function in the desired class so that its associated data approximately optimal. The theory also allows us to give tight bounds on the support of the optimal spectral measure given our approximations.

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MS84

Electric Circuits with Negative Capacitances and Inductances Exhibiting Exceptional Points of Degeneracy

We present an algorithm of the synthesis of lossless electric circuits such that their evolution matrices have the prescribed Jordan canonical forms subject to natural constraints. Every synthesized circuit consists of a chain-like sequence of LC-loops coupled by gyrators. All involved capacitances, inductances and gyrator resistances are either positive or negative with values determined by explicit formulas. A circuit must have at least one negative capacitance or inductance for having a nontrivial Jordan block for the relevant matrix. The mathematics involved in our analysis is intimately related to the canonical forms for quadratic Hamiltonians.

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MS84

Discrete and Continuum Networks with Homological Boundary Conditions

In many applications, electrical networks appear with boundary conditions different from the usual Dirichlet and Neumann ones and their mixture. For instance, in multiport networks, one prescribes the voltage drop and sets the total current to zero within each port. For networks on surfaces, one often prescribes voltage drops along topologically nontrivial loops on the surface. Special boundary conditions also arise in electromagnetic circuits, introduced by Milton and Seppecher. We develop a general framework to deal with such homological boundary conditions in the discrete setup. We adopt the classical concepts and theorems, such as the response matrix and the existence and uniqueness theorem. Our main result is a generalization of all-minors Kirchhoff's matrix-tree theorem, a combinatorial formula for the minors of the response matrix in terms of certain subgraphs, in the spirit of Kenyon and Wilson's enumeration of groves. This generalization is challenging because the subgraphs can now contribute with arbitrary integer coefficients. The proof uses tools from statistical physics, such as Smirnov's parafermionic observables and the double-dimer model. We also address the approximation of continuum networks by discrete ones. Namely, we mention a convergence result for one type of homological boundary conditions, giving a tool to compute period matrices of Riemann surfaces.

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MS85

Multiscale Modeling of Stimuli Responsive Materials for Drug Delivery

Wormlike micelles (WLMs) have emerged as promising drug delivery systems (DDS) due to their unique structural properties. Their ability to efficiently encapsulate drugs and achieve controlled release offers significant advantages over traditional methods. One key advantage of micelles as DDS is their responsiveness to stimuli. These "living" polymers undergo equilibrium breakage and growth through combinations. When subjected to stimuli, for example flow or changes in pH, the system is driven out of equilibrium, and the energy barrier for scission/recombination is modified. Experiments have revealed that, at high shear rates or changes in pH, micelles can undergo a structure transition from long, flexible chains to short, rod-like polymers. We develop a rheological model to approximate the nonlinear rheology of wormlike micelles using two constitutive models to represent the structural transition. Under flow, we hypothesize that stretching energy introduces a linear potential that decreases the rate of recombination and reduces the mean micelle length. Under pH changes, the electrostatic free energy accounts for repulsion due to presence of similarly charged ions. The increased repulsive force

reduces the overall energy needed to break a chain. For successful cancer drug delivery, WLMs must remain elongated under flow until reaching the acidic tumor microenvironment, where they undergo a structural transition to shorter, rod-like micelles, signifying drug release.

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MS85

Buckling Instability of Colloidal Crystals on a Lipid Membrane

The interacting assembly of particles on fluid interfaces constitutes a recurring motif in material science and membrane biophysics. It serves as a model system to understand diverse phenomena such as protein packing in viral capsids, cellular processes like endo-/exo-cytosis, and crystallization in curved geometries. The latter has been extensively explored in colloidal physics to probe fundamental questions of defect structure in curved geometries. In this talk, we present a hybrid-continuum model to study such systems. The interface is a lipid membrane (modeled by the Helfrich-Canham energy) that is embedded with point particles that can freely move on the surface. The particles interact with each other via a pair-potential. We explore the influence of substrate elasticity and pair-potential parameters on the packing structure of the particles. Using a Bloch ansatz, we perform a linear stability analysis to show that a flat state loses stability to non-planar configurations, some resembling bud-like states observed in (protein-mediated) exocytosis of lipid vesicles in cells. We compare our prediction with experimental data.

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MS85

A Discrete Platelet-Bonding Model for Simulating Platelet Aggregation under Flow

Hemostasis is the healthy clotting response to a blood vessel injury. A major component of clotting is platelet aggregation, which involves the formation of platelet-platelet and platelet-wall bonds between platelet receptors (GPVI and GP1b), and platelet integrins ($\alpha_2\beta_1$ and $\alpha_{IIb}\beta_3$) with plasma-borne molecules (von Willebrand factor and fibrinogen) and wall adherent collagen. There are platelet disorders that decrease the number and/or functionality of $\alpha_{IIb}\beta_3$, which results in excessive bleeding. Current treatments exist but are not evidence based and are not always successful in restoring hemostasis. In the cases where hemostasis is restored, the aggregation mechanism without $\alpha_{IIb}\beta_3$ remains speculative. Our long term goal is to uncover this mechanism with a mathematical and computational approach. As a first step, we simulated platelet aggregation using the molecular dynamics software, LAMMPS. We considered individual platelets and tracked the platelet-platelet and platelet-wall bonds that formed during aggregation. Currently, the strength of the bonds depend on the local shear rate of a prescribed background flow. Simulations show stable aggregation for healthy platelets under flow. Future work is to improve our modeling framework by parameterizing with experimental measurements and computationally coupling our platelet model to a dynamic flow.

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MS85

Anisotropic Drag in Complex Fluids: Mesoscale Models with Formed Chains

A mesoscopic model is proposed to describe the transient behavior of complex fluids with anisotropic hydrodynamic drags. Chains formed by the merging of beads from dumbbells at junctions are considered, as opposed to Rouse chains, in which there is only one bead at each junction. The anisotropy of the bead-spring chain is formulated by summing the anisotropic drag (which depends on the spring alignment) of each attached bead. This tensor drag coefficient is then inverted to yield the associated mobility coefficient. In this talk, formed (non-breaking/reforming) chains of fixed length are considered, and the number of beads at each junction is restricted to two. The effect of this drag-conserving anisotropy on the flow is explored. The eventual goal is to consider transient network effects in an anisotropic breaking/reforming bead-spring network, where the anisotropy arises from the drag.

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MS86

Speckle Imaging with Blind Source Separation and Total Variation Deconvolution

This talk is concerned with optical imaging in strongly diffusive environments. We consider a typical setting in optical coherence tomography where a sample is probed by a collection of wavefields produced by a laser and propagating through a microscope. We operate in a scenario where the illuminations are in a speckle regime, namely fully randomized. This occurs when the light propagates deep in highly heterogeneous media. State-of-the-art coherent techniques are based on the ballistic part of the wavefield, that is the fraction of the wave that propagates freely and decays exponentially fast. In a speckle regime, the ballistic field is negligible compared to the scattered field, which precludes the use of coherent methods and different approaches are needed. We propose a strategy based on blind source separation and total variation deconvolution to obtain images with diffraction-limited resolution. The source separation allows us to isolate the fields dif-

fused by the different scatterers to be imaged, while the deconvolution exploits the speckle memory effect to estimate the distance between these scatterers. Our method is validated with numerical simulations and is shown to be effective not only for imaging discrete scatterers, but also continuous objects.

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MS86

High-Order Continuum Approximations of Tight-Binding Models

This talk is concerned with the derivation of PDE models from tight-binding descriptions of 2D materials. We show that our PDE models accurately capture the tight-binding wave-packet dynamics over long times. Our results require a degenerate point (e.g. a Dirac cone) in the dispersion surfaces of the tight-binding Hamiltonian, and initial conditions that are spectrally localized to that degenerate point. Applications include single- and multi-layer graphene.

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MS86

Shower Curtain Effect and Source Imaging

An interesting phenomenon in optics is that it is possible to see a person behind a shower curtain better than that person can see us. This effect has been referred to as the shower curtain effect. We address the challenge of giving a precise mathematical description of this phenomenon. In addition we identify what governs the effect and discuss how imaging algorithms can be designed and analyzed when the objective is to image a source hidden behind a complex section.

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MS86

Reflection Optical Diffraction Tomography

We present an Optical Diffraction Tomography (ODT) algorithm to reconstruct the refractive index (RI) map of a medium in reflection mode microscopy. Our goal is to make quantitative imaging possible for thick biological samples and in-vivo applications. One of the main challenges in reflection ODT is the ill-posed nature of the inverse problem of light propagation. Under the linearized first-order Born forward model, only the RI spatial frequencies close to the wave number can be recovered, preventing us from quantitative imaging. Here, we demonstrate that multiple scattering can be used to recover the missing information, including the low spatial frequencies of the RI. To do so, we introduce an optimization-based reconstruction algorithm that retrieves these missing components, even though the problem is non-convex.

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MS87

Data-Enabled Stochastic Estimation for Nonstationary Inverse Problems

Nonstationary inverse problems present a number of significant mathematical and computational challenges in successfully estimating and quantifying uncertainty in unknown system components from limited, corrupt observations. This work introduces a data-enabled stochastic estimation procedure for solving inverse problems of this type, emphasizing statistical analysis and uncertainty quantification of the resulting estimates, as demonstrated on a suite of numerical examples.

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MS87

A Scalable Interior-point Gauss-Newton Method for PDE-constrained Optimization with Bound Constraints

We present a scalable method for large-scale elliptic PDE- and bound-constrained optimization. Such problems are a means to learn unknown aspects of PDE-based models. It is assumed that such model uncertainty is mathematically manifest in an unknown spatially distributed parameter field, $\rho(x)$. Bound-constraints $\rho(x) \geq \rho_\ell(x)$ are a natural means to introduce additional knowledge of an unknown parameter field, e.g., nonnegativity of a diffusivity parameter field. Bound-constraints are, however, the source of additional computational challenges as they introduce complementarity conditions in the nonlinear optimality system. We utilize a robust, full-space, interior-point method to solve the optimization problem. In order to avoid the computational costs required to regularize the inertia of the linearized optimality system matrix, we use a Gauss-Newton search direction. We discuss two related preconditioned Krylov-subspace solution strategies for said linear system. We show that the number of preconditioned Krylov-subspace iterations is independent of not only discretization but also the ill-conditioning that notoriously plagues interior-point linear systems. We conclude with parallel scaling results on a nonlinear elliptic PDE- and bound-constrained optimization example problem. The results were generated with a native implementation of the computational framework that makes extensive use of MFEM, a scalable C++ finite element library.

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MS87

Optimal Sensor Placement for Gaussian Processes using Column Subset Selection

Gaussian processes use data measured at a finite number of sensor locations to reconstruct a spatially dependent function with quantified uncertainty. However, since one can only deploy a finite number of sensors, it is important to determine how to optimally place the sensors to minimize a measure of the uncertainty in the reconstruction. We consider the Bayesian D-optimal criterion to determine the optimal sensor locations by choosing k sensors from a candidate set of m sensors. Since this is an NP-hard problem, our approach uses sensor placement as a column subset selection problem (CSSP) on the covariance matrix, computed using the kernel function on the candidate sensor points. We propose an algorithm that uses the Golub-Klema-Stewart framework (GKS) to select sensors and provide an analysis of lower bounds on the D-optimality of these sensor placements. To reduce the computational cost in the GKS step, we propose and analyze randomized Nystrm approximations on the kernel matrix. We demonstrate the performance of our method on two applications: fiber coating dynamics and sea surface temperature.

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MS88

Experience of Using Multigrid for Transonic and Supersonic Flows

Multigrid method has been used for accelerating convergence of solutions for the Euler and Navier-Stokes equations for compressible flows including transonic and super supersonic flows. However, its efficiency decreases for supersonic flows significantly. I will present a few practical techniques in the implementation of multigrid for high-speed flows that increase the robustness and efficiency of the standard multigrid method for solving the Navier-Stokes equations.

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MS88

Entropy-Stable Discretizations of Conservation Laws Via Residual Correction: Extension to Non-Polynomial Basis Functions

Entropy-stable discretizations of nonlinear partial differential equations (PDEs) provide a promising pathway toward developing robust fluid flow solvers. A popular approach to achieve entropy stability is to use two-point flux functions along with summation-by-parts (SBP) operators and simultaneous approximation terms (SATs). However, this approach requires substantially larger computational costs than standard divergence-form discretizations. Furthermore, SBP operators, which are typically constructed using polynomial basis functions, require a sufficiently strong quadrature rule to retain the SBP property needed for entropy stability. This often leads to lower efficiency relative to exiting alternatives. The residual correction method provides a simple and direct approach to make design-order modifications to standard divergence-form discretizations resulting in conservative and entropy-stable schemes. In this talk, we present numerical results highlighting the performance of this alternative entropy-stable method. We extend the approach to non-polynomial basis functions and demonstrate its numerical properties for a number of PDEs.

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MS88

Non-Reflecting Recirculation-Tolerant Outflow Boundary Condition for Compressible Navier-Stokes

We introduce an outflow boundary condition that uses Riemann flux solvers and is tolerant to recirculation at outflow boundary conditions. Additionally, it can be used in regions of high viscous stress (e.g. outflows of viscous boundary layers). The use of Riemann flux solvers allows acoustic waves to exit the simulation domain. The boundary condition is demonstrated on a few scale-resolving simulation examples.

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MS89

Determining the Sources of Heterogeneity in Neural Responses

Neurons ubiquitously display heterogeneities in spiking activity even within a given cell type. To date, the relative contributions of extrinsic mechanisms (e.g., synaptic bombardment) and intrinsic mechanisms (e.g., conductances, cell morphology) towards determining spiking activity remain poorly understood. We have recently addressed this important question using a novel approach that combines biophysical techniques, in which extracellular in vivo recordings of electrosensory pyramidal cells within weakly electric fish, are combined with computational modeling. Specifically, we explored how varying parameters of a Hodgkin-Huxley type model that produces ghost bursting dynamics successfully reproduced the highly heterogeneous spiking activities seen experimentally. Model parameters that varied the most were then used to gauge the relative contributions of extrinsic vs. intrinsic mechanisms, and the predictions made were experimentally validated. To simplify the analysis, we also developed a phenomenological model of ghost bursting that was capable of replicating the extrinsic dynamics of these neurons. In this talk, I will provide an overview of these findings.

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MS89

Dendritic Excitability Controls Overdispersion

The brain is an intricate assembly of intercommunicating neurons whose input-output function is only partially understood. In particular, the role of active dendrites in shaping spiking responses is unclear. Although existing models account for active dendrites and spiking responses, they are too complex to analyze analytically and demand long stochastic simulations. Here we combine cable and renewal theory to describe how input fluctuations shape the response of neuronal ensembles with active dendrites. We find that dendritic input readily and potently controls interspike interval dispersion. This phenomenon can be understood by considering that neurons display three fundamental operating regimes: one mean-driven regime and two fluctuation-driven regimes. We show that these results are expected to appear for a wide range of dendritic properties and verify predictions of the model in experimental data. These findings have implications for the role of interspike interval dispersion in learning and theories of attractor states.

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MS89

The Axon Initial Segment Controls Backpropagation and Learning

We consider two intrinsic neural properties: the spatial distribution of sodium channels in the axon initial segment (AIS), and the heterogeneity of adaptation kinetics in memory. In pyramidal neurons, the proximal AIS has more high threshold NaVs (Nav 1.2) compared to the distal AIS (Nav 1.6). As neurons develop, the spatial distribution of these subtypes also changes, which alters neural excitability. We implemented a range of hypothetical spatial NaV distributions in three multi-compartmental pyramidal cell models to quantify how channel kinetics regulate forward and backpropagation of spikes. Backpropagation is crucial for spike-time-dependent plasticity. With axonal stimulation, proximal NaV 1.2 availability dominates and promotes backpropagation. However, with somatic stimulation, the higher activation threshold of NaV 1.2 can impede backpropagation. Developmental changes to the spatial separation of NaV1.2 and NaV1.6 in the AIS thus differentially impact activation and availability, and thus learning. I will also show how the population heterogeneity of adaptation time scales enables the encoding of durations between stimuli encountered e.g. during path learning, or episodic memory more generally. Such heterogeneity is observed in thalamic-like neurons that drive memory circuits, and is shown through a Fisher-information analysis to be necessary for representing information about sequences of time intervals.

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MS90

Geometric Methods for Computing Most Probable Escape Paths in a Carbon Cycle Model

Noise perturbations in nonlinear systems can trigger critical transitions between stable states. This talk presents a unified framework combining dynamical systems theory with computational methods to analyze noise-induced tipping phenomena. We focus on novel techniques for computing Most Probable Escape Paths (MPEPs) in systems with periodic basin boundaries, demonstrating their application through a carbon cycle model. Our geometric approach illuminates key features of these transitions, offering potential insights for understanding critical shifts in Earth system dynamics.

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MS90

How the Follower Remembers: Up to the Tipping Point

A tandem run is a coordinated movement between a leader and a follower, observed in social arthropods. In B. obscuricornis, a blind termite species, coordination is maintained through tactile interaction. Previous work using empirical data reveals asymmetry in information flow from leader to follower, analogous to a unidirectional network system. We frame the pair interaction as a discrete-time dynamical system: the follower updates its position through a memory kernel that weights the leaders past movements. We show that this formulation can be recast as a three-node unidirectional network, enabling a homeostatic interpretation of tandem coordination. We analyze the stability of the system in a moving frame of reference. The fixed point reflects a form of homeostasis in which the projected distance between leader and follower along the direction of motion remains constant at d_h. The tipping point marks a loss of balance, reflecting a breakdown in the internal regulation that sustains coordinated movement.

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MS90

The Spatial Hyperbolic Restricted Three-Body Problem and Earth's Long-Term Climate Cycle

It is known as Milankovitch cycles that Earth's long-term climate cycle matches with combination of Earths eccentricity, obliquity, and precession. However, due to the chaotic behavior of the solar system, Olsen et al (2019) showed that there are mismatches between the celestial computation and the geological climate data beyond 60 million years ago. Chandramouli (2020) speculated that the geologic data might be able to detect the effect of a passing star, and applied the planar hyperbolic restricted three-body problem (HR3BP) to the Sun, a passing star, and Jupiter. In our study, we extend Chandramoulis planar model to motions in space. We investigated the change in Jupiter or Earth's orbital parameters by a stellar perturbation (of Sun-like mass, moving on a hyperbolic curve) near the Kuiper Belt. Similar to Sorokovich (1982) in their planar model, Jupiter's (and Earth's) eccentricity is stabilized after this stellar perturbation. We investigate if the change of inclination and argument of periapsis could be reflected in the Earths long-term climate cycle.

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MS90

From Icebergs to Water Bugs: Stable Floating Configurations for Floating Objects

Icebergs floating in the ocean float in certain stable configurations, governed by complex shape evolution associated with processes such as melting and/or calving. In this talk, I will discuss mathematical and computational techniques for the stability of floating objects, along with describing simple table-top experiments. Our focus is on long objects with uniform cross section. We explore both simple cross sectional shapes as well as highly complex shapes. We apply Archimedes' Principle along with a potential energy formulation that offers excellent insight into some of these observations. We compare our mathematical model predictions to experimental measurements. We also demonstrate an extension of our theory to objects that float at a two-fluid interface (e.g. oil–water). This theory also applies to small objects such as waterbugs, but in this case we have to incorporate the effects of surface tension.

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MS91

Centrosymmetric and Reverse Matrices in Bivariate Orthogonal Polynomials

We present bivariate orthogonal polynomials associated with an inner product that satisfies a symmetry property such that it is invariant when both variables are interchanged. Under that hypothesis, the structure of the polynomial vectors of the orthogonal polynomial systems is described by using centrosymmetric matrices. We show that the coefficient matrices of the three term relations, one for each variable, are connected by a reverse operation over matrices. Some particular cases and examples are presented.

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MS91

Lax-Type Pairs in the Theory of Bivariate Orthogonal Polynomials

In this seminar we consider sequences of bivariate orthogonal polynomials written as vector polynomials of increasing size satisfy a couple of three term relations with matrix coefficients. Furthermore, by introducing a time-dependent parameter, we investigate a Lax-type pair system governing the coefficients of the three-term relations. We also derive various characterizations of these Lax-type pairs, including the structure of the weight function, the Stieltjes function, moments, and a differential equation for the weight.

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MS91

Higher-Order Differential Operators Having Bivariate Orthogonal Polynomials As Eigenfunctions

We introduce a systematic method for constructing higher-order partial differential equations for which bivariate orthogonal polynomials are eigenfunctions. Using the framework of moment functionals, the approach is independent of the orthogonality domain's geometry, enabling broad applicability across different polynomial families. Applications to classical weight functions on the unit disk and triangle modified by measures defined on lower-dimensional manifolds are presented.

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MS91

Bivariate Multiple Orthogonal Polynomials of the Mixed Type

We study bivariate multiple orthogonal polynomials of mixed type in the step-line, providing a characterization in terms of a GaussBorel LU factorization of a suitable moment matrix. This matrix is inspired by analogous constructions in the bivariate standard setting and in the theory of mixed-type multiple orthogonal polynomials. The LU factorization yields recurrence relations and ChristoffelDarboux formulas for these polynomials. In addition, we establish a corresponding version of the ABC theorem.

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MS92

Dynamic Patterns in a Non-Reciprocal Cahn-Hilliard System

The Cahn-Hilliard equation is a classical model for phase separation. Arising as a mass-conserving energy minimizing flow, the Cahn-Hilliard equation is known to exhibit length-shortening and coarsening dynamics. More recently, there is growing interest in non-reciprocally coupled systems for which dynamics do not arise as energy minimizing flows. In this talk we describe a Mullins-Sekerka type reduction of a minimal non-reciprocal Cahn-Hilliard model introduced by Brauns and Marchetti in 2024. We explicitly determine stability thresholds for stationary and traveling multi-front solutions in periodic domains. In contrast to the classical Cahn-Hilliard equation we demonstrate that such minimal non-reciprocal coupling leads to dynamic behavior that is in stark contrast to that found in the classical Cahn-Hilliard equation.

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MS92

Diffusion-Induced Synchrony for a Cell-Bulk Compartmental Reaction-Diffusion System in 3-D

We investigate diffusion induced oscillations and synchrony for a 3-D PDE-ODE bulk-cell model, where a scalar bulk diffusing species is coupled to nonlinear intracellular reactions that are confined within a disjoint collection of small spheres. The bulk species is coupled to the spatially segregated intracellular reactions through Robin conditions across the boundaries of the small spheres. For this system, we derive a new memory-dependent ODE integro-differential system that characterizes how intracellular oscillations occur in the collection of cells are coupled through the PDE bulk-diffusion field. By using a fast numerical approach relying on the "sum-of-exponentials' method to derive a time-marching scheme for this nonlocal system, diffusion induced synchrony is examined for various spatial arrangements of cells. This theoretical modeling framework, relevant to applications such as quorum sensing when spatially localized nonlinear oscillators are coupled through a PDE diffusion field, is distinct from the traditional Kuramoto paradigm for studying oscillator synchronization through ODEs coupled on networks or graphs. (Joint work with Merlin Pelz, UBC and UMinnesota).

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MS92

Spikes in Discrete Gierer-Meinhardt Model

In this talk, we will discuss the spike solutions and their stability for the Gierer-Meinhardt model on discrete lattices. We explore several phenomena that have no analogues in the continuum limit. For example in the discrete case, the system retains spike patterns even when diffusion of the activator is set to zero. In this limit, we derive a simplified algebraic system to determine the presence of a K-spike solution. The stability of this solution is determined by a K by K matrix. We further delve into the scenarios where $K = 2$ and $K = 3$, revealing the existence of stable asymmetric spike patterns. Our stability analysis indicates that the symmetric two-spike solution is the most robust. Furthermore, we demonstrate that symmetric K-spike solutions are locally the most stable configurations. Additionally, we explore spike solutions under conditions where the inhibitors diffusion rate is not significantly large. In doing so, we uncover zigzag and mesa patterns that do not occur in the continuous system. Our findings reveal that the discrete lattices support a greater variety of stable patterns for the Gierer-Meinhardt model.

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MS93

High Accuracy ODE Solvers for Diffusion Models

In this study, we propose a novel approach that integrates exponential integrators with local radial basis function (RBF) interpolation to enhance the numerical accuracy of ODE solvers in diffusion methods. Our method leverages local RBF interpolation to refine the numerical approximation, ensuring stability and high accuracy. Unlike conventional polynomial-based methods, which can become unstable at higher orders, RBF interpolation offers greater flexibility, robustness, and adaptability to complex data structures. We introduce a new exponential integrator and provide a detailed analysis of the proposed solver, including error estimation and numerical validation.

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MS93

Unconditionally Gradient Stable But Explicit Numerical Method for Solving Gradient Flows

We propose an explicit linear scheme to solve the gradignt flows that satisfies energy stability. The proposed method can be easily extended to the 2nd order accuracy in time. Numerical experiments demonstrate its accuracy and energy stability.

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MS93

Physics-Informed Deep Inverse Operator Networks for Solving PDE Inverse Problems

Inverse problems involving partial differential equations (PDEs) can be seen as discovering a mapping from measurement data to unknown quantities, often framed within an operator learning approach. However, existing methods typically rely on large amounts of labeled training data, which is impractical for most real-world applications. Moreover, these supervised models may fail to capture the underlying physical principles accurately. To address these limitations, we propose a novel architecture called Physics-Informed Deep Inverse Operator Networks (PI-DIONs), which can learn the solution operator of PDE-based inverse problems without labeled training data. We extend the stability estimates established in the inverse problem literature to the operator learning framework, thereby providing a robust theoretical foundation for our method. These estimates guarantee that the proposed model, trained on a finite sample and grid, generalizes effectively across the entire domain and function space. Extensive experiments are conducted to demonstrate that PI-DIONs can effectively and accurately learn the solution operators of the inverse problems without the need for labeled data.

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MS95

Panel Moderator in Discussion on Journey of Black Mathematicians

The first half of the minisymposium will be the movie screening. The second half will be the panel session with three panelists.

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MS95

Panelist 1 in Discussion on Journey of Black Mathematicians

The first half of the minisymposium will be the movie screening. The second half will be the panel session with three panelists.

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MS95

Panelist 2 in Discussion on Journey of Black Mathematicians

The first half of the minisymposium will be the movie screening. The second half will be the panel session with three panelists.

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MS95

Panelist 3 in Discussion on Journey of Black Mathematicians

The first half of the minisymposium will be the movie screening. The second half will be the panel session with three panelists.

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MS96

Sex Differences in Oxidative Stress Management and their Consequences

Oxidative stress, an imbalance between oxidants and antioxidants in cells, can damage cells and contribute to conditions such as metabolic dysfunction, neurological disorders, cardiovascular disease, and aging when present at high levels. Interestingly, women tend to have lower levels of oxidative stress and higher concentrations of certain antioxidants, such as glutathione, compared to men. These differences point to the important role of sex hormones in regulating oxidative stress and its effects on the body. In this talk, I use mathematical modeling to uncover the mechanisms behind various experimental and clinical findings, including why women have higher levels of glutathione and lower levels of oxidative stress than men, as well as the differential effects of estrogen supplementation on a key cardiovascular biomarker, homocysteine, in premenopausal and postmenopausal women. I will also explain contradictory clinical observations regarding fluctuating oxidative stress throughout the menstrual cycle. By connecting clinical data with mathematical modeling, this work provides insights into the underlying mechanisms and paves the way for sex- and menopausal status-specific approaches in medicine.

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MS96

An Analysis of a Non-Specific Disease via Non-Negative Matrix Factorization

Our work explores the application of Nonnegative Matrix Factorization (NMF) toward the identification of patient subgroups and phenotypic definitions from patient data.

The analysis of patient self-classification results in the observation of symptom clusters and patient subgroups. These observations motivate the construction of several phenotypic definitions for patient classification. The robustness of the symptom clusters and patient subgroups are evaluated by the performance of the phenotypic definitions on the dataset. This research illustrates how matrix factorization approaches can refine the understanding and classification of complex disease phenotypes.

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MS97

Engaging High School Students and Teachers Through M3 Challenge

MathWorks Math Modeling Challenge (M3 Challenge) is a free, entirely internet-based competition for high school juniors and seniors and sixth forms in England and Wales. M3 Challenge, which celebrated its 20th anniversary in 2025, engages more than 3000 students each year, helping them understand how math and data are used to solve real-world problems. The mission of M3 Challenge is to inspire young people to choose and persist in studies and careers in STEM fields. We highlight the differences between M3 Challenge and other, more traditional math competitions, and describe benefits for students, teachers, and community partners.

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MS97

Supporting Student Growth in Mathematical Modeling Through COMAPs HiMCM and MidMCM

COMAP's High School Mathematical Contest in Modeling (HiMCM) and Middle Mathematical Contest in Modeling (MidMCM) provide students with an opportunity to apply mathematics in meaningful, real-world contexts. These international contests challenge teams of up to four students to develop mathematical models and present solutions to open-ended problems using grade-appropriate mathematics while fostering problem-solving, collaboration, and communication skills. In this session, we will explore ways to support students in your community before and after the competition. Whether through mentorship, structured preparation activities, engagement with local teachers, or post-contest reflection, we will share strategies to help students deepen their mathematical modeling skills and maximize the impact of their contest experience.

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MS97

Middle School Math Modeling Outreach Day

For three years, we have developed and run a middle school mathematical modeling day for local eighth grade students. We will describe why we decided to do this outreach, the logistics of the event from start to finish, and the positive feedback we have received. The program could be easily replicated at low cost, and our hope is to expand this modeling outreach day to other colleges/universities.

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MS97

How Community Engagement Benefits Industry and Academia

Fostering strong connections between academia and industry is critical to advancing innovation. An often overlooked but impactful way to cultivate these connections is through community engagement with K12 partners. In this talk we describe ways that a small STEM university in a rural region has created outreach programs that not only enrich the student experiences but also provide valuable opportunities for faculty and industry professionals to engage with each other and the next generation of problem solvers. Through specific examples we highlight how successful K12 partnerships provide mutual benefit while creating research opportunities and positive societal impact. We describe how to get started as well as challenges and pathways.

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MS98

Predicting Individualized Safety and Efficacy Using Mechanistic Modeling and Machine Learning.

T-cell engagers (TCEs) are a transformative cancer therapy that directs the immune system to target cancer cells. However, the activation of the immune system following the dosing of TCEs can result in rapid release of cytokines which can potentially lead to Cytokine Release Syndrome (CRS), posing severe patient safety concerns. Existing models have struggled to predict CRS risk for individual patients due to variability in responses and lack of informative data. Data-driven models can regress clinical CRS incidence based on patient attributes and cytokine dynamics, but data sparsity and variability limit their accuracy. This study proposes a hybrid modeling approach combining mechanistic models with machine learning (ML) classifiers to predict CRS risk. The mechanistic model captures immune system dynamics, TCE dosing, and cancer cell interactions, predicting cytokine release. These predictions inform the ML classifier, which considers drug exposure metrics, baseline factors, and cytokine peaks to forecast clinical CRS incidence. We showcase the utility of this model using data across various studies and also simulated data to demonstrate that this hybrid approach improves prediction accuracy and in conjunction with models for drug efficacy can be used to optimize dosing regimens. Recognizing CRS as a limiting factor for TCE development, this work presents a practical tool for optimizing TCE dosing and designing safer clinical trials.

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MS98

Physics-Informed Neural Networks Approaches to Predict Dynamics of Epidemiological Models Incorporating Human Behavior

Compartmental models are a tool used to understand how infectious diseases spread through populations. However, the task of estimating epidemiological parameters, such as the infection or recovery rate of the disease, increases in complexity as more parameters and compartments are included in the model. This work is based on a Physics-Informed Neural Network (PINNs) approach to predict disease dynamics of modified compartmental models from observed data. This methodology is suitable for incorporating human behavior into the models, offering a more realistic representation of the disease.

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MS98

A PDE QSP Study of Dose Non-Monotonicity of ADC

The binding site barrier phenomenon introduces nonlinearity to the delivery of ADCs to solid tumors. In this talk we discuss numerical studies done with our QSP model of growing and shrinking tumors of this phenomenon and of the optimization of ADC efficacy in light of it.

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MS98

Comparison of Cancer-Targeting and Stromal-Targeting Antibody-Drug Conjugates Using Bystander QSP Models

This talk presents ADC mathematical models incorporating both antigen-positive and antigen-negative cells. Simulations suggest that response to ADC treatment might not be durable when antigen-positive and antigen-negative cells grow independently. However, stromal-targeting ADCs could overcome this limitation, as antigen-positive stromal cells may be recruited into the tumor. Additionally, we demonstrate that ADCs with more permeable payloads and less stable linkers may enhance efficacy in cases of heterogeneous target expression.

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MS99

Multiple State Transfer

When the Hamiltonian of a continuous-time quantum walk is symmetric, perfect state transfer can occur from a vertex to at most one other vertex. When the Hamiltonian is non-symmetric, it is possible for pairwise perfect state transfer to occur in a set of three or more vertices, a phenomenon called multiple state transfer. In this talk, we present some new results on multiple state transfer in chiral quantum walks.

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MS99

Simple Quantum Coins Enable Pretty Good State Transfer on Every Hypercube

One desired phenomenon in quantum walks is pretty good state transfer, where the system gets arbitrarily close to a target state. In this talk, we consider pretty good state transfer in coined quantum walks between antipodal vertices on the hypercube Q_d. When d is a prime, this was proven to occur in the arc-reversal walk with Grover coins. We extend this result by constructing weighted Grover coins that enable pretty good state transfer on every Q_d. Our coins are real, and require modification of the weight on only one arc per vertex. We also generalize our approach and establish a sufficient condition for pretty good state transfer to occur on other graphs.

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MS100

New Capabilities of the Linear Solver Packages at Lawrence Berkeley National Laboratory

In this talk, I will give an overview of the new capabilities of linear system solvers developed at Lawrence Berkeley National Laboratory (LBNL), particularly focusing on a supernodal sparse solver SuperLU_DIST, a rank-structured multi-frontal sparse solver STRUMPACK, and a rank-structured dense solver ButterflyPACK. These new features include improved distributed-memory CPU and GPU scalabilities, batched functionalities and Python interfaces in SuperLU_DIST, GPU-accelerated block-low-rank compression algorithm and new sketching-based H2 compression in STRUMPACK, and new tensor algorithms in ButterflyPACK. These new capabilities are developed in various DOE funded projects including ECP, SciDAC and other ASCR projects, and can greatly enhance the solvers' scalability, interoperability, efficiency and flexibility.

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MS100

rocSPARSE - Sparse Linear Algebra Library on AMD GPUs

In this presentation, we introduce AMDs GPU-accelerated libraries for sparse linear algebra, rocSPARSE and rocALUTION, tailored to workflows spanning machine learning, data analytics, and large-scale simulations. These libraries offer high-performance kernels and easy-to-use APIs, seamlessly integrating into modern scientific codes. We will explore their design principles, highlight key capabilities, and demonstrate how developers can leverage them to expedite parallel application development. Code examples illustrate the flexibility of their interfaces, while performance benchmarks underscore their efficiency in real-world computing

environments.

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MS100

Frosch, a Domain Decomposition Library in Trilinos

FROSch (Fast and Robust Overlapping Schwarz) is a software package in Trilinos, which implements multi-level domain-decomposition based linear solvers. It takes advantage of the Trilinos software stack in order to be portable to different computer architectures. In this talk, we discuss the functionalities and implementation of FROSch, and show its performance for Albany Landice simulation on Perlmutter supercomputer at NERSC.

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MS101

Minimax Rates for the Learning of Spectra of Differential Operators from Data

The field of graph-based learning is one that is closely connected to manifold learning. It explores the following question: given a collection of data points $x_1, \ldots, x_n$ and a similarity graph over it, how can one use this graph to learn relevant geometric features from the dataset and in turn learn about the distribution that generated it? In this talk, I will discuss that, despite the multiple questions and answers that have been explored in the area of graph-based learning, there are several fundamental questions in statistical theory that have been largely unexplored, all of which are essential for manifold learning. Examples of these questions include: 1) What is the best possible estimator (potentially not graph-based), from a sample efficiency perspective, for learning features of unknown manifolds from observed data? 2) What is the asymptotic efficiency of popular graph-based estimators used in unsupervised learning? I will focus on the first type of question in the context of the task of learning the spectra of elliptic differential operators from data and will present new results that can be interpreted as a first step in bridging the gap between the mathematical analysis of graph-based learning and the analysis of fundamental statistical questions like the ones mentioned above. This talk is based on very recent work with my PhD student Chenghui Li (UW-Madison) and with Raghavendra Venkatraman (Utah).

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MS101

Neighbor Embeddings and Persistent Homology for High-Dimensional Data and Abstract Graphs

In this talk, I am going to summarize our recent work on neighbor embeddings, which is a powerful approach to manifold learning and dimensionality reduction of high-dimensional data. I will introduce a contrastive approximation to t-SNE based on the InfoNCE loss function, which allows to construct parametric and high-dimensional embeddings. I will discuss an important trade-off in neighbor embedding methods, the attraction-repulsion spectrum, appearing in both contrastive and non-contrastive setting. I will then show how the neighbor embedding framework can be applied to abstract graphs (as opposed to k-nearest-neighbor graphs), producing high-quality node embeddings and graph layouts. Finally, I will discuss whether neighbor embeddings can be trusted to preserve topological structures such as loops. I will show that persistent homology can be a reliable tool to detect the correct topology even in the presence of high-dimensional noise but only when using spectral distances (such as diffusion distance and effective resistance) on the k-nearest-neighbor graph of the data.

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MS101

Geometric Learning Beyond Visualization: Explanations and Eigenflows

Manifold learning is widely used for visualization of scientific inferences performed by other means. This talk shows that mathematically and statistically grounded geometric data analysis can support quantitative algorithms, that both recover the underlying low-dimensional structure of point clouds and validate inferences about these embeddings that are usually left to the scientist to sort out. This talk will illustrate this paradigm in two directions. First, we ask if it is possible, in the case of scientific data where quantitative prior knowledge is abundant, to explain a data manifold by new coordinates, chosen from a set of scientifically meaningful functions? Second, I will show how some popular manifold learning tools and applications can be recreated in the space of vector fields and flows on a manifold. Central to this approach is the order 1-Laplacian of a manifold, Δ_1, whose Helmholtz-Hodge Decomposition provides a basis for all vector fields on a manifold. We present an estimator for Δ_1, and, based on it, applications including: visualization of the principal harmonic, gradient or curl flows on a manifold, smoothing and semi-supervised learning of vector fields. In topological data analysis, we describe prime manifold decomposition, the k-th order analogue of spectral clustering. From it, a new algorithm for finding shortest independent loops follows. Joint work with Yu-Chia Chen, Vlad Murad, Samson Koelle, Hanyu Zhang and Ioannis Kevrekidis

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MS101

Manifold Learning in Wasserstein Space

Many datasets in modern applications - from cell gene expression and images to shapes and text documents - are naturally interpreted as probability measures, distributions, histograms, or point clouds. This perspective motivates the development of learning algorithms that operate directly in the space of probability measures. However, this space presents unique challenges: it is nonlinear and infinite-dimensional. Fortunately, it possesses a natural Riemannian-type geometry which enables meaningful learning algorithms. This talk will provide an introduction to the space of probability measures and present approaches to manifold learning within this framework. The proposed algorithms are demonstrated in pattern recognition tasks in imaging and medical applications.

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MS102

Emergent Bottleneck Structure in Dnns: How Neural Nets Learn Symmetries

: Add the following abstract: Deep Neural Networks have proven to be able to break the curse of dimensionality, and learn complex tasks on high dimensional data, such as images or text. But we still do not fully understand what makes this possible. To answer this question, I will describe the appearance of a Bottleneck structure as the number of layers in the network grows, where the network learns low-dimensional features in the middle of the network. This allows the network to identify and learn symmetries of the task it is trained on, without any prior knowledge. This could explain the success of Deep Learning on image and text tasks which feature many 'hidden' symmetries.

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MS102

A Function Space View of Norm-Constrained Deep Neural Networks

Many mathematical analyses of deep learning focus on how neural network (NN) parameters evolve during training. A complementary perspective is to view NN training as fitting a function belonging to a function space implicitly defined by the architecture and training procedure. In particular, when parameter norms are explicitly or implicitly constrained, NNs exhibit a bias toward functions with low "representation cost", defined as the minimal parameter norm required to realize the function with a given NN architecture. This talk surveys recent results that characterize representation cost of shallow NN architectures in terms of Banach space norms, and through non-linear notions of function rank for deeper NN architectures. Finally, we discuss how bias towards low representation cost functions helps to explain generalization in training denoising auto-encoders and solving inverse problems with implicit neural representations.

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MS102

Compositional Sparsity of Computable Functions and Learnability

TBA.

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MS102

Unveiling the Role of Learning-Rate Schedules via Functional Scaling Laws

Scaling laws have played a cornerstone role in guiding the training of large language models (LLMs). However, existing theoretical analyses only focus on the final-step risk, overlooking the intermediate-step risk and, crucially, the impact of learning rate schedule(LRS). In this paper, we aim to bridge this gap by studying a teacherstudent kernel regression task trained with stochastic gradient descent. Leveraging a novel e?ective time viewpoint, we derive a Functional Scaling Law (FSL) that applies to general learning rate and batch size schedules. The schedules influence enters through an explicit convolution-type functional term, making their e?ects fully tractable. To illustrate the utility of FSL, we analyze three widely used LRSs constant, exponential decay, and warmup-stable-decay(WSD) under both data- and compute-limited regimes. Our analyses provide theoretical support for widely adopted empirical practices in LLMs pretraining such as (i) higher-capacity models are more data- and compute-e?cient; (ii) learning rate decay can improve training e?ciency; (iii) WSD-like schedules can outperform direct-decay schedules. We also examine the practical relevance of FSL to LLM pretraining and provide partial theoretical support for the recently proposed LRS-aware scaling law [LWH+24]. Overall, our FSL o?ers a principled approach for understanding the role of learning rate and batch size schedule in neural scaling laws and, more broadly, in stochastic optimization.

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MS103

Characterization of Electric Circuits with Two Kinds of Passive Elements

We study the response of response of multi-terminal networks composed of two kinds of passive two-terminal elements (e.g. resistor-capacitor, resistor-inductor, inductor-capacitor). The response is a rational function with poles at resonances and matrix valued residues that both need to satisfy certain thermodynamic constraints. Conversely we show that it is possible to construct a network having a response with prescribed pole and residue structure provided they satisfy the thermodynamic constraints and we do not prescribe the residues at the two extreme poles. This work may have applications to designing materials with exotic properties.

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MS103

Multivariable Rational Matrix Functions: Synthesis Constraints Using Reciprocal Electrical Networks

We present our recent theorem, and its proof, that resolves an open problem posed to me as an undergraduate by my research advisor, Aaron Welters (Florida Institute of Technology), in Jan. 2022. Our results can be summarized as follows. First, every square matrix whose entries are multivariable rational functions over a field $\mathbb{F}$ in n indeterminates $z_1, , z_n$ has a Bessmertnyi realization, i.e., is the Schur complement of an affine linear square matrix pencil with coefficients in $\mathbb{F}$. Second, if the matrix is also symmetric and either $n = 1$ or the characteristic of the field $\mathbb{F}$ is not two then it has a symmetric Bessmertnyi realization (i.e., the pencil can be chosen to consist of symmetric matrices). For all other cases (i.e., when $n \geq 2$ and the characteristic of $\mathbb{F}$ is two), we give counterexamples and, in particular, show there is a class of multivariate rational functions that cannot be synthesized from the response matrix of any reciprocal electrical network over fields of characteristic two (e.g., Boolean networks). A specific example of this is given that illustrates the result using the Y-Δ transform. Finally, we conclude with a complete characterization of the class of functions with symmetric Bessmertnyi realizations. This is joint work with Jason Elsinger and Aaron Welters.

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MS104

Bayesian Estimation for Parameters of ODE Models in the Presence of Time Warping

Curve registration is a set of techniques to align functional data in the presence of time warpingstochastic variation of the time component. In this talk, we will present a Bayesian framework to estimate the parameters of an ODE model when the observations contain stochastic fluctuations in both amplitude and phase with a Gaussian process defining the time warping model. Particular attention will be paid to the effect of time warping on the accuracy of estimation of the structural parameters from the original ODE model. Such a framework can help us develop a more complete picture of stochastic variability across subjects, such as the variation across patients when collecting highly sampled physiological data. Case studies via simulation and of collected data will be presented.

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MS104

Bayesian Inference and Role of Astrocytes in Amyloid-Beta Dynamics with Modelling of Alzheimer's Disease Using Clinical Data

Alzheimer's disease (AD) is a prominent, worldwide, age-related neurodegenerative disease that currently has no systemic treatment. Strong evidence suggests that permeable amyloid-beta peptide (Abeta) oligomers, astrogliosis and reactive astrocytosis cause neuronal damage in AD. A large amount of Abeta is secreted by astrocytes, which contributes to the total Abeta deposition in the brain. This suggests that astrocytes may also play a role in AD, leading to increased attention to their dynamics and associated mechanisms. Therefore, in the present study, we developed and evaluated novel stochastic models for Abeta growth using ADNI data to predict the effect of astrocytes on AD progression in a clinical trial. In the AD case, accurate prediction is required for a successful clinical treatment plan. Given that AD studies are observational in nature and involve routine patient visits, stochastic models provide a suitable framework for modelling AD. Using the approximate Bayesian computation (ABC) approach, the AD etiology may be modelled as a multi-state disease process. As a result, we use this approach to examine the weak and strong influence of astrocytes at multiple disease progression stages using ADNI data from the baseline to 2-year visits for AD patients whose ages ranged from 50 to 90 years. Based on ADNI data, we discovered that the strong astrocyte effect could help to lower or clear the growth of Abeta, which is a key to slowing down AD progression.

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MS104

Conservative Hamiltonian Monte Carlo

Among many Markov Chain Monte Carlo algorithms used to sample high dimensional distributions, Hamiltonian Monte Carlo (HMC) is a prominent algorithm often utilized for Bayesian inference. However, such distributions tend to have thin high density regions, posing a significant challenge for symplectic integrators to maintain the small energy errors needed to retain a high acceptance probability. Instead, we introduce a variant of HMC called Conservative Hamiltonian Monte Carlo, using $R-$reversible energy-preserving integrators to maintain a high acceptance probability for high dimensional target distributions. While such integrators are generally not volume-preserving, an approximate Jacobian is introduced in the acceptance probability as a trade-off between computational efficiency and exact stationarity. This leads to our notion of approximate stationarity, which quantifies the error from stationarity determined by the Jacobian approximation of the energy-preserving proposal map. We show numerical results with improved convergence and robustness over integration parameters on target distributions with thin high density regions and in high dimensions. Moreover, we introduce a variant of our algorithm which can be applied to target distributions without gradient information, in contrast to HMC.

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MS104

Inference for Dynamic Systems Via Gaussian Processes: Progress and Challenges

We discuss some recent developments in statistical methods for inferring the trajectories and parameters of differential equation (DE) models from time-series data. While least-squares estimation via deterministic numerical solvers is the traditional approach, alternatives that bypass the need for numerical integration have gained attention. Among these, Gaussian process (GP) models represent the solution trajectory in a probabilistic way, with the help of priors that allow us to encode the dynamics specified by the DEs. GPs can thus be well-suited for facilitating inference in applied scientific problems, where experimental data from the system are often noisy and sparse, and only partially observed. By imposing a manifold constraint for the DEs, we can construct GP-based Bayesian posteriors that accurately characterize the parameters of interest in a variety of settings. These include dynamical models with features such as time-delay parameters, time-varying parameters, or inter-subject variability. We use examples from biology and epidemiology to illustrate the potential of such GP-based methods for fast and reliable inference, along with their applicability to selecting the appropriate DE model for the data and generating future predictions. We conclude by reviewing some limitations of GPs and challenges that may be tackled by future research in this area.

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MS105

High Order Unconditionally Strong Stability Preserving Method for Kinetic Equations

In this talk we present a novel unconditionally strong stability preserving additive method which relies on the downwind operator for the first component and a second derivative term for the second component. We show how this method performs in numerical simulations of kinetic equations.

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MS105

Two-Derivative Explicit, Implicit, and IMEX SSP Runge-Kutta Methods

In this work we review sufficient conditions for a two-derivative multistage method to preserve the strong stability properties of spatial discretizations in a forward Euler and different conditions on the second derivative. In particular we present the strong stability preserving theory for explicit and implicit two-derivative RungeKutta schemes, including a special condition on the second derivative under which these implicit methods may be unconditionally strong stability preserving. This special condition is natural for the stiff component of wide range of plasma physics problems, and can be useful in the context of strong stability preserving implicit-explicit multi-derivative RungeKutta schemes, where the time-step restriction is then independent of the stiff term. Finally, we present the strong stability preserving theory for implicit-explicit multi-derivative general linear methods, and some novel second and third order methods where the time-step restriction is independent of the stiff term.

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MS105

Asynchronous Time Integration Via Stage-Local Partitioned Two-Step Runge-Kutta Methods

In this talk we present stage-local partitioned two-step Runge-Kutta methods, an extension of standard two-step Runge-Kutta methods and an alternative to standard additive two-step Runge-Kutta methods. These new schemes are designed with an eye towards truly N-partitioned systems and leverage local stage approximations to make several computationally interesting approximations viable. Specifically, we will present the construction of both asynchronous, in the parallel sense, methods as well as implicit schemes that require the inversion of only local nonlinear systems.

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MS105

An Explicit Energy-Conserving Particle Method for the Vlasov-Fokker-Planck Equation

We propose an explicit energy-conserving particle method for the Vlasov–Fokker–Planck equation by extending a recent particle-in-cell scheme originally developed for the collisionless Vlasov equation. The proposed method preserves exact energy and achieves second-order accuracy in time, even in the presence of Fokker–Planck collisions. The key idea is to discretize the collision operator in a way that is compatible with the energy-preserving time integrator. Numerical tests confirm the methods accuracy on collisional plasma problems including Landau damping and the

two-stream instability. This is joint work with Lee Ricketson and Jingwei Hu.

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MS107

Polygonal Monotone Schemes for Convection-Dominated Transport Equations

In this talk, we present polygonal monotone schemes for solving the transport equation, formulated as a convection-diffusion problem in a convection-dominated regime. A key challenge in such problems is ensuring numerical stability while accurately capturing sharp solution features. To address this, we introduce the discrete maximum principle (DMP), which guarantees stable numerical solutions and prevents non-physical oscillations. The DMP follows from a monotonicity property, which, in turn, is ensured by satisfying the M-matrix condition. Based on this foundation, we develop and analyze numerical schemes that enforce these conditions on general polygonal meshes. To construct these schemes, we employ edge-averaged finite element (EAFE) methods, which offer a straightforward implementation while naturally preserving the DMP and minimizing numerical dissipation. The proposed schemes extend the EAFE concept to the finite volume method, the virtual element framework, and polygonal triangulation. We will present theoretical insights and numerical results to demonstrate the effectiveness of this approach.

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MS107

HDG for theCoupled Time-dependent Navier-Stokes and Darcy Problem

We present a hybridizable discontinuous Galerkin (HDG) method for the time-dependent Navier-Stokes equations coupled to the Darcy equations via the Beavers-Joseph-Saffman interface condition [A. Cesmelioglu, J. J. Lee, and S. Rhebergen, A strongly conservative hybridizable discontinuous Galerkin method for the coupled time-dependent Navier-Stokes and Darcy problem. ESAIM: Mathematical Modelling and Numerical Analysis 58 (2024), pp. 273-302.]. The discretization results in a discrete velocity that is globally H(div)-conforming and exactly divergence free in the absence of source terms. We will show stability of the discretization under a small data assumption, prove well-posedness, and discuss a priori error estimates.

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MS107

Conservation-Preserving FVE Schemes Through a Two-Layer Dual Strategy

Conservation laws are fundamental physical properties that are expected to be preserved in numerical discretizations. We propose a two-layered dual strategy for the finite volume element method (FVEM), which possesses the conservation laws in both flux form and equation form. In particular, for problems with Dirichlet boundary conditions, the proposed schemes preserves conservation laws on all triangles, whereas conservation properties may be lost on boundary dual elements by existing vertex-centered finite volume element schemes. Theoretically, we carry out the optimal L^2 analysis with reducing the regularity requirement from $u \in H^{k+2}$ to $u \in H^{k+1}$. While, as a comparison, all existing L^2 results for high-order ($k >= 2$) finite volume element schemes require $u \in H^{k+2}$ in the analysis.

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MS107

A Weak Galerkin Finite Element Method for Poroelasticity Problems on Quadrilateral Meshes

We propose a stabilizer-free weak finite element method that utilizes H(div) elements on quadrilateral meshes to approximate the space of weak gradient functions. For temporal discretization, backward differentiation formulas (BDF) are employed, while spatial discretization is achieved using weak Galerkin (WG) finite elements on quadrilaterals. The discrete weak gradients of shape functions are constructed within the vector- or matrix-valued Arbogast-Correa spaces. The combination of BDF and WG discretizations yields numerical solutions with well-balanced spatial and temporal errors across all six primary quantities: displacement, dilation (divergence of displacement), stress, pressure, velocity, and normal flux.

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MS108

Intrinsic Neural Heterogeneity Controls Computation in Spiking Neural Networks

Neurons are the basic information-encoding units in the brain. In contrast to information-encoding units in a computer, neurons are heterogeneous, i.e., they differ substantially in their electrophysiological properties. How does the brain make use of this heterogeneous substrate to carry out its function of processing information and generating adaptive behavior? In recent work, we used a mean-field model to investigate computation in heterogeneous neural networks, by studying how the heterogeneity of cell spiking thresholds affects three key computational functions of

a neural population: the gating, encoding, and decoding of neural signals. We show that neural heterogeneity provides a previously unconsidered means of controlling computational properties of neural circuits, and uncover different capacities of inhibitory vs. excitatory heterogeneity to regulate the gating of signals vs. the encoding and decoding of information, respectively. Drawing from these findings, we propose intra-cell-type heterogeneity as a mechanism for sculpting the computational properties of local circuits of excitatory and inhibitory spiking neurons, permitting the same canonical microcircuit to be tuned for diverse computational tasks.

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MS108

Interplay of Intrinsic Properties and Circuit Dynamics Dictates Spike Frequency Adaptation in the Lateral Prefrontal Cortex

Intrinsic neuronal properties, such as intrinsic spike frequency adaptation (I-SFA), play a key role in neuronal circuit dynamics and in vivo activity. To investigate how I-SFA in neurons isolated from brain networks contributes to extrinsic-SFA (E-SFA) in behaving animals, we recorded responses of macaque lateral prefrontal cortex neurons during a visually guided saccade task and in acute brain slices in vitro. Broad spiking (BS) putative pyramidal cells and narrow spiking (NS) putative inhibitory interneurons exhibited E-SFA in vivo. In vitro, the cell types displayed differing magnitudes of I-SFA but with timescales similar to E-SFA. To elucidate how in vitro I-SFA contributes to in vivo E-SFA, we developed a data-driven hybrid circuit model in which NS neurons are driven by local BS input. The model NS cell responses show longer SFA than observed in vivo. However, addition of inhibition of model NS cells removed this discrepancy and reproduced the in vivo E-SFA, suggesting a vital role of local circuitry in task-related in vivo activity. Furthermore, I-SFA contributes to E-SFA in a I-SFA timescale dependent manner and modulates in vivo response magnitudes and E-SFA timescales, indicating that both I-SFA and inhibitory circuit dynamics contribute to E-SFA in LPFC neurons during a visual task. Consequently, large cortical network models may benefit from including intrinsic neuronal properties.

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MS108

Multiple Kinds of Interneurons Participate in Supporting Spike Time Dependent Plasticity

The increase or decrease in the strength of a connection between two neurons often depends on the relative timing of the pre- and post-synaptic neurons, usually called spike-time-dependent plasticity. It remains to be understood what mechanisms can produce the correct timing for STDP. This talk describes STDP in the basolateral amygdala (BLA), a major site for fear leaning, a paradigmatic form of associative learning. We use Hodgkin-Huxley-like dynamical systems models to show that the necessary timing comes about from interactions of three types of (inhibitory) interneurons having different sets of intrinsic currents and different connectivity, as supported by experiments. The desired plasticity is between two kinds of projection cells, one (F) that responds to an unconditioned (aversive) stimulus and the other (CS) that responds to a conditioned (neutral at first) stimulus; after fear training, the unconditioned stimulus produces a response in the F cell. It has been experimentally documented that three brain rhythms in the BLA are associated with fear learning: gamma (30-90 Hz), low theta (2-6 Hz) and high theta (6-12 Hz). Our models show that there is a connection between the types of interneurons (PV, SOM and VIP) and the three brain rhythms: each kind of interneuron is associated with one of rhythms. Then we show why, at least for certain kinds of plasticity rule, each kind of interneuron and rhythm is necessary for plasticity, explaining experiments.

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MS108

The Role of Neuronal Excitability in Macroscopic Circuit Dynamics in Recurrent Neural Networks

Conventional neural network training adjusts both weights and biases. Recent evidence shows that fixing weights and training only biases can yield effective learning, offering resource efficiency, streamlined neuromorphic implementations, and insights into brain mechanisms via striatal gating of cortical processing. We implemented recurrent and feedforward networks with fixed weights and trainable biases, evaluating performance on learning dynamical systems and image classification using gradient/Jacobian-based methods. Results indicated that bias-only training could match—and sometimes outperform—weight-trained networks with an equal number of learnable parameters. One bias-trained network achieved over 90% accuracy on five MNIST-based tasks and successfully learnt the dynamics of 10 chaotic dynamical systems with learnt biases for each task. These findings suggest that biases alone can encode sufficient information for effective learning, with implications for simplified network training and low-power neuromorphic designs. Moreover, this approach may serve as a computational analogy for basal ganglia–cortex gating in the brain. Ongoing work extends these methods to

reinforcement learning and spiking neural networks.

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MS109

Bispectral Bivariate Polynomials

The bispectral polynomials of the Askey scheme play important roles in many areas of mathematics and mathematical physics. They have been classified by Leonard to obtain a characterization of P- and Q-polynomial association schemes. This classification has been done for univariate polynomials. In this seminar, I would like to discuss bivariate polynomials that also exhibit bispectral properties. There are numerous additional difficulties, and I will present approaches to obtain a classification of such polynomials.

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MS109

Multivariate Racah Polynomials and Their Associated Algebras

In this talk, I will discuss the higher-rank Racah algebra and associated orthogonal polynomials. I will give a brief introduction and then focus on the bivariate orthogonal polynomials that arise in the representations. The orthogonal polynomials arise as overlap coefficients between two commuting generators in the algebra. We will compare different choices of these bases to see the different families of OPs and some differences in degree structure and domains of support within the families.

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MS109

The Nucleus of a Q-polynomial Distance-regular Graph

Let Γ denote a Q-polynomial distance-regular graph with diameter $D \geq 1$. For a vertex x of Γ the corresponding subconstituent algebra $T = T(x)$ is generated by the adjacency matrix A of Γ and the dual adjacency matrix $A^* = A^*(x)$ of Γ with respect to x. We introduce a T-module $\mathcal{N} = \mathcal{N}(x)$ called the nucleus of Γ with respect to x. We describe $\mathcal{N}$ from various points of view. We show that all the irreducible T-submodules of $\mathcal{N}$ are thin. Under the assumption that Γ is a nonbipartite dual polar graph, we give an explicit basis for $\mathcal{N}$ and the action of A, A^* on this basis. The basis is in bijection with the set of elements for the projective geometry $L_D(q)$, where $GF(q)$ is the finite field used to define Γ.

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MS110

Advances in Truncated Gaussian Quadrature Rules for Exponential Weights

The idea of truncated Gaussian formulas emerged from numerical observations for integrals with classical Laguerre weights [G. Mastroianni and G. Monegato, Truncated quadrature rules over $(0, \infty)$ and Nyström-type methods, SIAM J. Numer. Anal. 41 (2003), no. 5, 1870-1892]. Over the past two decades, their theoretical foundations have been systematically investigated, and these rules have been extended to a broader class of exponential weights, including non-classical ones, defined on both bounded and unbounded intervals of the real line, building on the results of [E. Levin and D.S. Lubinsky, Orthogonal polynomials for exponential weights, CMS Books Math. 4, Springer-Verlag, New York, 2001]. Further numerical challenges arise in computing the nodes and weights of these quadrature formulas when the coefficients of the three-term recurrence relation for the associated orthonormal polynomials are not explicitly known. In this talk, we present new advances in truncated Gaussian quadrature rules, with a focus on their convergence properties, error estimates, and computational advantages. We will also explore their applications in numerical methods for integral equations, emphasizing recent results from [P. Junghanns, G. Mastroianni and I. Notarangelo, Weighted Polynomial Approximation and Numerical Methods for Integral Equations, Pathways in Mathematics, Birkhäuser, Cham, 2021].

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MS110

Bivariate Bernstein-Jacobi Approximants for Negative Parameters

We study bivariate Bernstein-Jacobi operators based in the weighted classical Jacobi inner product on the simplex. Apart from standard results, we deduce derivation properties, and prove that classical simplex orthogonal polynomials are the eigenfunctions of these operators. We also study the limit cases when one of the parameters is a negative integer. Finally, we analyse several numerical examples.

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MS110

On Classical Generalized Bivariate Symmetric Polynomials

We study families of bivariate orthogonal polynomials with respect to the symmetric weight function

$$B_\gamma(x, y) = w(x)w(y)|x - y|^{2\gamma+1}, \quad x, y \in (a, b),$$

for $\gamma > -1$, where $w(t)$ is a classical weight function in $t \in (a, b)$. The case $\gamma = \pm 1/2$ is easily reduced to products

of classical orthogonal polynomials. The Jacobi case corresponds to the Jacobi polynomials for root system BC_2 introduced by Koornwinder in 1974, a very special case of the Jacobi polynomials associated with root systems of Heckman and Opdam. In this work, lowering and raising second order partial differential operators are introduced in the general case, and after the change of variables $u = x + y, v = xy$, we obtain the representation in terms of the variables u, v for the algebra of partial differential operators having as eigenfunctions the respective Hermite, Laguerre and Jacobi generalized bivariate orthogonal polynomials.

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MS111

Faceting, Folding, and Surface Diffusion Within Incompressible Deformable Membranes

We present a comprehensive framework for the development of gradient flows of parameterization independent surface energies. While these energies are naturally expressed in terms of intrinsic quantities (curvature and metric) we show that the analysis of quasi-steady patterns is greatly simplified when conducted in the framework of the extrinsic vector field (normal and tangential velocities). We make application to faceting type evolution of brine inclusions in sea ice, to adhesion-repulsion energies that guide folding flows of cellular organelles, and to locally incompressible flows of fluidic membranes. Joint work with : Vinh Nguyen, Brian Wetton, Qiliang Wu.

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MS111

Splintering and Coarsening in a Growth and Inhibition System

A geometric variational problem is utilized to study pattern formation as an outcome of growth and inhibition in physical and biological systems. A perimeter term in the problem gives a growth force while a negative power of the Laplace operator provides an inhibition force. Two phenomena, splintering and coarsening, which are sources of morphological instability, are investigated. Splintering, which means large pieces of structures break into small pieces, is favored by the inhibition force and opposed by the growth force. On the other hand coarsening, which means large pieces increase in size and small pieces shrink and vanish, is favored by the growth force and opposed by the inhibition force. Several thresholds in terms of the parameters of the problem for these phenomena are found.

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MS111

Effect of Domain Geometry on the Stability and Dynamics of Spot Patterns

For localized spot patterns in reaction diffusion systems, we discuss how their stability and dynamics are impacted by the shape of the bounding domain as well as the domain curvature. For the former, we focus on how the bounding domain selects the dominant mode of oscillations in a certain translational instability. For the latter, we discuss how spotted vegetation patterns evolve under the influence of terrain topography, isolating effects of water transport and accumulation, as well as those of the terrain curvature itself.

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MS112

A Method of Field Expansions for Quasiperiodic Gratings

In many applications of scientific and engineering interest, the accurate modeling of linear waves scattered by quasiperiodic media plays a crucial role. The ability to numerically simulate such configurations robustly and rapidly is of overwhelming importance in photonics applications. In this contribution we focus upon the specific problem of electromagnetic radiation interacting with a two-dimensional diffraction grating with quasiperiodic layers. We describe, for the first time, how the classical boundary perturbation method of Field Expansions can be extended to this two-dimensional problem with a quasiperiodic interface. With specific numerical experiments we will show the remarkable efficiency, fidelity, and high-order accuracy one can achieve with an implementation of this algorithm.

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MS112

BIE Approaches for Eigenvalues and Resonances

Boundary integral approaches provide several advantages - includign dimension reduction and high-accuracy - while computing the spectra of elliptic operators. They are particularly effective in challenging situations involving exterior domains or open arcs. In this talk we survey some recent progress in the use of boundary integral techniques to compute the spectra of interior and exterior Dirichlet-to-Neumann maps, as well as photonic eigenvalues.

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MS112

Dispersion in Floquet Materials

Floquet media, materials subject to time-periodic forcing, naturally give risevia homogenizationto Dirac Hamiltonians that differ from those traditionally studied in quantum mechanics. A key question is whether wavepackets disperse in such media. This, in turns, lead to the study of dispersive dynamics of nonautonomous Hamiltonians, a largely open problem.

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MS112

Mathematical Analysis and Computational Modeling in Photonics

Understanding the phenomena of light propagation in photonics is crucial to design of optical devices. This minisymposium will address topics arising in photonics. Some of the topics speakers will address include:

- Propagation of plasmons on graphene
- Topological photonics - insulators and edge states
- Floquet media
- Design of photonic devices
- Twisted multi-layer and Moir materials
- Scattering by optical gratings
- Numerical methods for wave propagation and scattering in complex media

The two-part mini-symposium will start with an overview of the diverse topics and discuss the over-arching theme PDE, analysis, and numerical methods that hold these topics together.

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MS114

How Can We Efficiently Generate Virtual Patient Cohorts?

Virtual patient cohorts (VPCs) are computer-generated representations of patients that mirror real-world populations. VPCs use mathematical models to establish the effects of inter-patient variability on disease and treatment outcomes, thereby allowing for the comprehensive exploration of disease mechanisms and therapeutic strategies at low-cost and without burden to patients. Further, they may aid the development and validation of mechanistic mathematical models that aim to capture the underlying mechanisms of biological systems. Efficient generation of such populations is critical. While several methods exist, computational efficiency remains a challenge. One common approach combines Approximate Bayesian Computation (ABC) with Markov Chain Monte Carlo (MCMC), which samples from parameter distributions that yield plausible model outcomes. However, this method suffers from a high rejection rate, as samples must meet ABC and MCMC acceptance criteria. To address this, we developed a more efficient technique: Trajectory Matching ABC-MCMC, which relaxes acceptance to only require that model trajectories fall within observed data bounds. In this talk, I will present results from applying TM-ABC-MCMC to three mechanistic models of varying complexity. Compared to standard ABC-MCMC, our method substantially reduces the rejection rate while preserving accuracy, offering a faster and more scalable path to generating realistic virtual patient cohorts.

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MS114

Reflections of Traveling Waves in Models of Cardiac Dynamics

When propagated action potentials in cardiac tissue interact with a local heterogeneity, reflected waves can sometimes be induced. These reflected waves have been associated with the onset of cardiac arrhythmia, and while their generation is not well understood, their existence is linked to that of one-dimensional (1D) spiral waves. Thus, understanding the existence and stability of 1D spirals plays a crucial role in determining the likelihood of unwanted reflected pulses. In this talk, we will review computational results that studied the existence and stability of 1D spiral waves in a qualitative ionic model and present ongoing extensions to learn about physiological conditions that promote reflections in a detailed conductance-based model.

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MS114

Where GLP-1 Meets PCOS: Insights from Modeling

GLP-1 receptor agonists (GLP-1 RAs) have gained widespread attention for their effectiveness in treating metabolic abnormalities such as type 2 diabetes and obesity. Central to their success is the regulation of glucose-insulin metabolism and improvement of insulin resistance. In reproductive endocrinology, GLP-1 RAs have also shown promise as off-label treatment of polycystic ovary syndrome (PCOS), which results from reproductive hormone dysregulation and is often accompanied by insulin resistance. The use of insulin-sensitizing drugs has been a common approach to treating some forms of PCOS, even though its precise pathogenesis remains unclear. Here we describe a mathematical framework to examine the specific effects of GLP-1 RAs on ovulatory function/defects, and we discuss the underlying mechanisms that may determine treatment efficacy.

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MS114

Modeling Mechanisms of Microtubule Dynamics and Polarity in Neurons

Microtubules (MTs) are dynamic protein filaments essential for intracellular organization and transport, particularly in long-lived cells such as neurons. The plus and minus ends of neuronal MTs switch between growth and shrinking phases, adding and removing tubulin protein, and the nucleation of new filaments is believed to be regulated in both healthy and injury conditions. In fruit fly neurons, the healthy MT cytoskeleton is stable with a particular orientation throughout the lifetime of the cell. However, when injured, these MTs are dynamic, rearrange their orientation, and nucleation of MTs is upregulated. Using experimental data and a stochastic mathematical model, we seek to understand how nucleation can impact MT dynamics in dendrites of fruit fly neurons. In the stochastic model, we assume two mechanisms that limit MT growth: limited tubulin availability and the dependence of shrinking events on MT length. To investigate our model analytically, we utilize a simplified partial differential equation model to understand steady-state MT length distributions under different nucleation and length-regulating mechanisms. In both modeling frameworks, the models predict parameter regimes where the system is scarce in tubulin and suggest that low filament nucleation regimes are characterized by high variation in MT lengths, while high nucleation regimes drive high variation in MT numbers. Insights from these models can then be used to understand what mechanisms are used to organize MTs into polarized structures in neurons, and how MT dynamics, like nucleation, may impact MT structure post-injury.

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MS115

Computation of Generalized Mathieu Functions

The Mathieu functions are defined to be the solutions of the Mathieu equation that have period 2π, and only those functions. But the Mathieu equation has isolated double eigenvalues when the parameter q has certain complex values, as first noticed in 1929 by Mulholland and Goldstein. In the 60s, the first systematic computation of these double eigenvalues was carried out by Gertrude Blanch (the author of the chapter in Abramowitz and Stegun on Mathieu functions) and D. Clemm. Later, work by Hunter and Guerrieri in 1981 confirmed and extended those computations. At a double eigenvalue, Mathieu functions coalesce, and so for completeness of the basis a new function must be introduced for that value of the complex parameter q. This talk discusses computation of such functions and whether or not the effort to do so is justified in practice.

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MS115

Improving the Quality of Numerical Software for Distribution Functions

Special functions are fundamental in probability theory, especially in defining and analyzing probability distributions. This is why the use of numerical methods commonly employed to compute special functions allows for the development of stable and accurate numerical algorithms for calculating important distribution functions. In this talk, we will discuss recent advances in the development of numerical software for Beta distribution functions. We will see how this software represents a significant improvement over existing implementations in R and MATLAB. This is joint work with Javier Segura and Nico M. Temme.

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MS115

Fast Measure Modification of Orthogonal Polynomials Via Matrices with Displacement Structure

It is well known that matrices with low Hessenberg-structured displacement rank enjoy fast algorithms for certain matrix factorizations. We show how $n \times n$ principal finite sections of the Gram matrix for the orthogonal polynomial measure modification problem has such a displacement structure, unlocking a collection of fast algorithms for computing connection coefficients (as the upper-triangular Cholesky factor) between a known orthogonal polynomial family and the modified family. In general, the $\mathcal{O}(n^3)$ complexity is reduced to $\mathcal{O}(n^2)$, and if the symmetric Gram matrix has upper and lower bandwidth b, then the $\mathcal{O}(b^2n)$ complexity for a banded Cholesky factorization is reduced to $\mathcal{O}(bn)$. In the case of modified Chebyshev polynomials, we show that the Gram matrix is a symmetric Toeplitz-plus-Hankel matrix, and if the modified Chebyshev moments decay algebraically, then a hierarchical off-diagonal low-rank structure is observed in the Gram matrix, enabling a further reduction in the complexity of an approximate Cholesky factorization powered by randomized numerical linear algebra.

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MS115

Special Functions and the Numerical Solution of Initial-Boundary Value Problems

Classical special functions emerge naturally in the study of constant-coefficient PDEs on the line, particularly in short-time asymptotic expansions near discontinuities. For initial-boundary value problems (IBVPs), special functions, and their generalizations, play an even more important role. In this talk, we explore how these generalized special functions arise through the Unified Transform Method. We highlight the challenges associated with small-time behavior computations and demonstrate how these generalized special functions can be computed using the method of steepest descent. Finally, we incorporate

these special functions to develop time-stepping routines for more general IBVPs, incorporating lower-order non-constant coefficient terms and nonlinearities as forcings.

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MS116

Recent and Future Activities of the Nist Digital Library of Mathematical Functions Project

The NIST Digital Library of Mathematical Functions https://dlmf.nist.gov/ is a website maintained by the Applied and Computational Mathematics Division at the National Institute of Standards and Technology, a Department of Commerce National Laboratory located in Gaithersburg, Maryland. This website is the 21st century successor of the National Bureau of Standards "Handbook of Mathematical Functions," commonly known as Abramowitz and Stegun, which was published in 1964. The DLMF has considerably extended the scope of the original handbook as well as improving accessibility to the worldwide community of scientists and mathematicians. The DLMF contains 36 chapters, each on a specific class of special functions, with each chapter authored by a world renown expert. The website covers everything in the handbook and much more: additional formulas and graphics, math-aware search, interactive zooming and rotation of 3D graphs, internal links to symbol definitions and cross-references, and external links to online references and sources of software. The DLMF contains more than twice as many formulas as the old one, includes coverage of more functions, in more detail, and an up-to-date list of references. DLMF updates and errata are published quarterly. In this talk we will discuss the current activities of the NIST DLMF and as well ongoing and planned additions and improvements.

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MS116

Accessing Mathematics Using MathSciNet

The manner in which mathematics is done and used is in a state of flux, with rapid changes apparent in every direction. The major mission of Mathematical Reviews is to maintain a reliable, searchable record of the mathematical literature. What began as a journal transformed into a database, MathSciNet, which provides increased potential for using the information for more than just literature searches. I will explain some of these alternative uses, as well as some ways that we are working to make the database more accessible to diverse users and usages.

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MS116

arXiv.org As HTML Papers – the Next 20.25%

arXiv's growing collection of scientific articles is being gradually enriched from LaTeX sources into web-friendly HTML. This has been an international effort now spanning nearly two decades. The LaTeX to HTML conversion has been instrumented via NIST's LaTeXML tool. Nearly 80% of the ∼2.5 million articles now have an HTML version. Crucially, more than a billion formulas written in LaTeX have been mapped to an accessible MathML representation. This talk will provide an overview of the remaining challenges to full HTML coverage. It will also cover the recent advancements towards the fourth version of the MathML standard, and walk through a few notable examples of close relevance to the SIAM community.

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MS116

Mathematical Research Data in zbMATH Open, Wikipedia, and Beyond

Mathematical research data spans a diverse range of structured information, including bibliographic records, formalized mathematical statements, computational results, encyclopedic articles, and interactive notebooks. As open-access platforms such as zbMATH Open, Wikipedia, and other repositories continue to grow and interconnect, they unlock new possibilities for knowledge discovery, verification, and collaboration. This talk explores how these platforms structure and integrate mathematical research data, enhancing accessibility and reusability. We will address key challenges such as data curation, standardization, and interoperability, along with the emerging role of artificial intelligence in mathematical knowledge management. Drawing from our experience with Germany's Mathematical Research Data Initiative (MaRDI), we will highlight the role of knowledge graphs in organizing and linking mathematical information, offering insights into their potential for the broader research community

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MS117

Time-Lag Monotonicity-Breaking in Time-Delay Systems with Impulses

In this talk, we prove that the well-posedness of the Cauchy problem for a differential equation with state-dependent delay (DE-SDD) and impulses crucially relies on the monotonicity of the time lag. We demonstrate pathologies that occur in the monotonicity-breaking case, which can lead to dynamical behaviour completely different from what is possible in DE-SDD or impulsive differential equations with constant delays.

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MS117

Hybrid Control Architecture: A Pathway to Reliable Artificial Intelligence

Integration of artificial intelligence (AI) into complex real-world applications although demonstrating significant promise across diverse industries, continually seeks robust framework to ensure reliability and safety, particularly in sensitive and safety-critical applications. This talk will explore hybrid control methodologies, designed to bridge the gap between deterministic control mechanisms and AI-driven adaptive strategies, to ensure dependable performance in complex dynamical systems. We introduce a cohesive framework integrating model-based and data-driven methodologies to form a robust, scalable system capable of handling intricate dynamics and uncertainties. The architecture employs a dual-layer control strategy: One layer manages real-time deterministic control objectives, including stability and rapid responsiveness, while the second layer leverages machine learning to enhance performance and adaptability. We also demonstrate how our architecture improves reliability of AI procedures in autonomous vehicles, and robotics, through theoretical analysis and practical implementation. Through focusing on specific case studies, this talk highlights the advantages of our approach including fault isolation, and improved adaptability and operational safety. By examining the intersection of certified learning and hybrid control architectures with complex dynamical systems, this talk illuminates innovative pathways toward reliable artificial intelligence.

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MS117

Leader-Follower Flocking Control of Multi-Agent Systems Via Hybrid Protocols

The leader-follower flocking control problem of multi-agent systems via hybrid impulsive and pinning control is studied. In particular, the hybrid impulsive and pinning mechanisms efficiently reduce control resource consumption and transmission redundancy. Furthermore, parametric uncertainties, actuator failures, and deception attacks are compensated for to enhance overall network stability. Additionally, gyroscopic and braking forces are employed for obstacle avoidance. Based on the transmission topology structure and impulsive control theory, sufficient criteria are derived to allocate admissible error bounds for maintaining flocking stability. Numerical simulations are conducted to confirm the validity of the theoretical analysis.

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MS117

Event-Triggered Impulses for Pinning Stabilization in Complex Networks

Complex networks (CNs) consist of vast nodes typically modelled as dynamical systems, with specific topological structures governing their connections. Impulsive control, a distinctive feedback control, employs abrupt state changes or jumps at discrete time intervals to achieve stabilization. This impulsive control paradigm has demonstrated robustness and efficiency in facilitating network stabilization. In this talk, we will address the stabilization problem for a class of CNs using a pinning impulsive control approach, where only a subset of the network nodes is controlled. We propose a novel event-triggering algorithm to identify the timing for impulses, and we outline sufficient conditions related to the network topology, impulsive control gains, and parameters in the event-triggering conditions that ensure network stabilization.

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MS119

Numerical considerations for the elastodynamics of skeletal muscle tissue

Realistic simulations of biological tissue deformation require moving beyond traditional one-dimensional models and adopting fully three-dimensional, nonlinear finite element approaches. Skeletal muscle tissue, in particular, is a fibre-reinforced composite whose active, velocity-dependent components significantly influence the behaviour of numerical solvers. In this talk, we will examine the numerical aspects of a fully dynamic finite element formulation of the problem, focusing on the spatio-temporal discretization and the challenges posed by the material's nonconvex properties.

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MS119

Finite Time Blow-Up of the Axisymmetric Euler Equations: A (High-Order) Numerical Investigation

The importance of the formation of singularities in the three-dimensional Euler and Navier-Stokes equations beginning with a smooth divergence-free velocity field cannot be overstated since it would indicate that the governing equations are not well-posed. The issue is of great interest to engineering communities because of the possible connection with the onset of turbulence. In 2014, Luo and Hou presented numerical evidence to show that a certain swirling rotationally symmetric flow of an incompressible inviscid fluid in an axially periodic cylinder of finite radius leads to finite time blow-up in the vorticity ω. The numerical schemes employed by Luo and Hou (2014), Barkley (2020) and Kolluru et al. (2022) for the simulation of this flow used a vorticity-stream function formulation and pseudospectral or B-spline based Galerkin methods in combination with a Runge-Kutta method. In this talk, we use a Fourier-Chebyshev spectral collocation method and compare both explicit and implicit adaptive Runge-Kutta

methods in an investigation of finite time blow-up of the vorticity in the swirling flow proposed by Luo and Hou.

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MS119

Numerical Computation of Two-Electron Four-Center Coulomb Repulsion Integrals

In this talk, we will present a novel approach for computing electron repulsion integrals, which are fundamental for ab initio quantum chemistry calculations and essential for accurately predicting molecular properties. We describe our method for calculating two-electron, four-center Coulomb repulsion integrals for 1s orbitals using Slater-type orbitals (STOs), leveraging GPU acceleration to enhance computational efficiency. A key element of our approach is the exploitation of the structure and properties of the product of two STOs. By applying a transformation derived from classical electromagnetism, we regulate the singularity in the integrals and employ numerical quadrature techniques to achieve high precision. Our method achieves an accuracy of six to seven decimal digits, limited only by machine round-off errors inherent to single-precision arithmetic. We will demonstrate the efficiency and effectiveness of our approach through several computational examples.

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MS119

High-Order Financial Option Pricing on Sparse Grids

The sparse grid combination method [Griebel et al, 1992] is a popular technique for reducing the impact of the curse of dimensionality (the exponential increase in the number of unknowns as dimensions increase). High-order methods are another technique for reducing the computational cost to obtain a similar level of error, with benefits that are especially pronounced in multi-dimensional settings. However, for parabolic PDEs with nonsmooth initial conditions that arise in financial option pricing, the direct application of these methods results in damaging effects on the order of convergence. Researchers [Hendricks, 2017; Wang, 2024] have used smoothing methods [Kreiss et al, 1970] on the initial condition to restore the order of convergence for both the sparse grid combination method and high-order methods. We present a high-order method based on cubic spline collocation [Houstis et al, 1988] to solve multi-dimensional parabolic PDEs, with emphasis on computational efficiency using the compact stencil that arises in the two-step formulation. To account for the nonsmooth initial conditions, we develop a high-order smoothing method that projects the initial condition onto the space of basis functions [Rannacher, 1984]. In addition, we compare the performance of projection with the smoothings in [Kreiss et al, 1970] and describe algorithms for the previously unexamined problem of computing smoothings efficiently in multiple dimensions.

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MS120

Space-time Adaptive Algorithms and a Posteriori Estimators Including Mesh Modification

We present a space-time adaptive algorithm for parabolic PDEs, using finite elements. The error estimators derived in [2] are modified taking into account successive adapted, non nested, and possibly anisotropic meshes. The evaluation of the error estimators requires to compute the intersection between non matching meshes, which is handled as in [1]. Numerical experiments for the convection-diffusion with the Euler scheme are presented. Extension to the Crank-Nicolson scheme is also mentioned.

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MS120

A Simpler Approach for the Evss Formulation for Viscoelastic Fluid

The numerical simulation of manufacturing polymeric object (molding, extrusion, etc.), involve describing the mechanical behaviour of a viscoelastic fluid: a fluid driven by a Navier-Stokes system combined (coupled) with a constitutive law describing the behaviour of the stress tensor of the polymer (usually based on an upper convected derivative). The basic model is well known for its numerical challenge stemming from the nature of the PDE. The DEVSS model avoids these difficulties, increase stability and leads to simpler finite element schemes. A feature of the DEVSS is the introduction of secondary unknown (a symmetric tensor of order 2, leading to 6 more scalar unknown), and a relaxation coefficient. The value of the relaxation parameter and interpolation space for the added unknown must be adress. In this presentation, we will introduce a simpler model based on the EVSS model. Relying on a added grad-div term, this formulation is consistent and does not need a supplementary variable. One of the important challenges when doing numerical simulation of such phenomenon is the ability to cope with certain values of parameters characterizing the polymer. The Wissenberg number (Wi) allows to characterize those critical values. We will illustrate the efficiency and the ability of our formulation to cope with critical values of Wi, making this formulation a viable alternative to the DEVSS in certain situation.

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MS120

A Moore-Penrose Continuation Algorithm for Large Deformation Contact Problems

Problems involving the large deformation of hyperelastic materials in contact are of interest in both industry

and research. Due to the significant non-linearities they present, numerical tools such as finite element discretization, a quasi-static framework, and Newton-like solvers are commonly used to solve these problems. However, convergence difficulties can arise from bifurcations and severe non-linearities. Predictor-corrector or arc-length methods, which introduce a path-following constraint and treat the load increment as an additional unknown within the finite element space, can improve convergence. While these methods add computational complexity, we demonstrate that incorporating a continuation algorithm accelerates the overall iterative process. We present a Moore-Penrose continuation algorithm, its implementation in an existing finite element code, and its effectiveness in solving large deformation contact problems, including industrial examples, in 2D and 3D. This algorithm is compatible with common contact-solving methods. Through further examples, we show that achieving large deformations of hyperelastic materials, often associated with severe mesh distortion, is possible using the proposed continuation algorithm, an updated Lagrangian formulation, and an adaptive remeshing strategy. These applications are of interest to our research partner, Michelin. All simulations are performed using our research group's software, MEF++.

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MS120

The Cutfem Method for Two-Phase Flows of Viscoelastic Fluids

Non-Newtonian fluids are fluids whose viscosity varies depending on the applied stress. Their unique properties make them particularly valuable for numerous industrial applications, especially in the field of polymers and, more specifically, in the tire manufacturing industry. However, their behavior during shaping processes can be complex and difficult to predict. Numerical simulations offer a powerful tool to anticipate this behavior, significantly reducing the costs associated with developing new products. This presentation will focus on the application of the Cut Finite Element Method (CutFEM) to two-phase flows of viscoplastic fluids, a specific type of non-Newtonian fluid. The CutFEM method was first introduced in [P. Hansbo and A. Hansbo, An unfitted finite element method, based on Nitsches method, for elliptic interface problems. 2002]. A significant advancement occurred in 2010 with the introduction of the Ghost Penalty stabilization technique [E. Burman, Ghost penalty. 2010]. Since then, CutFEM has been applied to solve numerous complex problems and has proven to be particularly robust for solving problems involving complex and evolving geometries. First, we will present the fundamental principles of the CutFEM method. Using a model problem, we will detail its key concepts, including geometry discretization, weak formulation, and time integration. Finally, we will showcase a series of examples that demonstrate the methods effectiveness.

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MS121

Adaptive Tolerances and Media Effects in Schelling's Model of Segregation

Thomas Schelling introduced his agent-based model of segregation in 1971 and concluded that even when there is a low amount of intolerance within society that segregation will develop if people follow their individual preferences. A large body of literature building of this framework has been built and has bolstered this claim. This paper aims to take the same framework but instead look for ways to get to an integrated state. We focus on Allport's contact hypothesis that states that if there is equal status among groups, common goals among groups, and an institutional mechanism supporting intergroup contact then intergroup contact can reduce prejudice. We incorporate the contact hypothesis by having individuals adjust their intolerance based on their current neighborhood composition and the ease of conforming to their surroundings. Furthermore, we add in positive and negative media effects, as individuals are likely to get information about an outgroup from the media (e.g., news, TV, movies, etc.) that they consume. We find that having a society composed of individuals who do not easily conform to their surroundings and displaying positive examples of both groups in media promote integration within society.

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MS121

A Network Diffusion Model of Urban Development and Inequality

Wealth inequality between the richest and poorest U.S. Americans has continued to increase over the last several decades. In designing intervention strategies to address this growing social problem, it is useful to recognize that there is a distinct geographic structure to the distribution of wealth. Within a city, neighborhoods tend to cluster into wealthier "nice" parts of town and poorer "bad" parts of town, often limiting the upward mobility of residents in "bad neighborhoods." To better understand and address this phenomenon, we build a dynamical model to study the geospatial patterns of urban development and inequality. Specifically, we model the flow of wealth in an urban area as a diffusive process on a network. Using this model, we characterize the effects of investment and other development strategies on the distribution of wealth and economic opportunities within a city. Furthermore, we link these effects to changes in population and racial distributions to study the process of gentrification. We test our model using data from the National Historic GIS. Ultimately, our model shows that combatting wealth inequality must involve a fundamental shift in how and where money is invested.

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MS121

The Role of Social Learning in Climate Change Inaction: Modeling Opinion Polarization and Issue Prioritization

Despite scientific consensus on anthropogenic climate change and its risks, public opinion in the United States remains polarized, leading to inconsistent climate policies and limited collective action. This paper presents a dynamic model to explain how social learning, conformity, and affective polarization shape climate change opinions by hindering cross-party learning and influencing the prioritization of climate issues relative to economic concerns. The model shows that high levels of social learning amplify initial differences in concern between the left and right, resulting in persistent polarization. It also reveals that, even when a majority of the population expresses concern about climate change, this does not always lead to prioritizing climate mitigation, largely due to the complexity of climate risks compared to the more explicit risks of economic issues. However, increasing cross-party social connectionsand thus cross-party learningcan mitigate polarization and nudge public support toward more desirable levels. By identifying key psychological and social mechanisms in climate opinion formation and prioritization, this research offers insights into addressing public inaction and informs strategies for more effective climate communication and policymaking.

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MS121

Beyond Trust in Science: Modeling the Effect of Institutional Structure for Global Environmental Governance

Trust in science remains relatively high around the world, but it has not been sufficient to spur the collective action needed to address critical issues like climate change. In order to solve global environmental challenges, scientific and technological solutions alone will not suffice: the solutions require a diplomatic and policy response across scales. International scientific institutions play a role in fostering scientific cooperation and providing policy-relevant analysis to decision makers. In this context, the question becomes: how does the structure of scientific institutions impact their influence on policy? This talk will describe a dynamical model to quantitatively assess the tradeoffs in structures of scientific institutions along three dimensions which have been shown to influence policy: salience, legitimacy, and credibility. We apply the model to the case of global environmental assessments, defined as a formal effort to assemble knowledge to support decision making, focusing on the Intergovernmental Panel on Climate Change (IPCC). Our study underscores how path dependence and tradeoffs in institutional structure can affect the influence of science on policy over time.

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MS122

K-Sample Inference Via Multimarginal Optimal Transport

This work proposes a Multimarginal Optimal Transport (MOT) approach for simultaneously comparing $k \geq 2$ measures supported on finite subsets of $\mathbb{R}^d$, $d \geq 1$. We derive asymptotic distributions of the optimal value of the empirical MOT program under the null hypothesis that all k measures are same, and the alternative hypothesis that at least two measures are different. We use these results to construct the test of the null hypothesis and provide consistency and power guarantees of this k-sample test. We consistently estimate asymptotic distributions using bootstrap, and propose a low complexity linear program to approximate the test cut-off. We demonstrate the advantages of our approach on synthetic and real datasets, including the real data on cancers in the United States in 2004 - 2020.

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MS122

Sharp Deconvolution of Optimal Transport Matchings with Applications to Photonic Imaging

We consider the statistical problem of recovering the optimal transport matching between two atomic measures from noisy convolutions of these measures with a smooth kernel. This question is motivated by super-resolution microscopy applications, where optimal transport matchings have recently been proposed as a figure of merit for quantifying the spatial proximity between discrete signals under observation (Tameling et al., *Nature Computational Science* 1.3 (2021) 199-211). Our main result quantifies the minimax risk of estimating optimal transport matchings in this setting, under appropriate regularity assumptions. As a byproduct, we also derive the minimax rate of recovering a discrete signal under our deconvolution model, with respect to the Wasserstein distance. These minimax rates are achieved by simple estimators based on the method of moments and maximum likelihood estimation.

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MS122

Application of the GenCol Algorithm to Adversarial Multi-Class Classification

Adversarial training procedures can alleviate the problem of overfitting in multi-class classification. Exploring this approach from a distributional perspective leads to a ro-

bust optimization problem using a Wasserstein distance. Recent theoretical results showed a similarity to the multi-marginal formulation of Wasserstein-barycenter in optimal transport. Unfortunately, both problems suffer from the curse of dimension, making it hard to exploit the linear program structure of the problems for numerical calculations; the number of unknowns scales polynomially with the number of data points and even exponentially with the number of classes. We investigate how ideas from *Genetic Column Generation* for multi-marginal optimal transport can be used to overcome the curse of dimension in computing the minimal adversarial risk in multi-class classification. Hereby, column generation –a standard method to solve large linear programs– is combined with a genetic proposal rule. This yields an efficient routine by maintaining a reduced set of configurations.

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MS122

New Developments in Optimal Transport for Inverse Problems

Optimal transport has long played a significant role in the solution of inverse problems in imaging and computer vision. The Wasserstein distance has been widely used as a metric for image and shape registration and interpolation, and optimal mass transport models have proven effective for capturing mass-preserving dynamics in spatio-temporal imaging. More recently, optimal transport has gained prominence in machine learning approaches to inverse problems, particularly as a loss function or similarity measure in learned feature spaces. In this talk, I will provide a brief overview of these developments and place particular emphasis on the use of optimal transport in machine learning for inverse problems. I will highlight emerging trends, recent advances, and key open challenges in this rapidly evolving area.

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MS123

DeepHyper: Distributed Neural Architecture and Hyperparameter Optimization for Machine Learning

In the past decade, machine learning has experienced exponential growth, propelled by abundant datasets, algorithmic advancements, and increased computational power. Simultaneously, high-performance computing (HPC) has evolved to meet rising computational demands, offering resources to tackle complex scientific challenges. Nevertheless, the development of machine learning workflows is often a sequential trial-error process based on heuristics, making it hard to track, and time-consuming. Machine learning workflows are built from modules offering numerous configurable parameters, also known as hyperparameters, from data transformation policies to training procedures and model architectures. This presentation focuses on DeepHyper, an open-source software that solves the hyperparameter optimization challenge efficiently. Its core methodology is based on the asynchronous parallelisation of Bayesian optimization. It combines it with early discarding strategies to stop iterative loops of machine learning workflows that are tested as soon as possible and save time. Finally, it builds on top of hyperparameter optimization to create ensembles of models for improved accuracy or uncertainty quantification.

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MS123

AuroraGPT

I will present AuroraGPT, a foundation model for science, trained on the Aurora supercomputer at the Argonne Leadership Computing Facility (ALCF). This model is designed to process and generate human-like scientific text, with the goal of supporting scientific discovery. Trained on a large corpus of scientific literature, this model has the potential to assist researchers in exploring, summarizing, and generating new hypotheses, making it a useful tool for various scientific domains.

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MS123

Scalable Deep Learning: Challenges and Strategies

In this talk, we will explore the growing computational demands of large-scale models, the difficulties in optimizing training efficiency, and the bottlenecks in distributed learning environments. Additionally, we will highlight key strategies that address these challenges, including scalable optimization techniques, automated hyperparameter tuning, and model distillation for deployment efficiency. By introducing these foundational topics, this talk will provide context for the minisymposium presentations.

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MS123

Scaling Beyond Diagonal Preconditioners for Training Neural Networks At-Scale

Over the past decade, diagonal scaling-based adaptive subgradient methods like AdaGrad and Adam(W) have been widely adopted for neural network training due to their simplicity, linear memory requirements, and robustness to hyperparameter tuning. However, full-matrix preconditioned adaptive subgradient methods, which offer superior performance, are often hindered by their quadratic memory and cubic computational complexity. Recent advances in approximate Kronecker factorization-based methods, including K-FAC and Shampoo, offer a promising alternative, achieving faster convergence than diagonal approximation-based methods while remaining computationally tractable. This talk provides an overview of the Shampoo algorithm and presents our distributed PyTorch implementation, highlighting key heuristics, performance optimizations, and systems/scalability developments that enable efficient training of million- and billion-parameter models. We will also share key insights and learnings from our AlgoPerf PyTorch Shampoo submission, including generalizable configurations and future research directions.

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MS124

Incorporating the Health Belief Model into Infectious Disease Dynamics: Addressing Disparate Impacts on Vulnerable Populations

This work presents an extended SIR model that integrates behavioral insights from the Health Belief Model (HBM) to examine the unequal impacts of epidemics on disadvantaged populations. By incorporating a propensity-to-adopt-behavior (PAB) metric and a socio-economic structure variable, the model captures how risk perception and responsiveness to public health messaging affect disease burden. Simulations highlight the influence of messaging strategiespositive, negative, and combined cueson behavioral change and epidemic outcomes. This work emphasizes the critical role of human behavior and socio-economic factors in shaping disease dynamics and informing equitable public health policy.

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MS125

A Computational Analysis of Behavioural Phenotype: Modeling the Interaction Between the Butterfly Pieris Brasicae and Trichogramma Wasps

The diverse expression of behavioural phenotypes in a population has the potential to influence the whole population. Rather than using discrete levels of expression, we propose a model that treats the behavioural phenotype as a continuous distribution. This is more appropriate for dealing with phenotypes associated with continuous quantities, such as the amount of a pheromone secreted by a butterfly. We model the interaction of the butterfly Pieris brasicae and one of its predators, the Trichogramma wasp, using a reaction-diffusion equation coupled with an integro-differential equation with the distribution of behavioural phenotypes of the butterflies modeled as a diffusion process. The phenotypes are associated with the male butterflies propensity to secrete a pheromone as part of the species mating practices. We use computational methods to compute the steady states of our system and to determine their stability properties. This information facilitates a qualitative analysis of our model while avoiding the difficulties of using larger systems of equations. Our results also yield ecological inferences beyond what can be gained from merely solving the system in time.

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MS125

Modeling the Spread of Crimean Congo Hemorrhagic Fever Accounting for Tick Co-Feeding

Crimean Congo Hemorrhagic Fever (CCHF) is a tick-borne illness that affects animals and humans in countries across Africa, Asia, and now Europe. Ticks transmit this disease to susceptible hosts by feeding on them and can acquire the disease by feeding on an infected host. Ticks feed on different hosts at different stages in their life cycle: larvae and nymphs feed on small mammals, while adults feed on large mammals. Another aspect of the spread of CCHF is tick co-feeding. Co-feeding occurs when ticks feed on the same susceptible host within close proximity. If one tick is infected and the other is susceptible, the susceptible tick can become infected during co-feeding while the host remains susceptible. Very few mathematical models exist in literature that explore the epidemiological effects of tick co-feeding. In this talk, I will present an ODE compartment model of the spread of CCHF that accounts for the life cycle of ticks and co-feeding dynamics. Preliminary results to fit the model to data and observations in Uganda and Namibia will be presented as well. This work is supported by the MASAMU program with funding from a National Science Foundation (NSF) grant based at Auburn University.

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MS125

Sensitivity of Spotted Lanternfly Establishment to Climate and Phenotype Variability

When successfully established in an initial location, invasive species often spread over large areas that cover diverse climatic conditions. Moreover, at many fixed locations, the climate in a few decades will be different from today's climate. Both aspects encourage phenotype changes, potentially leading to an interplay of mixed populations. We show how principled mathematical models can capture these aspects, with a specific application to the spotted lanternfly, an invasive species that has been spreading across the Eastern United States since its introduction a decade ago. The study of different calibrated models can reveal which mechanisms in the lanternfly's life cycle may be particularly relevant towards their spread and establishment under varying climatic conditions.

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MS125

Macro-Scale Implications of Micro-Scale Movement Models for the Spotted Lanternfly

The Spotted Lanternfly, an invasive species currently present in the Northeastern United States, causes significant environmental and economic damage. Understanding the spread of the species is important at multiple scales. For instance, stakeholders at local scales care about the annual re-invasion of crop fields. In contrast, state and national stakeholders are concerned with the invasion of new areas over years and hundreds of kilometers. For the plant-hopping Spotted Lanternfly, the local arrangement of hosts is a primary driver of movement. We present how macroscopic movement models for a population can be systematically derived from a principled model for the movement of individual agents in periodic domains. In particular, we demonstrate how certain host geometries can lead to the emergence of asymmetric spread patterns even if the agent behavior exhibits no directional bias.

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MS127

A Method for the Incompressible Euler Equations with an Arbitrary Resolution Property

Problems of interest in hydrodynamics, particularly in the inviscid case, can develop exponentially-fine-scale features over time. Accurately resolving these fine features, on a fixed computational grid, quickly becomes prohibitively expensive in terms of computation time and memory usage. The Characteristic Mapping (CM) method is a general framework for nonlinear advection equations that seeks to alleviate this problem. In a CM method, rather than directly evolving advected quantities, one evolves the inverse flow map. This map may be arbitrarily decomposed into submaps, which recover the flow as a whole via composition. This decomposition may be performed adaptively at runtime. As such, the method is able to resolve arbitrarily-fine scales, yet only requires coarse computational grids. We review the CM framework and its application to the solution of the 2D incompressible Euler equations. In particular, we illustrate the methods exponential resolution and ability to represent sub-grid scales, all the while using coarse computational grids. Time permitting, we will discuss conservation properties and the application to domains with curved boundaries.

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MS127

Block-Centered Compact, Domain Decomposition and Optimal Control in Contamination Flows

Time-dependent partial differential equations (PDEs) are widely used for contamination flows in many practical applications such as in groundwater modeling, petroleum reservoir simulation, soil science and environment modeling. Due to the computational complexity and the large scale and long term prediction, it is important to develop efficient numerical methods for solving time-dependent PDE problems in parallel computing. In this talk, we would like to present our developments of block-centered compact method and its domain decomposition algorithm for the time-dependent PDEs. Meanwhile, we will also present our study of time dependent PDE-constrained optimal control model for contamination flows in porous media. Numerical experiments demonstrate the performance of the developed methods. Numerical simulation in more realistic shaped aquifer validates the control models efficacy.

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MS128

Meta-Learner Methods for PDEs

In this talk, we will explore a meta-learning framework that leverages weighted combinations of lower-order methods to derive an optimized higher-order method. The weighting mechanism is dynamically learned through a deep neural network, enabling an adaptive and efficient solution. We will demonstrate the efficiency of this approach through illustrative examples.

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MS128

Enhancing Machine Learning Models for Nonlinear Optimization Problems in Biomedical Applications Using Novel Iterative Schemes

Equilibrium problems encompass a broad spectrum of critical issues, including cost optimization, variational inequality, fixed points, Nash equilibria, and complementarity problems. The Extreme Learning Machine (ELM), a rapidly learning single-hidden-layer feedforward neural network, has garnered significant attention due to its efficacy in diverse machine learning applications. However, its reliance on randomly initialized hidden layer weights and biases frequently results in instability, suboptimal performance, and susceptibility to noise. These limitations impede ELMs capacity to generalize effectively, particularly in high-dimensional and complex problem domains, such as biomedical applications and financial market forecasting. This presentation examines the relationship between equilibrium problems, cost optimization problems, and ELM. A novel, efficient iterative approach termed the Accelerated Self-Adaptive Iterative Method (ASAIM) will be introduced for addressing split pseudomonotone equilibrium problems with multiple output sets (SPEP-MOS). This technique incorporates an inertial mechanism and a self-adaptive step size, eliminating the necessity for an initial

Lipschitz constant estimate, which can hinder convergence in conventional algorithms. Furthermore, computational simulations demonstrating the utility of ASAIM in optimizing the output weight in ELM training are presented. The analysis also encompasses comparative findings with established methodologies.

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MS128

Convergence Guarantees for Gradient Descent in Neural Networks with Non-convex Loss Functions

Theoretical understanding of optimization dynamics remains challenging due to non-convex loss landscapes. We address this gap with locally quasi-convex regions (LQCRs), characteristic regions where gradient descent (GD) exhibits reliable convergence properties. We describe a rigorous characterization of LQCRs, showing they naturally emerge under standard initialization schemes, and develop some convergence guarantees as well as an initialization strategy. Through theoretical analysis and experiments on synthetic data we demonstrate that gradient methods can avoid bad local minima when initialized properly for neural network in practice.

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MS128

An Efficient Popov Type Inertial Extragradient Algorithm with Applications in Regression-Based Extreme Learning Machine

Variational inequalities (VI) serve as a framework for expressing numerous scientific and engineering problems. This approach encompasses fundamental concepts in applied mathematics, such as convex minimization, equilibrium problems, convex-concave saddle point problems, and inclusion problems, which are commonly found in optimization and machine learning. Our study introduces an innovative Popov-type inertial extragradient algorithm designed to approximate solutions to VI. We investigate the convergence characteristics of this iterative technique under specific conditions. The algorithm is then modified and implemented to train an extreme learning machine (ELM) network. We employ our proposed method to determine the optimal output weight and required time, which are essential components of ELM training. To assess the efficacy of our algorithm and other comparative techniques, we utilize standard metrics typically employed to evaluate machine learning performance in regression tasks.

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MS129

Infinite Dimensional Representations of the Meta Hahn Algebra and Special Functions

Recently, Zhedanov and Vinet described the Meta Hahn algebra together with their finite dimensional representations in order to study rational functions which have bi-spectral properties. In this talk, I will present some new results obtained using infinite dimensional representation theory of the Meta Hahn algebra. In particular, we will see how it can be used to study continuous Hahn polynomials and their rational analogues.

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MS129

Commutative Subalgebras of Symmetric Groups and Hecke Algebras Arising from Shuffling Processes

This talk will explore two interrelated families of commutative subalgebras of the group algebras of the symmetric groups, and their generalizations to Hecke algebras. These subalgebras arise naturally from their connections to card shuffling processes, particulary the random-to-random operator and the Bidigare-Hanlon-Rockmore theory of random walks on hyperplane arrangements. The spectral theory of these subalgebras is especially elegant: the eigenvalues have an explicit combinatorial interpretation; and the associated eigenspaces can be constructed recursively. This talk is based on ongoing joint work with Sarah Brauner (Brown), Patricia Commins (Minnesota), Darij Grinberg (Drexel), and previous joint work with Ton Dieker (Columbia) and Nadia Lafrenire (Concordia).

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MS129

Euler-Bernoulli Beam Problem and Noncommutative Stieltjes's Continued Fractions

In the first part of the talk, I will briefly review the use of orthogonal polynomials in the integrable equations of the Camassa-Holm type. In the second part, I will describe an integrable system describing isospectral deformations

of the Euler-Bernoulli beam problem. I will show how one can solve the inverse problem for the special case of a discrete Euler-Bernoulli beam. The solution involves a noncommutative generalization of Stieltjes ' continued fractions, leading to the inverse formulas expressed in terms of ratios of Hankel-like determinants.

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MS130

Orthogonal Polynomials and Hankel Determinants for Certain Bernoulli and Euler Polynomials

Using continued fraction expansions of certain polygamma functions as a main tool, we find orthogonal polynomials with respect to the odd-index Bernoulli polynomials $B_{2k+1}(x)$ and the Euler polynomials $E_{2k+\nu}(x)$, for $\nu = 0, 1, 2$. In the process we also determine the corresponding Jacobi continued fractions (or J-fractions) and Hankel determinants. In all these cases the Hankel determinants are polynomials in x which factor completely over the rationals. (Joint work with Lin Jiu).

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MS130

Zeros of the Deformed Exponential Function

The deformed exponential function $f(x) = \sum_{n\geq 0} x^n q^{n^2}/n!$ arises in various contexts in combinatorics and statistical physics. In particular, its zeros $x_k = x_k(q)$ are closely related to generating polynomials of complete graphs (also, to Tutte polynomials and enumerations of trees). Alan Sokal proposed a number of intriguing conjectures concerning the expansions of these zeros in powers of q. In this talk, we will explore these conjectures and their implications and will discuss known properties of $x_k(q)$, including the results of Wang and Zhang on their asymptotic expansions in power of $1/k$. We will also present our recent results of expansions of $x_k(q)$ in powers of q, providing further evidence for the validity of Sokal's conjectures.

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MS130

The Limiting Behavior of Zeros of a Family of Polynomials Coming from a Rational Integral

Some time ago G. Boros and the speaker conjectured that the zeros of a sequence of polynomials appearing in the evaluation of a rational integral converge to a lemniscate. The talk will outline the solution of this conjecture using Riemann-Hilbert Problems. This work is part of John Jairo Lopez thesis a Tulane. It is joint work with Ken McLaughlin

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MS130

On MeixnerPollaczek Polynomials and the Sturm-Liouville Problem

This work provides a detailed survey of MeixnerPollaczek polynomials and employs the forward-shift operator to study the Sturm-Liouville problem. It presents two linearly independent solutions to the recursion relation, along with the associated difference equations. Additionally, the formulation of second-kind functions is discussed. This work is in collaboration with Mourad Ismail.

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MS131

Newer Rank Notions on Tensors and Their Computational Applications

Matrix rank comes with its own supply of computational problems on which one can find a vast literature, such as the famous matrix completion problem asking for completions of the entries of a matrix with some missing entries that minimise the rank of the resulting matrix. The rank of matrices may be extended to a notion of rank of tensors called the tensor rank, and the tensor rank has itself been the object of considerable attention for computational purposes, in some cases motivated by applications to matrices, such as the determination of the exponent of matrix multiplication. More recently however, other notions of rank of tensors have been defined, including the slice rank and the partition rank. We will discuss open problems in the basic theory of these other rank notions, then follow by analogues to these other rank notions of computational problems for matrix rank and tensor rank, and finally conclude by providing examples of contexts in data interpretation where these problems are more relevant for these other ranks than for the tensor rank. For instance, coming full circle, when might a tensor with hidden entries, completed to minimise partition rank be more likely to be the original tensor than the same tensor with hidden entries but completed to minimise tensor rank?

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MS131

Causal Discovery in Time-Series Data Using Signature Tensors

In this work, we model causal relations among time-series data using a path-dependent stochastic differential equation (SDE). Any function of a path can be approximated by some linear functional of its signature tensor i.e. some linear functional of the iterated integrals of the path. We

leverage this fact to model the causal relations among the time series data using an SDE with a finite number of parameters. We then propose a causal discovery method, where these parameters are estimated by solving a polynomial system of equations. We show that this parameter estimation method is consistent under certain conditions on the driving noise. This is joint work with Darrick Lee, Vincent Guan, and Elina Robeva.

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MS131

Contracting Tensor Networks from Clifford Circuits Using Gf(2) Gaussian Elimination

Quantum circuits are considered more powerful than classical circuits but require exponential resource to simulate. Clifford circuits are a special class of quantum circuits that can be simulated in polynomial time but still show important quantum effects such as entanglement. In this work, we present an algorithm that simulates Clifford circuits by performing Gaussian elimination on a modified adjacency matrix derived from the circuit structure. Our work builds on ZX calculus tensor network representations of quantum circuits based on quantum graph states. We give a concise formula of amplitudes of graph states based on an LDL decomposition of matrix using GF(2), and, using it, efficient algorithms for sampling Clifford circuits. Our formula also provides a local equivalence result for graph states with invertible adjacency matrices. Finally, we discuss how Clifford-based simulation may be combined with low-rank tensor methods for general quantum circuit simulation.

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MS131

Improving the Leading Constant of Matrix Multiplication

Algebraic matrix multiplication algorithms are designed by bounding the rank of matrix multiplication tensors, and then using a recursive method. However, designing algorithms in this way quickly leads to large constant factors: if one proves that the tensor for multiplying $n \times n$ matrices has rank $\leq t$, then the resulting recurrence shows that $M \times M$ matrices can be multiplied using $O(n^2 \cdot M^{\log_n t})$ operations, where the leading constant scales proportionally to n^2. Even modest increases in n can blow up the leading constant too much to be worth the slight decrease in the exponent of M. Meanwhile, the asymptotically best algorithms use very large n, such that n^2 is larger than the number of atoms in the visible universe! In this paper, we give new ways to use tensor rank bounds to design matrix multiplication algorithms, which lead to smaller leading constants than the standard recursive method. Our main result shows that, if the tensor for multiplying $n \times n$ matrices has rank $\leq t$, then $M \times M$ matrices can be multiplied using only $n^{O(1/(\log n)^{0.33})} \cdot M^{\log_n t}$ operations. In other words, we improve the leading constant in general from $O(n^2)$ to $n^{O(1/(\log n)^{0.33})} < n^{o(1)}$.

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MS132

Topics in Topological Photonics

In the field of light matter interactions, novel photonic architectures and their guiding of light follows behavior seen in condensed matter physics and attributes connected to topology. In this presentation, we will highlight research in both the linear and nonlinear regimes of light propagation in one and two dimensional lattices and the role played by the topological properties of these structures. Results in the inherently discrete description as well as in relevant continuous approximations will be discussed.

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MS132

Coupled harmonics in time-modulated scattering systems

We consider the resonance and scattering properties of a composite medium containing scatterers whose properties are modulated in time. The temporal modulation induces a coupling between wave harmonics whose frequencies differ by the modulation frequency, described as a folding of the frequency axis into a temporal Brillouin zone. We develop an integral-operator characterization of the resonances and band structure of time-dependent scatterers, and present small-volume asymptotic (formal) expansions analogous to the classical results for the static (unmodulated) case. As an effect of broken energy conservation, we show that the scattering coefficients may blow up when (complex) resonances cross the real axis. We also show how the integral-operator approach can be leveraged for efficient numerical calculation of the scattering properties of time-dependent materials.

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MS132

Continuum models of moiré materials

Moiré materials, made by stacking 2D materials with slightly mismatched Bravais lattices, have attracted huge attention in recent years because of their remarkable ability to realize diverse quantum phenomena such as "unconventional" superconductivity. These phenomena are generally predicted using continuum PDE models which extract the essential physics at the scale of the material's moiré pattern. I will show how these models can be derived using systematic multiple-scales analysis with rigorous error estimates. I will first present the derivation for models of single-particle electronic properties, such as the Bistritzer-MacDonald model of twisted bilayer graphene. I will then present the case of mechanical models describing structural relaxation and vibration (phonons). Our derivations and proofs clarify the parameter regime of validity of such continuum approximations and allow for systematic derivations of higher-order corrections.

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MS132

Mathematical Theory of Edge States in Topological Photonics

The discovery of topological insulators in condensed matter physics has opened new avenues for generating interface and edge modes in photonic and phononic media. These modes, confined near the interface between two distinct structures or along the boundary of a single structure, offer robust ways to guide and control light. Their origin lies in the symmetries and/or nontrivial topology of the underlying wave operators. In this talk, we report on recent advances toward rigorously establishing the existence of interface and edge spectra in a variety of topological photonic and phononic structures.

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MS133

A Mathematical Model to Study the Heredity of Protocells

Research has unveiled cell components, yet their origins and assembly remain mysteries. The gene-centric "RNA World" hypothesis has been pivotal, suggesting life began with self-replicating RNA molecules that evolved to perform all biological functions. This hypothesis highlights the need for a hereditary mechanism, foundational for evolution. However, it's unproven due to the absence of a de novo RNA replicator in laboratory conditions. An alternative, the "metabolism-first" hypothesis, proposes life started from autocatalytic reaction networks, not from singular RNA molecules. These networks, increasing in concentration collectively, might have enabled the first replicators to pass on information through chemical compositions, including the molecular makeup of lipid membranes, suggesting a different form of inheritance before genetic biopolymers became the primary information carriers. This project assesses heredity limits in vesicle-based protocells and aims to engineer molecular systems, focusing on liposome production. We explore how self-assembling lipids might have driven the reproduction of early cellular structures, providing insights into life's origins aligned with the metabolism-first perspective. Our findings, which will include which lipids form the most stable vesicles and an image-recognition algorithm for vesicle analysis, aim to illuminate the early stages of biological evolution and Darwinian principles sans DNA.

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MS133

Beyond Message Passing: Learning Representations from Dynamics on Graphs

This talk introduces two complementary frameworks that harness geometric and topological structure in dynamics on graphs for representation learning. I will first introduce Neurospectrum, a modular architecture that models brain activity as graph signals and learns latent neural trajectories shaped by multiscale spatial and temporal structure. By extracting geometric and topological invariants of these naturally occurring dynamics, such as curvature, path signatures, persistent homology, and recurrent dynamics, Neurospectrum reveals interpretable patterns in brain function, offering insights into neural synchrony, coordination, sensory processing, and aberrant dynamics associated with psychiatric disorders like OCD. Building on the idea of using dynamical behavior to reveal structure, I will next introduce DYMAG, a novel graph neural network that replaces traditional message passing with solutions to heat, wave, and chaotic partial differential equations defined over graphs. By treating graphs as continuous dynamical systems, DYMAG captures intrinsic geometric and topological features of the graph, enabling richer node and graph-level representations that improve performance on various benchmarks.

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MS133

Mathematical Model of Endosomal Escape

We developed a novel method to quantify endosomal escape of designed fusogenic peptides that electrostatically bind with siRNAs and promote their endosomal escape and delivery into the cytosol. The novel fusogenic peptides enable efficient knockdown of target oncogenes in epithelial ovarian cancer, resulting in decreased cell migration and recolonization in vitro. siRNAs are also known to degrade rapidly in the endosome. Rapid degradation is avoided due to a combination of cationic and hydrophobic amino acid residues, which allows disruption of the endosome and release of siRNAs into the cytosol. Studies regarding the use of the peptides complexed with siRNAs targeting and silencing oncogenes demonstrate the technology's therapeutic potential in ovarian cancer and strategies to reduce ovarian cancer aggressiveness. More information is needed about endosomal escape after successful delivery. Combining kinetic modeling of biochemical systems and stochastic modeling of intracellular organelles for analysis

will enable the development of novel strategies to understand the complexity of in vitro delivery and intracellular processes. Using a Bayesian inference method, we estimate the production rate of endosomal escape, and use the estimated parameters to train our logistic growth model which predicts how endosomal escape reacts per experiment. Successful quantification of endosomal escape will lead to more effective strategies for delivering RNAi therapeutics.

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MS133

Agent-Based Modeling on Keloid Scar Propagation

Keloids are debilitating skin scarring disorders, triggered by an aberrant wound healing program and exhibit continuously spreading growth. Recent single cell RNA-sequencing experiments reveal heterogeneity in human keloid fibroblasts, and interactions among various subclusters of fibroblasts together with interactions with immune cells might be key factors regulating the keloid propagation. We developed an agent-based model to investigate the propagative dynamics of keloids, where single cell data inferred cell communications are implemented into the model. Using the model, we propose the potential regulating mechanisms behind keloid propagation.

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MS134

NSF Mathematical Sciences Research Institutes: Expanding Research Opportunities for All Career Stages

NSF Mathematical Sciences Research Institutes play a vital role in advancing mathematical research and its applications by fostering collaboration, innovation, and interdisciplinary engagement. They provide dynamic environments where researchers from around the world come together to explore fundamental mathematical questions, develop new research directions, and apply mathematical techniques to other scientific disciplines. This talk will highlight the opportunities available at NSF Math Institutes for researchers at all career stages, from undergraduate to senior faculty. We will discuss how to apply for institute programs (including funding considerations), as well as how to propose and organize research programs. Examples will primarily be drawn from the Institute for Pure and Applied Mathematics, providing concrete insights into how participants can maximize their engagement with the institutes.

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MS134

What You Look Like Those Looking You Up Online Matters and Why!

Do you want to have a career in applied math – especially in academia? If so, people will be looking for you frequently. You do want to make it easy for awards committees to give you awards, right? You want to make it easy for hiring committees to find the right you. Perhaps you even aim to become known outside your topic area. A strong online presence can help with all of these goals. I'll talk through what that can look like, what are must-dos, nice to haves, and above and beyond efforts. I'll also share insights from my experiences with award searches, hiring committees, and many other engagementsboth successful and not-so-successful.

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MS134

Assimilation by the SIAM Collective: How to Engage Siam and Be Engaged by SIAM

I will provide an overview of my 30+ year connection to the SIAM community, and discuss tips on how to engage with SIAM, and in return be engaged by SIAM. I will review the challenges and rewards of being active in SIAM and how to balance service in professional societies with an active research career. I welcome active audience participation and I am looking forward to a lively QA session.

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MS134

Transition From Following to Leading Initiatives

Many of us are excellent researchers - writing good papers and giving good talks. However, more often than not, we need to take initiatives outside our comfort zone. Writing a grant proposal is the first step. Once your proposals or initiatives are granted, what are the skills needed to successfully execute the projects? I will share my experiences and lessons learned.

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MS135

CoCalc for Course Management

CoCalc is a cloud-based platform designed to streamline the use of scientific software while making it more collaborative. It enables educators to manage courses, create assignments with auto/self-grading capabilities, perform research, and write publications, all in one place. We will explore the platform's integrated course management system, which facilitates real-time collaboration between students and instructors, resulting in a more engaging learning experience. Additionally, when combined with the interactive features of CoCalc's Jupyter implementation and custom

version control (TimeTravel), the platform can provide better insight into student engagement.

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MS135

NIST DLMF Tables: Standard Reference Tables on Demand

In 2010 the National Institute of Standards and Technology (NIST) launched the Digital Library of Mathematical Functions (DLMF) to upgrade the widely cited Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables (AS). AS addressed a critical need for accurate tables of reference values to support the research and computation of special functions. Today, reliable computing engines, computer algebra systems, and multiple precision computational packages diminish the need for such tables, but applied scientists, numerical analysts, and software developers still need the ability to test software for computing mathematical function values. DLMF Standard Reference Tables on Demand (DLMF Tables), http://dlmftables.uantwerpen.be/, is a collaborative project of the NIST Applied and Computational Mathematics Division (ACMD) and the University of Antwerp Computational Mathematics Research Group (CMA) to address this issue – developing an online system where users can generate tables of special function values at user-specified precision with an error certification to test their own algorithms or confirm the accuracy of results from a commercial or publicly available package. Ultimately, the goal is a standalone system also accessible from the DLMF. We discuss our beta site at the University of Antwerp, based on CMAs MpIeee, a multiple precision IEEE 754/854 compliant C++ floating point arithmetic library and suggest the next steps for further development.

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MS135

Exploring Angle Ranks Using the LMFDB and a Brief Introduction to Code4Math

I would first like to use this opportunity to introduce Code4Math, a relatively new professional society dedicated to the advancement of mathematical research through the development of high-quality sociotechnical infrastructure, and invite you all to join us. Following this, I will speak about some joint work with Taylor Dupuy, Kiran Kedlaya, and David Roe, in which we developed and deployed a database of isogeny classes of abelian varieties over finite fields on the L-functions and modular forms database website. I will introduce some quantities of interest related to these objects, and then show how the digital data we generated led to, on the one hand, disproving a conjecture found in the literature, and on the other to the formulation and ultimately the proof of new theorems by Dupuy, Kedlaya, and David Zureick-Brown.

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MS136

Cascaded Impulsive Systems and Applications

Many evolutionary processes such as those in engineering, sciences, and ecosystems are often modelled by complex nonlinear dynamical or control systems. Analyzing and controlling such systems are even more challenging. One way to overcome those difficulties is to divide the system into interconnected multiple-state (or multiple-control-loop) structures. If these states (or controllers) are viewed as leader and follower subsystems, then the interconnected systems are called cascaded systems. These systems are used, for example, in manipulating (e.g. purifying and enriching) fuel substances, synchronizing electrical or/and mechanical systems, and synchronizing leader-follower spacecrafts. In this talk, we present: (i) input-to-state stability for a class of nonlinear cascaded systems undergoing external disturbing signal and impulses and (ii) the synchronization of two mechanical systems with impulsive effects. The direct Lyapunov method is used to study the two problems.

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MS136

Constructing Convex Relaxations of ODE Solutions via Hybrid Dynamical Systems

In state-of-the-art deterministic methods for continuous global minimization (as implemented in the solvers BARON, ANTIGONE, MAiNGO, and EAGO.jl), a problem is solved to ϵ-optimality in finite time by evaluating upper and lower bounds on the unknown globally optimal value, and then successively refining these bounds. In this setting, lower bounds are typically computed by constructing and minimizing an appropriate convex relaxation. Intuitively, for these lower bounds to be useful in global optimization, the supplied convex relaxations must be accurate and tight, and they must be constructed both automatically and cheaply. For problems involving embedded ODEs, however, useful convex relaxations are challenging to furnish. This presentation introduces our recent advances in constructing effective convex relaxations for solutions of parametric ODEs, including new formulations that employ gradient/subgradient information and derivative-free sampling techniques. The resulting convex relaxations of ODEs perform well in practice, and are described as solutions of hybrid dynamical systems, with mode transitions that essentially prevent relaxations from drifting too far from the original system's trajectories. Several numerical examples are presented for illustration.

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MS136

Physics-Informed Neural Network Lyapunov Functions with Formal Guarantees

One of the longstanding challenges in nonlinear systems and control is the effective construction of Lyapunov functions for stability analysis and the efficient computation of optimal value functions for control. In this talk, we will

discuss a physics-informed neural network framework for learning Lyapunov and optimal value functions for nonlinear systems. Specifically, we obtain neural Lyapunov and value functions by solving their characteristic PDEs using neural networks. We derive sufficient conditions for the efficient verification of the learned certificates with satisfiability modulo theories solvers. We address approximation error bounds, convergence guarantees of neural approximations to maximal Lyapunov functions and optimal value functions, and the formal correctness of neural Lyapunov certificates. We also introduce a software toolbox, LyZNet, for integrated learning and verification of neural Lyapunov functions for stability analysis and control. The framework is illustrated with examples from nonlinear systems and control, ranging from low- to high-dimensional systems.

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MS136

Sensitivity-Based Methods for Parametric Identifiability and Model Reduction of Nonsmooth Systems

Nonsmooth systems, which are continuous but nondifferentiable and experience "switches between modes, arise in a variety of applications in science and engineering. However, the presence of nonsmoothness invalidates standard theory from smooth dynamical systems, including analyzing the identifiability of a system using derivative-based information (to determine if the system parameters can be uniquely determined from system outputs). In this talk, we present a sensitivity-based method to determine identifiability of a nonsmooth system using lexicographic directional derivatives, which are a type of generalized derivative that possess a strong theoretical and numerical toolkit. In order to do this, we develop a first-order Taylor-like approximation theory for nonsmooth functions. The resulting theory, called the lexicographic sensitivity rank condition (LSERC), is applicable to both ODEs and differential-algebraic equations (DAEs) and can be used for model reduction, which is useful in system design, control, and optimization. Moreover, the new theory recovers the classical sensitivity rank condition (SERC) test for ODEs when participating functions are smooth and establishes the SERC test for smooth DAEs. The new theory and methods are illustrated through examples and practical applications.

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MS137

A Mesh-Free Collocation Method for Vector Fields on Surfaces

Surface flow phenomena across science and engineering are described by partial differential equations (PDEs) involving scalar and vector fields. Numerically studying such PDEs requires efficient spatial discretization of vector fields on curved surfaces and differential operators over them. We present a mesh-free numerical collocation method for approximating intrinsic differential operators over scalar and vector fields defined on oriented Riemannian manifolds. Given a surface point cloud and the surface normal at each point, the method provides a computationally embedding-free approximation of the fields and their spatial derivatives at each point. The presented method, called Surface DC-PSE, was originally proposed for scalar fields [Singh et al., J. Sci. Comp. 96(2023)]. It is based on the discretization-corrected particle strength exchange (DC-PSE) scheme that generalizes finite differences to point clouds [Schrader et al., J. Comp. Phys. 229(2010)]. Here, we show how Surface DC-PSE can be extended to vector fields in the tangent space of a surface, and we discuss the influence of operator support and collocation point regularity on the convergence properties. We also discuss properties of computational efficiency. Due to its mesh-free nature, Surface DC-PSE scales well on distributed-memory parallel computers, for which we present an efficient software implementation. We showcase its capability by solving parabolic PDEs on parametric and non-parametric manifolds.

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MS137

Fast Construction of Efficient Cut Cell Quadratures

Several new and improved algorithms for constructing efficient quadrature rules for cut cells are presented. The rules are "native" (do not involve mapping or meshing the cut cell), have positive weights, and do not have excessively more nodes than the minimum number required for a given polynomial degree (they are "efficient", but not Gaussian). For a modest degree, our algorithms can construct quadrature nodes at a rate of about 10,000 points per second per core.

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MS137

A High-Resolution Numerical Framework for LNP-mRNA Nanoparticle Growth in Jet Mixers

Lipid nanoparticle (LNP) formulations encapsulating messenger RNA (mRNA) have become a cornerstone of modern drug delivery and vaccine development. The rapid and controlled self-assembly of LNP-mRNA complexes in jet mixers is a crucial determinant of their physicochemical properties, stability, and therapeutic efficacy. This study introduces a high-order compact finite difference numerical framework to model the intricate hydrodynamic and

physicochemical mechanisms governing LNP-mRNA formation in jet mixers. Our approach integrates computational fluid dynamics (CFD) with detailed nanoparticle growth kinetics, effectively capturing the coupled effects of turbulent mixing, nanoprecipitation, and nucleation dynamics. By resolving local concentration gradients and transport phenomena, our model quantitatively predicts key LNP characteristics, including size distribution, encapsulation efficiency, and stability. Validation against experimental data confirms the frameworks accuracy in predicting LNP properties across diverse flow conditions and formulation parameters. This work establishes a computational foundation for optimizing jet mixing strategies, enabling precise control over LNP-mRNA synthesis and advancing the rational design of next-generation nanomedicines.

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MS137

High-Order, Meshfree Integration on Surfaces, Including Singular Integrands

We propose high-order, meshfree methods for computing surface integrals. Our approaches utilize symmetric meshfree methods for solving surface partial differential equations (PDEs) combined with solvability conditions for these PDEs to achieve accurate integration. Through a modification to existing meshfree methods, we also demonstrate how singular functions can be integrated with high accuracy on arbitrary surface point clouds. We validate our approaches through numerical examples and convergence studies on surfaces with and without boundary, demonstrating their accuracy and efficiency.

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MS138

Isometric Simplices for Anisotropic and High-order Mesh Adaptation

Anisotropic mesh adaptation with Riemannian metrics has proven efficient to create straight-sided meshes whose anisotropy is induced by the geometry of interest and/or the resolved physics. The adapted meshes typically exhibit orders of magnitude fewer degrees of freedom than structured or isotropic grids, while providing solutions of comparable accuracy. In the so-called continuous mesh framework, anisotropic meshes are seen as the discrete counterpart to Riemannian metrics, and ideal, or unit, simplicial meshes consist only of simplices whose edges have unit or quasi-unit length with respect to the input metric. Recently, mesh adaptation with high-order (i.e., curved) elements has grown in popularity in the meshing community, as the additional flexibility of high-order elements allow to further reduce the approximation error. These meshes are curved inside the computational domain to better represent the resolved fields. However, a complete and competitive methodology for both anisotropic and high-order mesh adaptation is not yet available. In this presentation, the adequacy between a metric and a high-order mesh is discussed, and the notions of unit simplices and unit meshes, central to the continuous mesh framework, are extended to high-order elements. The existing definitions of unit simplex are reviewed, then a broader definition based on Riemannian isometries is proposed to handle curved and high-order simplices. Similarly, quasi-unitness is extended to curved simplices for the practical generation of high-order meshes. Lastly, a frontal meshing algorithm to generate high-quality quadratic and geodesic meshes in two dimensions is presented.

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MS138

A Finite Element Method for Solving the Richards Equation Using a New Bounded Auxiliary Variable

The Richards equation, a nonlinear elliptic parabolic equation, is widely used to model infiltration in porous media. We develop a finite element method for solving the Richards equation by introducing a new bounded auxiliary variable to eliminate unbounded terms in the weak formulation of the method. This formulation is discretized using the backward Euler scheme and the resulting nonlinear system is solved using a modified Picard method. Our approach eliminates the need of regularization techniques and offers advantages in handling both dry and fully saturated zones. In the proposed techniques, a non-overlapping Schwarz domain decomposition method is used for modeling infiltration in layered soils. We apply the proposed method to solve the Richards equation using the Havercamp and Van Genuchten-Mualem models for the capillary pressure. Numerical experiments are performed to validate our approach, including a test for modeling flows in fibrous sheets where the initial medium is totally dry, two tests in the presence of fully saturated zones as well as dry regions in the domain and a numerical test for infiltration problem in layered soils. The numerical results demonstrate the stability and accuracy of the proposed numerical method. The numerical solutions remain positive in the presence of totally dry zones. Our numerical investigations clearly demonstrated the capability of the proposed method to effectively predict the dynamics of flows in unsaturated soils.

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MS138

Semi-Implicit Second-Order Mixed Finite Element Methods for Modeling Infiltration and Solute Transport in Soils

In this study, the Richards equation modeling infiltration is discretized using the mixed finite element method to handle both pressure and saturation variables. To efficiently address nonlinearities of some terms in the weak formulation, second-order time-stepping schemes with two free parameters are developed. Noniterative methods for

the coupled system of infiltration and solute transport are proposed using extrapolation for the hydraulic conductivity term and Taylor series expansion for the Leverett J-function. A regularization technique is applied to handle solutions in the presence of fully saturated regions where steep gradients can cause numerical issues. We evaluate the proposed class of second-order time-stepping techniques, through extensive numerical simulations in both homogeneous and heterogeneous soils. The semi-implicit scheme (SBDF) based on the second-order backward differentiation formula demonstrates superior computational efficiency and stability, particularly in coarse-textured soils where gravity forces dominate over capillary forces. The SBDF scheme is extended to solute transport using the advection-dispersion-reaction equation to model scenarios including single and multispecies nitrogen transport, pore water electrical conductivity, and nitrate leaching. Validations against analytical solutions and experimental data confirm that the SBDF scheme accurately captures transport dynamics and presents advantages in terms of computational efficiency.

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MS138

A Semi-Implicit Finite Element Technique for the Advection-Diffusion-Reaction Model of Fertilizer Transport in Soil

In this study, a semi-implicit finite element technique is developed for solving the advection-diffusion-reaction system governing fertilizer transport in unsaturated soils. The model is highly nonlinear due to nonlinearities arising from the Richards equation for the infiltration process, where the specific moisture capacity and hydraulic conductivity strongly depend on the pressure head. Additionally, nonlinear source terms accounting for root water and nutrient uptake, further increase the complexity of the system. To ensure numerical stability and computational efficiency, we develop a semi-implicit technique for the hydrodynamics parts while second-order Taylor expansions are proposed to linearize the source terms in the coupled system. This approach leads to a robust second-order semi-implicit finite element scheme. The methodology is applied to subsurface drip irrigation to model the transport of urea, ammonium, and nitrate fertilizers by considering nitrogen first-order decay transformations. Numerical simulations are performed to validate the reliability of the proposed approach in modeling fertilizers in soils. The results confirm the stability, accuracy, and efficiency of the proposed scheme where available data and reference solutions are used for comparison. Our semi-implicit approach can be applied to effectively model the complex interactions of processes in water-fertilizer-soil-plant continuum.

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MS139

Knowledge As An Infection: Modeling Compliance to Public Health Recommendations

Management of the COVID-19 pandemic required, during its early stages, the deployment of non pharmaceutical interventions (NPIs) [social isolation, physical distancing, mask-wearing, hand-washing], and then, as they became available, administration of repeated doses of vaccine. We are interested in the consequences, for the dynamics of the disease, of variable adherence to these measures, and the motivation generating the lack thereof. We present two modeling approaches to represent this evolution of behaviour. First, a basic SEIRS model is expanded by introducing a structure in the infectious class, to reflect the variable severity of symptoms and the presence of asymptomatic cases considering the population divided into two classes according to their degree of adherence to the NPIs. Then, from a different perspective, we focus on the health literacy level in a population and the consequences, for the disease dynamics, of both knowledge dissemination and its integration in behaviour.

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MS139

Fear Dynamics and Bifurcations in a Mathematical Model of Disease Transmission

We explore a mathematical model of disease transmission with a fearful compartment. Susceptible individuals become afraid by either interacting with individuals who are already afraid or those who are infected. Individuals who are afraid take protective measures via contact reductions to reduce risk of transmission. Individuals can lose fear naturally over time or because they see people recovering from the disease. We consider two scenarios of the model, one where fear is obtained at a slower rate than disease spread and one where it is comparable. In the former we show that behavioural change cannot impact disease outcome, but in the latter, we observe that sufficient behavioural intervention can reduce disease impact. However, response to recovery can induce a bifurcation where contact reduction cannot mitigate disease spread. We identify this bifurcation and demonstrate its implication on disease dynamics and final size.

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MS140

Regularity Results for Entropic Optimal Transport

Problems

In this talk, I discuss Caffarelli's-type regularity results for Schrödinger potentials of Shanon-Entropy regularized optimal transport.

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MS140

Plug-in Estimation of Schrdinger Bridges

We propose a procedure for estimating the Schrdinger bridge between two probability distributions. Unlike existing approaches, our method does not require iteratively simulating forward and backward diffusions or training neural networks to fit unknown drifts. Instead, we show that the potentials obtained from solving the static entropic optimal transport problem between the source and target samples can be modified to yield a natural plug-in estimator of the time-dependent drift that defines the bridge between two measures. Under minimal assumptions, we show that our proposal, which we call the *Sinkhorn bridge*, provably estimates the Schrdinger bridge with a rate of convergence that depends on the intrinsic dimensionality of the target measure. Our approach combines results from the areas of sampling, and theoretical and statistical entropic optimal transport. This is joint work with Jonathan Niles-Weed.

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MS140

Entropy Solutions of Nonlocal Transport Equations with Congestion

In this talk we consider a class of scalar nonlinear models describing crowd dynamics. The congestion term appears in the transport equation in the form of a compactly supported nonlinear mobility function of the macroscopic density, thus making standard weak-type compactness arguments and uniqueness of weak solutions fail. Under reasonable conditions on the velocity field, the well-posedness can be recovered among Kruzkov entropy solutions of the target pde. We consider a variational approach to the problem in the spirit of minimising movements, which exploits the gradient flow structure of the evolution in a suitable metric framework, and discuss its connection with the dissipative nature of entropy solutions.

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MS140

Variational Regularity of Optimal Transport Maps and Applications

In this talk I will present a purely variational approach to the regularity theory of optimal transportation introduced by Goldman and Otto. Following De Giorgis strategy for the regularity theory of minimal surfaces, it is based on the approximation of the displacement by a harmonic gradient, which leads to a one-step improvement result that feeds into a Campanato iteration on the $C^{1,\alpha}$-level for the displacement. With Otto and Prod'homme, we extended this variational approach to almost minimizers (with respect to quadratic cost) of the optimal transport problem, which allowed us to reprove the $C^{1,\alpha}$-regularity result of De Philippis–Figalli, bypassing Caffarellis celebrated theory. I will give a brief overview of further recent developments using this variational approach and highlight some interesting applications.

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MS141

No Gpus, No Problem: Easy Trillion-Parameter Model Training and Scaling with Cerebras

Scaling traditional GPU clusters to support large-scale deep learning workloads, particularly at the trillion-parameter model scale and beyond, is notoriously complex. Data, model, and tensor parallelism require delicate tuning in addition to complex software dependencies not needed at smaller model scales. We demonstrate that a Cerebras wafer-scale cluster can train models at the trillion-parameter scale as easily as any smaller model, and using an arbitrary number of compute devices, without introducing any additional code complexity during either scale-up or scale-out. Cluster throughput projections indicate that a 64x CS3 Wafer-Scale Cluster would process this workload with efficiency on par with thousands of GPUs from the Frontier supercomputer. The Wafer-Scale Cluster's weight-streaming compute paradigm meant we could achieve this result with a straightforward upgrade to the model's parameter server capacity. This work shows promise for streamlining large-scale deep learning workloads, reducing the amount of ML engineering experience teams need to scale their work, and simplifying the hyperparameter tuning and software complexity traditionally associated with these large-scale experiments.

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MS141

Developing Scalable Machine Learning Methods for Accelerating Computational Chemistry

Developing machine learning methods that are scalable - meaning that they are accurate and efficient on large inputs and continue to improve as computing resources are increased - is crucial in the current age of massive-scale AI. This paradigm holds particularly true in the subfield of AI for Science, in which machine learning methodologies are increasingly being used to accelerate scientific discovery. In this talk, we will explore recent trends in developing scalable ML methods for simulating and designing molecules, materials, and proteins, with a focus on recent work from our group. We will discuss esCAIP, a new machine learning force field (MLFF) architecture that eschews traditional inductive biases such as SO(3) equivariance in favor of a more scalable, attention-centric architecture, enabling efficient and accurate molecular dynamics simulations and other applications. We also introduce a knowledge dis-

tillation (KD) technique that produces small, highly efficient MLFFs specialized for specific downstream scientific applications, such as modeling amino acid chemistry or particular elements of the periodic table, while leveraging the general-purpose representations learned by larger models. Finally, we discuss recent scalable ML methods for tackling the canonical problem of transition path sampling (TPS) by zero-shot repurposing existing, large-scale generative models of high-dimensional atomistic configurational distributions.

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MS142

Experimental and Theoretical Investigations of Rotating Algae Biofilm Reactors (RABRs): Areal Productivity, Nutrient Recovery, and Energy Efficiency

Microalgae biofilms have been demonstrated to recover nutrients from wastewater and serve as biomass feedstock for bioproducts. In this talk, we present a platform to quantitatively describe microalgae biofilm production that can provide guidance and insights for improving biomass areal productivity and nutrient uptake efficiency of a rotating algae biofilm reactor (RABR). Furthermore, we will present a novel mathematical model to accurately capture the growth dynamics of algae biofilms within RABR.

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MS143

A Poissonian Model for the Circadian Activity of Cupboard Spiders

Experimental data from multiple spider families suggest that locomotor activity is circadian. Surprisingly, the free-running period of spiders can vary significantly, even within species. Here, we present a model to describe this locomotor activity based on a nonhomogeneous Poisson process.

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MS143

Bacterial Contamination in Microchannels with Varying Wall Curvatures

Many motile bacteria have been successfully modeled as active rods - elongated bodies capable of self-propulsion. A hallmark of active rod dynamics under confinement is their tendency to accumulate at the walls and swim against the imposed flow, reflecting bacterial contamination in a tube-like micro-channel (catheter, blood vessel, etc.). In this work, we examine the effects of wall curvature on active rod distribution by studying elliptical perturbations of such three-dimensional micro-channels, that is, the cylindrical confinement with an elliptical cross-section. By developing a computational model for individual active rods and conducting Monte Carlo simulations, we discovered that active rods tend to concentrate at locations with the highest wall curvature, which is consistent with known results on the 2D dynamics of self-propelled particles under strong confinement. We then investigated how the distribution of active rod accumulation depends on the background flow and orientation diffusion. Finally, we used bifurcation analysis of our computational model to reveal how the reaction force exerted by the wall on the self-propelled rod may affect the distribution dynamics of accumulated rods.

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MS143

Effects of Seasonal Disruption on Continuous Food-web Interactions

Ecological behaviors can occur over multiple timescales. Over short timescales, quick behaviors such as feeding or growth may occur. Over longer timescales, slow behaviors such as seasonal reproduction or migration may occur. Additionally, it may be important to understand interactions across these timescales in determining long-term outcomes. For example, the effect of feeding on reproductive output may determine whether a species persists. In this work, we bridge timescales by combining continuous differential equations for quick changes with discrete difference equations for slow, seasonal behaviors. The resulting models are difficult to analyze, and so we use numerical methods to simulate and represent the range of long-term outcomes. We implement the method for increasingly complex feeding networks and examine how the assumption of discrete, seasonal behaviors impacts assessments of ecosystem stability.

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MS145

Natural Damping in Time-Harmonic Problems Helps Parallel Solvers

It is known since the introduction of the shifted Laplace preconditioner that damping can greatly help iterative solvers to perform well when solving time harmonic problems where they usually struggle. More recently, it was discovered that the typical time harmonic model problem, the Helmholtz equation, also becomes much easier to solve when posed in free space, compared to wave guides and cavities. In nature, there is always damping, and the mathematical models without damping are approximations. We study here the influence of naturally present damping on

the performance of Schwarz methods when solving damped Helmholtz problems, compared to the undamped case. We consider first order and viscoelastic damping. Our results show quantitatively the big impact on Schwarz methods of such damping: even the very hard cavity case becomes easy to solve with impedance Schwarz methods if natural damping is present.

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MS145

A Discrete Correction Function Method For Electromagnetic Problems with Boundary and Interface Conditions

In this talk, we propose a discrete correction function method (CFM) to handle various boundary conditions (impedance, and perfect electric and magnetic conductors) and interface conditions. The key idea of the discrete CFM is to enforce the governing equations (e.g., Maxwells equations) directly through the correction function polynomial coefficients. The remaining constraints are enforced pointwise. The correction functions are required to match the base methods numerical solution at the nodes in the vicinity of the surface, while the boundary or interface conditions are enforced using sampling points on the surface. This leads to a linear overdetermined system of equations, which is solved using a least-squares approach. The CFM least-squares problem is solved using a QR factorization, considerably reducing the condition number of the CFM matrices when compared to the original method. Additionally, the resulting method is devoid of numerical integrations, making it more computationally efficient than the previously proposed CFM. The discrete CFM is applied to high-order Hermite-Taylor methods to handle embedded boundary and interface conditions for Maxwells equations. Numerical examples in 2-D are performed and the expected convergence order is observed for $m = 1 - 3$, resulting in up to a seventh-order Hermite-Taylor discrete correction function method.

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MS145

Finite Difference and Wavelet Methods for the Helmholtz Equation

High-order schemes are known to be better in mitigating the pollution effect encountered when solving the Helmholtz equation. In this talk, we present high-order finite difference schemes for solving a 2D Helmholtz equation with an interface, and a special 2D Helmholtz equation on a separable domain. For the latter, we observe that our method can handle arbitrarily high wavenumbers. Additionally, we also present a high-order wavelet method for solving a 2D Helmholtz equation which models an electromagnetic scattering problem. Our wavelet method produces linear systems with uniformly bounded condition numbers for all scale levels (or equivalently matrix sizes) for a given wavenumber.

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MS146

Discrete Bispectrality and Pascal's Matrix

We describe the interplay between spectral data of Pascal's matrix and discrete-discrete bispectrality, with connections to orthogonal polynomials, counting points on elliptic curves over finite fields, and the discrete-time toda system.

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MS146

Algebraic Interpretation of Discrete Families of Matrix Valued Orthogonal Polynomials

In this talk, we discuss an algebraic interpretation of matrix-valued orthogonal polynomials. The construction is based on representations of a Lie (and q-deformed) algebra $\mathfrak{g}$ into the algebra $\mathrm{End}_{M_n(\mathbb{C})}(M)$ of $M_n(\mathbb{C})$-linear maps over a $M_n(\mathbb{C})$-module M. Cases corresponding to the Lie algebras $\mathfrak{su}(2)$ and $\mathfrak{su}(1,1)$ as well as to the q-deformed algebra $\mathfrak{so}_q(3)$ at q a root of unity are presented.

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MS146

The Spectrum of the Finite Open XX Quantum Spin Chain with Transverse Magnetic Boundary Fields Via Orthogonal Polynomials

We compute the spectrum of the finite open XX quantum spin chain with transverse magnetic boundary fields in terms of the roots of a two- parameter orthogonal family of Bernstein-Szeg polynomials. Estimates are presented for the locations of these roots. This enables the construction of an explicit eigenbasis diagonalizing the spin chain in terms of Slater determinants built from a one-parameter subfamily of the Bernstein-Szeg polynomials evaluated on the spectrum. The presentation is based on joint work with Andrs Soledispa and Adrin Vidal.

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MS147

Applications of Hypergeometric Functions to Modular Forms

In this talk, we will share some recent development regarding the applications of classical hypergeometric functions to the study of modular forms which form another important class of complex-valued functions playing central roles in number theory and physics.

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MS147

Hypergeometric Period Matrices

We will discuss the number-theoretic significance of n-by-n period matrices associated with the hypergeometric functions ${}_nF_{n-1}(t)$. Topics will include quadratic relations among the matrix entries, relations of determinants of certain minors with special values of L-functions, and the transcendence degree of the field generated by the matrix entries.

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MS148

A Fourth-Order Exponential Time Differencing Scheme with Dimensional Splitting for Multidimensional Black-Scholes Equation

An L-stable, fourth-order exponential time differencing (ETD) Runge-Kutta scheme with dimensional splitting is developed to solve nonsmooth, multidimensional reaction-diffusion equations. Our scheme uses an L-acceptable Pad (0,4) rational function to approximate the matrix exponentials in the dimensionally split ETDRK4 scheme. The resulting scheme, ETDRK4P04-IF, is verified empirically to be fourth-order accurate for several RDEs and demonstrated to be more efficient than competing fourth order schemes for solving the multidimensional linear Black-Scholes equation.

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MS148

Dimensional Splitting of aFourth-order Exponential Time Differencing Scheme with a Real and Distinct Poles Rational Approximation for Solving Nonlinear Systems of Reaction Diffusion Equations

Reaction-diffusion systems are mathematical models that describe the spatiotemporal dynamics of chemical substances as they diffuse and react. Variety of time discretization schemes have been developed to solve the stiff ODE system resulting from the spatial-discretization of the PDE. The quest to develop more efficient and accurate schemes to handle multidimensional, stiff problems with non-smooth data is ever increasing. In this work, we develop a dimensionally split, fourth-order, L-stable, parallelizable exponential time differencing scheme (ETD) by approximating the matrix exponentials in the class of ETD Runge-Kutta schemes with a fourth-order non-Pad rational function having real distinct poles (RDP). A variety of multidimensional,non-linear reaction-diffusion systems having Dirichlet, Neumann boundary conditions are used to empirically validate the order of convergence of the scheme and compare its performance with existing fourth schemes.

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MS148

The Efficient Computation of Accurate Continuous Numerical Solutions of Nonlocal Two-Point Boundary Value Problems and Parabolic Problems in One Space Variable

Ordinary and partial differential equations containing terms or coefficients that depend on an integral of a function involving one of the solution components are termed nonlocal. We first discuss the reformulation of nonlocal two-point boundary value problems to enable their solution using widely available software packages. Similarly, we consider nonlocal parabolic problems in one-space variable in which an integral of a function of the solution appears in one or more of the boundary conditions. The reformulation then involves replacing such a boundary condition with an ordinary differential equation. For each case, we use a software package that provides an error-controlled continuous numerical solution. Numerical examples are provided to demonstrate the efficacy of our approach and its advantages over numerous existing techniques.

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MS148

Efficient Option Pricing Using Deep Bsde Solvers: A High-Dimensional Approach to the Black-Scholes Model

In this paper, we apply backward stochastic differential equations (BSDEs) and deep neural networks to solve the Black-Scholes equations for option pricing. Using the Deep BSDE solver introduced by Han et al. (2017), we demonstrate its effectiveness in both low- and high-dimensional settings. This deep learning-based approach reformulates the PDE problem into a BSDE framework, enabling efficient numerical solutions for complex financial derivatives. We also extend our analysis to generalized Black-Scholes models incorporating transaction costs and stochastic volatility. To the best of our knowledge, this study is among the first to systematically apply Deep BSDE solvers to the Black-Scholes framework across multiple dimensions. Numerical experiments highlight key patterns in option pricing and the trade-offs between accuracy and computational efficiency.

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MS149

Placement, Trajectories, Retention, and the Geography of California

The University of California, Merced is a twenty-year old minority-serving R1 institution located in the primarily agricultural Central Valley. The majority of our students hold multiple minoritized backgrounds; many are first-generation, racially minoritized, low-income, undocumented, or a combination of these. Most UCM students

take entry-level precalculus and writing courses in their first year of college; these courses are highly predictive of student progress and retention through the program, but there are very large outcome gaps for minoritized students even when controlling for background knowledge and placement. In this talk, we will discuss a large-scale analysis of institutional data on placement, retention, success, and the geography of California. Viewing this through a lens of college readiness and early action in a first-semester course, we will also study the impacts of prior and ongoing interventions which aim to increase outcomes and equity.

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MS149

Quantitative Justice and Applied Mathematics: A 2025 Update

Quantitative justice is "the application of techniques, tools and topics from the quantitative sciences (e.g., mathematics, applied mathematics, data science, computer science, etc.) in subject domains that are derived from and/or typically associated with the social sciences (e.g., history, political science, law, economics, sociology etc.) with the explicit goal of promoting social justice. In this talk, we shall present an update on recent activities, articles, and applications of quantitative justice in the mathematical sciences. One example of a quantitative justice project in the mathematical sciences is #MetaMath, i.e. using mathematics to model the mathematical sciences community itself, sometimes called "the mathematics of Mathematics."

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MS149

Why An Anti-Dei Initiative Is Urgently Needed in the Mathematical Sciences. A Data-Driven Approach

In an era marked by intense scrutiny of initiatives that promote diversity, equity, and inclusion, this presentation provocatively redefines DEI as the Drivers of Exclusion and Inequity (DEI), advocating for a counterintuitive anti-DEI (as defined here) stance within the mathematical sciences. Leveraging comprehensive data from the Opportunity Atlas and the US Department of Education Civil Rights Database of 2018, we expose the impact of privilege and early access to mathematics on achieving success in STEM fields. The analysis reveals statistically significant evidence that current educational and professional pathways disproportionately benefit those with initial advantages. By dismantling the myth of meritocracy, this presentation challenges both critics and supporters of traditional DEI frameworks to reassess their views. Ultimately, it invites a reconsideration of the structural dynamics perpetuating inequity and aims to inspire a deeper, more informed dialogue about the true drivers of opportunity in mathematical sciences. This talk presents paths of action with great potential for eliminating drivers of exclusion and inequity.

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MS149

Using Data to Advance Equity: From Awareness to Action

Data can be a powerful tool for advancing equity, but how we use it matters. This talk will serve as a brief introduction to the session. First, Ill share some views on how department chairs and leaders, using data to identify trends, highlight disparities, and initiate discussions can be a first step toward meaningful change. Then Ill give an overview on the talented diverse speakers we have sharing how they apply data in their workwhether in education, research, or addressing broader social challenges. From analyzing educational outcomes to overcoming institutional resistance to data transparency, our speakers will share their expertise and strategies for leveraging data to promote equity. By making inequities visible, we can move from conversation to action.

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MS150

A Step Toward Agnostic Filters I: Siac Filters in Image Processing

This work, performed at the ICERM-SIAM Workshop on Empowering a Diverse Computational Mathematics Research Community, explores the application of Smoothness-Increasing Accuracy-Conserving (SIAC) filters. In this talk, we will discuss the application of SIAC in image processing, which forms the first part of our collaboration. First, we provide an overview of SIAC filters,

including their form, properties, and discretization procedure. Then, we demonstrate the utility of SIAC filters for enhancing edge detection in noisy images, improving image segmentation through the Normalized Cut algorithm, and augmenting feature detection in medical ultrasound images. We present results that illustrate the performance of SIAC filters for these applications, including visual comparisons and edge preservation capabilities. The results highlight the versatility of SIAC filters for addressing challenges in image processing with future work including the development of adaptive SIAC filters and applications to higher-dimensional datasets.

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MS150

A Step Toward Agnostic Filters II: A Bayesian Interpretation of SIAC Filters

This presentation introduces a Bayesian interpretation of the Smoothness-Increasing Accuracy-Conserving (SIAC) filter, building on work initiated at the ICERM-SIAM Workshop on Empowering a Diverse Computational Mathematics Research Community. In this talk, we provide an overview of SIAC filters from a statistical setting and the integration of SIAC filters into a Bayesian reconstruction framework for Fourier data. The goal of such an endeavour is to recover piecewise smooth signals from noisy and incomplete measurements and be able to provide some uncertainty quantification of the reconstructed Fourier data. Theoretical analysis and numerical experiments provide a proof-of-concept for the effectiveness of this approach. Future directions include developing a Bayesian framework for SIAC filters in the physical domain and extending their applications to more realistic settings. This work was done in collaboration with Ayaboe Edoh.

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MS150

Quantifying Uncertainty in Parametric Image Models for Inverse Problems

This presentation explores novel approaches to efficient uncertainty quantification in inverse problems for imaging. In the cases where target objects, such as tumor boundaries in medical imaging, are assumed to be piecewise constant, and the measured data is limited and noisy, traditional pixel-level inversion methods may not be feasible. To address these challenges, we introduce parametric image representations incorporating hierarchical Bayesian inference techniques. Numerical results demonstrate the effectiveness of our approach in uncertainty quantification for image reconstruction.

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MS151

A Collaborative, Cross-Institutional First Research Experience for Computational Mathematics

Computational mathematics research is perceived to have a high barrier to entry relative to research in other fields, because it often requires students to have advanced math coursework, be proficient programmers, and have some knowledge of a science or engineering application. Our new undergraduate program lowers this barrier to entry by (1) teaching fundamental applied and computational math research skills through carefully scoped computational projects that are open-ended and investigatory in nature and (2) fostering community among participants, both to support them in succeeding in their undergraduate studies generally and to demonstrate that research is fundamentally a community enterprise. In this talk, we will describe our experiences with our first cohort, which consisted of four first-year undergraduate students comprising two teams, each consisting of one student from Emory University and one from the Georgia Institute of Technology. Projects on (i) neural networks and (ii) uncertainty quantification were designed to encourage hands-on computational exploration applications of introductory-level college math classes including probability and statistics and calculus. At the conclusion of the program, each team attended and presented a scientific poster at the Georgia Scientific Computing Symposium. We will conclude the talk with

our vision for sustainably growing this program, including bringing in new universities, graduate students and postdocs.

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MS151

Mujer K-Es-Stem: Breaking Barriers, Building Stem Dreams for Girls

The Mujer K-Es-STEM project aims to address the gender gap in STEM fields by designing and implementing a comprehensive vocational strengthening program for female students in grades 9 to 11 from public and private schools in Bogot, Colombia. The main goal is to boost their participation and motivation in STEM through an interdisciplinary approach that combines exploration workshops in science, technology, engineering, and mathematics with practical tools to enhance their career aspirations. The program also includes essential life skills training, such as mental health education, healthy habits, personal branding, and innovative thinking strategies. In this presentation, I will share the outcomes and key insights from the first edition of the Mujer K-Es-STEM project, highlighting its impact on participants and the strategies implemented to inspire and empower young women to pursue careers in STEM.

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MS152

Simulating Quantum Evolution with Matrix Product States

Simulating quantum systems with many qubits is challenging because the computational resources grow exponentially with the number of qubits. Matrix Product States (MPS) offer a more efficient way to represent quantum states, especially for systems with low entanglement. In this work, we focus on using MPS with Time-Dependent Variational Principle (TDVP) methods to simulate time-dependent quantum systems. We explore how MPS can reduce storage, providing both mathematical and diagrammatic representations. This current work includes simulating Hamiltonians with static and control-dependent components.

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MS152

High-Order Hermite Optimization (HOHO) for Fast Quantum Gate Design

Quantum gates are the building blocks of quantum computing. A quantum circuits operate on quantum states by applying sequences of gates acting on local sets of qubits. Gates are implemented on quantum computers by varying the amplitudes of magnetic fields or EM radiation in time to form control pulses, which control the dynamics of the system. A quantum optimal control problem is solved to find control pulses which implement the desired behavior of a quantum gate. This work introduces the High-Order Hermite Optimization (HOHO) method, an open-loop discrete adjoint method for quantum optimal control. HOHO efficiently computes exact (discrete) gradients when using continuous, parameterized control pulses when solving Schrodinger's equation with an arbitrarily high-order Hermite Runge-Kutta method. The HOHO method is implemented in QuantumGateDesign.jl, an open-source software package for the Julia programming language, which we use to perform numerical experiments comparing the method to a Stormer-Verlet based method implemented in Juqbox.jl. For realistic model problems we observe speedups up to 775x.

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MS152

Unified Picture of Measurement-induced Ionization in the Transmon

Circuit quantum electrodynamics (cQED) has emerged as a powerful platform for quantum computation and for the investigation of quantum optics at microwave frequencies. A critical part of all cQED experiments is qubit readout, which relies on microwave drives. In principle, higher drive amplitudes should lead to faster and more accurate readout. However, experiments have consistently shown that as the drive amplitude increases, the readout quality rapidly deteriorates, something that severely limits qubit readout in the laboratory. We begin by reviewing the basics of qubit measurement in circuit QED, followed by presenting numerical simulations that capture the dynamics of the readout process. Our findings reveal signatures of qubit ionization, where the qubit is brought to highly excited states by the readout drive, leading to a breakdown of the measurement fidelity. Building on previous theoretical and experimental advances, we present a comprehensive theoretical framework providing a physical picture of the origin of transmon ionization, together with a set of tools which can readily be used to predict its occurrence. We further discuss how this phenomenon is not limited to qubit readout but also manifests itself in strongly driven nonlinear circuits across various settings. Finally, we compare our results with recent experimental data.

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MS153

Precision and Performance of a New Regularised Line Source

The immersed boundary method uses the Dirac delta distribution to interpolate singular forces that arise in fluid-structure interaction problems containing flexible 1D structures that are defined along moving curves. Most numerical approaches regularise the Dirac delta distribution by discretising the interface at a sequence of points and then introducing a regularisation of the Dirac delta point-source

over a finite support radius of size H centred at each interface point. The corresponding delta-forcing term is then interpolated onto an underlying fluid grid (with spacing denoted h) using appropriate quadratures. We derive an analytical form for a regularised line source that can be easily implemented in an immersed boundary framework. This regularisation is constructed independently of any specific numerical method and constrained to satisfy continuous moment properties of the Dirac delta line source distribution. The regularisation can be chosen up to a predetermined spatial order of accuracy with respect to its support H. Using multiple numerical methods on a 3D elliptic test problem, we compare theresults for our regularised line source to that from the usual point-delta approximation. Our results show that the new line-delta regularisation exhibits much smaller numerical errors. This improvement is largely due to the preservation of the physical properties along the tangential direction of the line source.

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MS153

Sketchy Natural Gradients for Physics-Informed Neural Networks

Natural gradient methods for physics-informed neural networks (PINNs) have achieved state-of-the-art performance with errors several orders of magnitude smaller than those achieved by standard optimizers such as ADAM or L-BFGS. However, computing natural gradients for PINNs is prohibitively computationally costly and memory-intensive for all but small neural network architectures. We develop a randomized algorithm for natural gradient descent for PINNs that uses sketching to approximate the natural gradient descent direction. We prove that the change of coordinate Gram matrix used in a natural gradient descent update has rapidly-decaying eigenvalues for a one-layer, one-dimensional neural network. This structure holds empirically across all our experiments. Our algorithm dramatically speeds up computation time and reduces memory overhead. Training time for a network with around 5,000 parameters is reduced from several hours to under two minutes. Training can be practically scaled to large network sizes; we optimize a PINN for a network with over a million parameters within a few minutes, a task for which the full Gram matrix does not fit in memory. Additionally, in our experiments, our method achieves errors on the order of 10^{-9} for linear PDE problems, and outperforms the original natural gradient in terms of accuracy.

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MS153

Landscape Refinement for Hp-Adaptive Eigenvalue Approximations

When approximating a collection of eigenvalue-eigenvector pairs (eigenpairs) of a differential operator via finite element methods, the prevailing wisdom is that the finite element space should be well-suited to approximating the entire invariant subspace (the span of the eigenvectors), as opposed to just being well-suited to approximating some particular basis of this space. Over the past 15 years or so, there have been a variety of approaches proposed for achieving this goal as part of an adaptive algorithm. Each approach uses the current computed approximation of the eigenvector basis in some (sophisticated) way to estimate subspace approximation error and determine how to refine the current finite element space to improve the next approximation. When the collection of desired eigenpairs is large, these approaches become increasingly costly. We propose an alternative means of driving adaptive refinement, based on the solution of a single source problem—the so-called landscape function. After providing some theoretical and heuristic justification that landscape refinement is not a ridiculous proposition, we illustrate its practical performance on a variety of examples, primarily in the hp-adaptive setting, where we think it can provide a particularly attractive alternative to current approaches.

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MS153

Layer Potential Approaches for Laplace and Helmholtz Equations

We discuss boundary and eigenvalue problems for the Laplace and Helmholtz equations in the plane using layer potentials for both interior and exterior domains. A new strategy is proposed to deal with Helmholtz wave numbers that correspond with Dirichlet-Laplace eigenvalues. We demonstrate the use of our method in numerical shape optimization and eigenvalue asymptotics for Steklov eigenvalue problems and to approximate the transmission eigenvalue problem.

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MS155

Considering the Effects of Pair Formation Dynamics on Mpox and Hiv Co-Infection in the Gbmsm Community

There is a growing need to explicitly consider how behaviour plays a role in the spread of diseases transmitted through close, prolonged contact. In particular, the duration individuals spend single or in relationships has yet to be incorporated into co-infection models, potentially underestimating the protective effects of stable partnerships. We propose an mpox and HIV co-infection model that explicitly incorporates the formation of pairs between individuals. We demonstrate that considering pair formation

and dissolution rates are critical in determining outbreak potential and severity. These considerations remain important beyond the initial stages of the outbreak and can lead to more accurate predictions. Our work highlights that the particular pairing context and serological status of the population should always be carefully considered prior to intervention on behavioural patterns.

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MS156

On the P-Wasserstein Barycenters

The talk is about the barycenters of N probability measures with respect to the p-Wasserstein metric ($p > 1$), which generalizes the notion of Wasserstein barycenters for $p = 2$, introduced by Agueh and Carlier. Providing a natural way to interpolate probability measures and computing a representative summary of input datasets, they are useful tools in data science, statistics, and image processing. This is a highly nonlinear problem but it can be rewritten as an equivalent multi-marginal optimal transport problem, paying with an (a priori) increase in dimension. Here we show that thanks to a new technique based on the geometric properties of the support of the optimal plan, the p-Wasserstein barycenters of absolutely continuous marginals are unique and absolutely continuous. This implies that the optimal MMOT plan is unique and can be parametrized as a graph over any marginal space (with a consequent dimension reduction). Some examples in one dimension are also discussed, with emphasis on the statistical meaning of the p-Wasserstein barycenters and on the two natural limits $p \to 1$ and $p \to \infty$. This is a joint work with G. Friesecke and T. Ried.

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MS156

Barycenters in Unbalanced Optimal Transport

A central challenge in many applications of optimal transport concerns finding a representative, or barycentric (probability) distribution of a given set of distributions. The basic optimal transport approach to this problem is to find the barycenter by minimizing the sum of weighted two-marginal optimal transport costs between the barycenter and each input distributions. In a seminal contribution by [Agueh & Carlier, 2011], it was subsequently shown that an equivalent and computationally favourable approach is to instead solve a single least-cost multi-marginal optimal transport problem. If the input distributions do not all have equal mass, an unbalanced barycenter can be found via a recourse to the emerging theory of unbalanced optimal transportation. This, however, can be done in a number of ways, depending on how one penalises mass deviations, what cost function is employed and whether one wishes to consider the conic formulation — see the detailed discussion in [Liero, Mielke Savaré, 2018]. In this talk, following a very brief introduction to the topic, I will present several results on how to recover the celebrated least-cost multi-marginal formulation of Agueh and Carlier in the unbalanced setting [Buze, 2025] and discuss on-going work on generalising such results to unbalanced settings where such a reformulation is not possible.

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MS156

Quantum Optimal Transport with Convex Regularization

In this talk, we discuss non-commutative optimal transport with convex regularization in a static and finite-dimensional setting. This can be seen as an extension of classical optimal transport to the quantum setting, where probability distributions are replaced by density matrices. We will emphasize the role of Von-Neumann entropy and other convex regularizers in the formulation of the problem. In particular, we focus our attention to stability of the problem, duality formulations and some numerical aspects. This is joint work with A. Gerolin, N. Monina and L. Portinale.

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MS156

Laplace Learning in Wasserstein Space

The manifold hypothesis posits that high-dimensional data typically resides on low-dimensional subspaces. In this work, we assume this hypothesis to investigate a class of graph-based semi-supervised learning algorithms, namely Laplace Learning, in high-dimensional (including, infinite dimensional) spaces, specifically the Wasserstein space. Our primary goal is to establish continuum limits for Laplace Learning in the Wasserstein space, thus extending the classical notion of graph-based semi-supervised learning algorithms from finite-dimensional Euclidean spaces to infinite-dimensional settings. To achieve this, we prove variational convergence of a discrete graph p-Dirichlet energy to its continuum counterpart using an appropriate scaling. In addition, we also characterize the explicit form of the discrete graph Laplacian operator and the continuum Laplace-Beltrami operator for this setting. Finally, we validate the proposed theoretical framework through numerical experiments conducted on benchmark datasets, demonstrating the consistency of our classification performance in high-dimensional settings.

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MS157

Double Descent and Scale-Time Equivalence

Double descent has traditionally been explained as a phenomenon where a model incorrectly learns spurious patterns from low-variance directions in the training data. This explanation successfully explains double descent as a function of model size and dataset volume, but unfortunately fails with respect to training time. This has led theorists to hypothesize alternate explanations of time-wise double descent, most notably that time-wise double descent only occurs when models are susceptible to learning noisy patterns early during training. We approach this question using scale-time equivalence: the idea that a small

model trained for a long time can achieve similar performance to a larger model trained for a shorter time. We theoretically justify this effect by modeling neural network training as gradient flow in random subspaces of larger nonlinear models. Next, using scale-time equivalence, we show that contrary to conventional explanations, double descent with respect to training time and model scale may share a common cause: namely, overfitting to noise early during training. Through this, we provide potential explanations for several previously unexplained empirical phenomena: reduced data requirements for generalization in larger models, heightened sensitivity to label noise in overparameterized models, and instances where increasing model scale does not necessarily enhance performance.

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MS157

VC-Theoretical Explanation of Double Descent

In spite of growing practical success of Deep Learning (DL) networks, their theoretical understanding remains limited. Such a lack of scientific understanding of inductive inference, dating back to Fishers (1935) paper, brings up multiple new theories that aim to explain various data-analytic heuristic methods. In particular, a recent phenomenon, known as double descent, discovered by DL practitioners, appears to contradict statistical bias-variance tradeoff. However, we show that double descent phenomenon is in perfect agreement with classical VC theory, that explains generalization of all methods based on minimization of training error. In particular, this theory explains both first and second descent regime, corresponding to under and over-parameterized estimators. Proposed conceptual and theoretical explanation is supported by empirical modeling of double descent curves using analytic VC bounds, under standard classification setting. Finally, we discuss methodological reasons for misunderstanding of VC theoretical concepts, such as VC dimension and Structural Risk Minimization (SRM), in statistical and machine learning research communities.

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MS157

Low Rank Structure and Double Descent

This talk considers linear regression with data that have a spiked covariance where the largest eigenvalue is allowed to go to infinity. We show that such models also exhibit double descent but the location of the peak of moves away from the interpolation point. Comparing this with standard double descent, we determine spectral properties that govern the location of the peak. Additionally, we also look at conditions for when such models exhibit benign overfitting.

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MS158

Modeling the Winter Tick Epizootic in Moose

Changing climatic conditions have increased the severity of winter tick (*Dermacentor albipictus*) parasitism of moose (*Alces alces*). We present two models of these dynamics, the first being a simplified, analytical model and the second being a more realistic, numerical model. Using the first model, we found a necessary and sufficient condition relating the reproductive rate of moose and the tick parasitism rate for the moose population to extirpate or persist. As changing climatic conditions are resulting in longer tick questing periods and increased tick reproduction, we also use this model to compare under what combination of these 'season' lengths the moose population will extirpate or persist. Using the second numerical model, we compare under what combination of tick reproduction and tick parasitism rates the moose population will extirpate or persist. We also investigate the effectiveness of mitigating the effects of tick parasitism by hunting, the most widely employed conservation effort at this time, by predicting the effects of different hunting rates at different times of year on the minimum and maximum moose herd sizes. We conclude that changes in season length can lead to local extirpations. However, reducing tick reproduction or tick survival and harvesting moose can stabilize moose populations.

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MS158

Coarse-Graining a Model for the Inside Dynamics of a Structured Population During Expansion

Understanding the expansion of structured cell populations requires bridging the gap between microscopic stochastic models and macroscopic continuum descriptions. This talk presents a systematic coarse-graining approach to derive a population-level model that captures the key dynamics of structured cell migration during invasion. Starting from an individual-based framework that incorporates stochastic processes such as proliferation and movement, we develop a coarse-grained model that describes the evolution of the populations density over time. This macroscopic formulation allows us to investigate how internal population dynamics shape invasion patterns. By analyzing traveling wave solutions, we highlight how different factors influence the speed and structure of the advancing front. Our findings provide insights into how collective invasion is governed in biological processes such as tumor progression and tissue regeneration.

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MS158

Parameter-Varying Models for Hybrid Promoters in Bacterial Genetic Circuits

Bacterial gene expression is often modeled using ordinary differential equations. These models contain unknown parameters which are estimated by fitting models to experimental data. Naturally, the resulting parameter estimates have uncertainty which can be quantified in several ways, each with their own tradeoffs. Our aim is to quantify both parameter and prediction uncertainties during the process

of model validation assuming time-dependent model characteristics and time-varying nonlinear models for genetic circuits with time-series biological data from our novel library of promoters. Different types of promoters exist such as one that encodes for gene activation while the cell population is in growth phase, and one for gene activation during stationary phase. We have stitched together a growth phase promoter and a stationary phase promoter to create a hybrid promoter, implying that it should exhibit different types of gene expression during the cell populations life cycle. We then created several mutated variants of this promoter to create a library of hybrid promoters in which each hybrid promoter has distinct gene expression profiles during the 2 targeted phases of the life cycle. Once we have our hybrid promoter library, we explore the parameter and prediction uncertainties associated with these promoters in different genetic circuit contexts.

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MS158

Data Assimilation for Estimating Change Points of Time-Varying Reproduction Numbers

The time-varying basic reproduction number, $R_0(t)$, is a key epidemiological metric that quantifies the transmissibility of an infectious pathogen at time t. Accurate estimation and uncertainty quantification of $R_0(t)$ are crucial for understanding disease dynamics and informing public health decision-making. In this study, we evaluate the performance of five methods for estimating $R_0(t)$ using synthetic data generated from a stochastic SIR model with imposed changes to pathogen transmissibility and empirical COVID-19 case data. The methods include ensemble filter methods and inflation techniques, which are employed to mitigate covariance underestimation and filter divergence. We compare the Ensemble Adjustment Kalman Filter (EAKF) with no inflation, fixed inflation, and adaptive inflation, the Ensemble Square Root Smoother (EnSRS) with adaptive inflation, and EpiEstim. Our results demonstrate that the EAKF and EnSRS methods with adaptive inflation outperform other approaches in accurately estimating $R_0(t)$, particularly in scenarios with abrupt changes in transmission rates. The adaptive inflation techniques effectively address the challenges of covariance underestimation and filter divergence, leading to more robust and reliable estimates of $R_0(t)$. These findings highlight the potential of adaptive inflation methods for improving the accuracy of time-varying parameter inference, ultimately contributing to more effective public health responses.

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MS159

Featurizing Koopman Mode Decomposition with Learned Distances

We introduce Featurized Koopman Mode Decomposition (FKMD), an integrated method for choosing KMD features using a learned Mahalanobis distance on a delay embedded space. The method is inspired by the recent observation that the outerproduct of the weights of a fully trained neural network agree with the average gradient outerproduct (AGOP) of the underlying interpolant (Mechanism for feature learning in neural networks and backpropagation-free machine learning models, Radhakrishnan et al., 2024). The Mahalanobis distance aids in featurizing KMD in cases where good features are not a priori known. We show that FKMD improves predictions for a high-dimensional linear oscillator, a high-dimensional Lorenz attractor that is partially observed, and a cell signaling problem from cancer research.

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MS159

Dynamical-adapted Regularization for Autoencoder with the Observed SDE Dynamics

We propose two dynamical adapted regularization terms to improve the accuracy and generalization of learning stochastic dynamics on the manifold. We assume an SDE solver is available and one has access to estimates of the extrinsic dynamical quantities such as the point on manifold with its associated drift vector field and covariance matrix. We add two regularization terms inspired from Itô formula and Manifold, to the AE loss. We will demonstrate with these two regularization terms, the learnt dynamics generalize better with benchmark examples.

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MS160

Using Spotlights to Search a Network

The spotlights game (also called the Hunter-Rabbit game) is a pursuit evasion game played on a graph, where a set of pursuers (hunters) search for an invisible evader (the rabbit). On the pursuers' turn, each pursuer selects a vertex to shine a spotlight on. If the evader is on this vertex, then they are detected, otherwise the pursuers receive no information. On the evaders turn, the evader must move from their current vertex to an adjacent vertex. The spotlight number of a graph G, denoted $s(G)$, is the minimum number of pursuers required to win the game when the evader playes perfectly. This game models how to detect the current state of an updating process, in the worst possible case for the detectors. Versions of this game have been independently introduced by several groups. A notable example being an Olympiad problem, which asked the student to prove $s(P_n) = 1$ for all n. A particular focus as been given to trees, grids, as well as the relationship between $s(G)$ and graph parameters such as treewidth and pathwidth. Extending this work, for all minor closed

classes $\mathcal{H}$, we determine an asymptotic characterization of the maximum $s(G)$ over all n-vertex graphs $G \in \mathcal{H}$. We also consider this problem for graph classes not closed on minors. Joint work with Ben Seamone (Dawson College).

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MS160

Signal Processing on Graphs Using Graphons

Many processes on graphs can be modelled through graph signals. Signals can represent measurements in a sensor network, congestion in a traffic network, or activity levels in regions of the brain. Analysis of such signals can allow us to detect noise, trends, missing data, etc. An important tool in graph signal processing is the graph Fourier transform (GFT). However, the GFT can be highly sensitive to changes in the graph. I will describe recent work on a GFT framework for an entire class of graphs with similar structure. The framework is derived from a graphon, a limit object of sequences of similarly structured graphs. This is joint work with Kathryn Beck, Mahya Ghandehari, Nauzer Kalyaniwalla, and Silo Murphy.

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MS160

Quantum Walks in Quantum Computation

A network of interacting qubits (usually subatomic particles) can be modelled by a connected weighted undirected graph G. The vertices and edges of G represent the qubits and their interactions in the network, respectively. The propagation of quantum states in G determines what is known as a (continuous) quantum walk. This quantum walk is completely described by a unitary matrix obtained from exponentiating a Hermitian matrix associated with G (usually the adjacency matrix of G). Quantum walks that manifest certain properties are desirable for transmitting quantum information. For example, the accurate transmission of quantum information is instrumental in the construction of operational quantum computers, while the generation of entanglements amongst multiple qubits speeds up quantum algorithms. In this talk, we survey the most recent breakthroughs in the study of continuous quantum walks, with emphasis on the role of underlying graph describing the spin network. This is a joint work with Dr. Sarah Plosker (Brandon University) and Dr. Steve Kirkland (University of Manitoba).

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MS161

Analysis of Some Non Linear Quasi-interpolation Strategies

In this presentation, we introduce new techniques for quasi-interpolation using nonlinear strategies to handle discontinuities in data across one or multiple dimensions. The key innovation is applying non-linear weights to quasi-interpolators of the form,

$$\mathcal{Q}(f) = \sum_{i=1}^{N} L_i(f) a_i(\mathbf{x}),$$

where L_i, a_i, or both form a partition of unity. We explore techniques to adapt data reconstruction, particularly for multivariate data and discontinuities along interfaces, and for mesh-free algorithms. We analyze the schemes' numerical properties, such as smoothness, accuracy near discontinuities and at smooth zones, and elimination of the Gibbs phenomenon. Numerical experiments in one, two, and three dimensions validate our theoretical findings.

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MS161

A Highly Efficient Finite Difference-Based PML Technique for Acoustic Scattering Problems

In this talk, we present a highly efficient perfectly matched layer (PML) technique for solving a two-dimensional Helmholtz equation in an unbounded domain with bounded scatterers. Conventional PML and its alternative, the perfectly absorbing layer (PAL) method, often require either increasing the layer width or handling nearly singular (or singular) differential equations to maintain theoretical accuracy. Our approach mitigates these issues by introducing a suitable compression transform, enhancing both efficiency and numerical stability. Moreover, the transformed equation retains a simple form, which allows us to apply the optimal sixth-order compact finite difference scheme. The efficiency and robustness of our method are demonstrated across diverse scenarios.

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MS161

Solving Nonlinear Two-Phase Problems with Monotonicity Formulas

After briefly introducing the two-phase free boundary problem, I am going to present a new version of the Alt-Caffarelli-Friedman monotonicity formula. The formula will then be applied to the existence and regularity theory of a solution of the two-phase problem. These topics reflect the recent joint research in the two-phase problem with David Patwin.

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MS162

Reduced Order Modeling in Forward and Inverse

Problems with the Distributed Fractional Derivative

Fractional time derivative operators are successfully used to model anomalous diffusion processes and the power-law attenuation of compressional and shear waves propagating in viscoelastic microstructured media and materials with memory. The order of the fractional derivative is related to the characteristic time scales; in multiscale media, the processes can occur at several (or continuously varying) time scales. Problems with continuously changing time scale can be formulated using the distributed fractional derivative operator. The talk discusses the attenuated wave equation and the inverse problem of identification of the distributed Caputo fractional time derivative. An efficient reduced order modeling numerical method for its solution is presented.

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MS163

Analysis of Continuous Data Assimilation with Large (or Even Infinite) Nudging Parameters

This talk considers continuous data assimilation (CDA) in partial differential equation (PDE) discretizations where nudging parameters can be taken arbitrarily large. We prove that solutions are long-time optimally accurate for such parameters for the heat and NavierStokes equations (using implicit time stepping methods), with error bounds that do not grow as the nudging parameter gets large. Existing theoretical results either prove optimal accuracy but with the error scaled by the nudging parameter, or suboptimal accuracy that is independent of it. The key idea to the improved analysis is to decompose the error based on a weighted inner product that incorporates the (symmetric by construction) nudging term, and prove that the projection error from this weighted inner product is optimal and independent of the nudging parameter. We apply the idea to BDF2-finite element discretizations of the heat equation and NavierStokes equations to show that with CDA, they will admit optimal long-time accurate solutions independent of the nudging parameter, for nudging parameters large enough. Several numerical tests are given for the heat equation, fluid transport equation, NavierStokes, and CahnHilliard that illustrate the theory.

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MS163

Some Principles and Rigorous Results for State and Parameter Reconstruction for Nonlinear PDEs

We will discuss some recent breakthroughs in the mathematical study of state and parameter reconstructions in the nonlinear PDEs. In particular, we will identify some unifying principles that allow one to define algorithms that leverage knowledge of the model with partial observations of its state with which one can provably guarantee convergence to the unknown state and parameters. This will be done in the context of hydrodynamic equations.

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MS163

Modelling the Nonlinear Richards Equation with Continuous Data Assimilation

Continuous data assimilation, which was introduced by Azouani, Olsen, and Titi in 2014, is a computationally-efficient algorithm that has been shown analytically and computationally to recover the true solution for a wide variety of regimes exponentially fast in time, in addition to being robust with respect to noisy data, stochastic forcing, and errors in parameters. In this talk, we will apply continuous data assimilation to the Richards equation, a nonlinear system that models fluid flow in unsaturated soil. We will examine convergence of the AOT approach numerically and analytically, assuming unknown initial data and sparse-in-time-and-space observations.

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MS164

RR-Type Identities from Zeta Functions over Quadratic Orders

We investigate a certain module-counting zeta function over quadratic orders, resulting in formulas involving infinite multi-sums. It turns out that certain specializations of the multi-sums are summable to infinite products, which amounts to new Rogers–Ramanujan type identities. Our recipe also gives a finitization of the multi-sum, which is instrumental in the proof of the identities.

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MS164

Hankel Determinants and Big q-Jacobi Polynomials for Q-Euler Numbers

The q-analogs of Bernoulli and Euler numbers were introduced by Carlitz in 1948. Similar to recent results on the Hankel determinants for the q-Bernoulli numbers established by Chapoton and Zeng, we perform a parallel analysis for the q-Euler numbers. It is shown that the associated orthogonal polynomials for q-Euler numbers are given by

a specialization of the big q-Jacobi polynomials, thereby leading to their corresponding Jacobi continued fraction expressions, which eventually serve as a key to our determinant evaluations.

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MS164

Diagonal and Constant Term Representations of Sequences

Many sequences in combinatorics and number theory can be represented as constant terms of powers of multivariate Laurent polynomials and, therefore, as diagonals of multivariate rational functions. On the other hand, it is an open question, raised by Don Zagier, to classify those diagonals which are constant terms. We provide such a classification in the case of sequences satisfying linear recurrences with constant coefficients. Various related examples, applications and open problems will be given as time permits. This talk is based on joint work with Alin Bostan and Sergey Yurkevich.

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MS165

On a New Symmetry in Splitting Methods

Splitting methods constitute a powerful tool for the numerical integration of differential equations, either arising directly from dynamical systems or from partial differential equations of evolution previously discretized in space. Efficient high-order schemes have been designed that provide accurate solutions whilst preserving some of the most salient qualitative features of the system. The presence of negative coefficients in methods of order greater than two, however, restricts their application to, e.g., equations defined in semigroups, thus motivating the exploration of splitting methods with complex coefficients with positive real part. Among them, we will present and analyze a new class of schemes which exhibit a good long time behavior when applied to linear unitary and integrable linear Hamiltonian systems. Some of the new methods show better efficiency than state-of-the-art splitting methods with real coefficients for several classes of problems. This work is done in collaboration with Joackim Bernier (Nantes), Sergio Blanes (Valencia) and Alejandro Escorihuela-Tomàs (Castellón).

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MS165

A Numerical Technique for Analyzing Critical Domains in Coupled Quenching Problems

In this talk, we introduce a coupled-parabolic quenching problem within square domains. The size of the critical domains depends on the existence of a steady-state solution. The integral solution is represented in terms of Greens function and a conformal mapping is employed to transform the square domain into a circle. Our objective is to numerically determine the critical domains associated with this problem.

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MS165

Novel Machine Learning Investigation to the Mathematical Fractional Model Analysis Breast Cancer and Chemotherapy Heart

The world's second-most common cause of death for women is breast cancer. Cancer can be treated by removing cancer cells surgically, killing them, or stopping them from receiving the signal necessary for cell division. Patients who receive cancer treatment may not always have beneficial effects. Treatment for breast cancer can affect the cardiovascular system. We created a fractional mathematical model. The model is built using a set of fractional differential equations. We used a modified ABC-fractional order to explain the fractional breast cancer model. A population is subdivided into five subsets. Stages include 1 and 2 (A), 3 and 4 (B), disease-free (D), and cardiotoxic (E). We have demonstrated the existence, uniqueness, and positivity of model simulation. We run simulations and use neural networks to provide a graphical comparison study and validate the numerical simulation. The findings also show how various model parameters affect the system, offering greater insight and a more effective solution for real-world issues. The efficacy, stability, precision, dependability, and relevance of the proposed approach are confirmed by the error distribution using histograms, obtaining low MSE,RMSE, MAE,MAPE,NSE, absolute error and linear regression outputs for the breast cancer model. We conclude with computational simulations that allow us to visualize our theoretical results.

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MS165

Artificial Neural Networks for the Epidemiological Analysis of Mumps Model Via Mittag-Leffler Kernel

This study develops a fractional-order mathematical model utilizing the fractal fractional Mittag-Leffler operator to analyze Mumps virus transmission. The model undergoes qualitative and quantitative assessments, emphasizing Ulam-Hyers stability, as well as the existence, uniqueness, and well-posedness of solutions, along with an analysis of disease-free equilibrium points and treatment sensitivity. Fixed-point theory ensures the constraints on solutions, while an advanced numerical approach highlights the significance of fractional dynamics. Simulations demonstrate convergent behavior across population classes, accurately capturing Mumps transmission. A comparative

study affirms the superiority of fractional-order modeling over integer-order approaches. Synthetic data generated using the Newton two-step solver with the Mittag-Leffler kernel are analyzed through a supervised learning framework utilizing artificial neural networks. The results from the neural network closely correlate with numerical findings, presenting minimal errors validated through convergence metrics and regression outputs. This framework offers a robust methodology for the epidemiological analysis of Mumps virus dynamics.

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MS166

Modeling the Effect of the Immune System on a Wound

A wound is a depletion of the integrity of living tissue in the body. The mechanisms in which the body repairs a wound are organized into the overlapping stages of wound healing, namely, homeostasis, inflammation, proliferation, and remodeling. Within minutes blood clots are formed and the bleeding stops. This is the first provisional matrix formed for the wound while the focus of the mechanisms implemented will be to remove pathogens and debris in the inflammation stage. The turnover of the provisional matrix proceeds in the proliferation and remodeling stages. Elucidating mechanisms in wound healing is of interest in improving wound care and determining causes of diseases. Mathematical modeling provides a means to help provide framework and implement theories that may not be feasible to test under experimentation. An ordinary differential equation mathematical model of the inflammation stage is constructed incorporating pathogens, debris, apoptotic neutrophils, classically activated macrophages, and alternatively activated macrophages. A representative set of parameters for this model is found based on output dynamics and parameter restrictions based on literature. Do not include keywords, references or citations separately at the end of the abstract. All citations must be within the abstract text in general form "[Authorname, Title, etc]." Improper citations will be deleted.

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MS166

Efficient Numerical Solutions of Laplace Equations with Mixed Boundary Conditions Using Steklov Eigenfunctions

This talk presents the Steklov expansion method as a solution technique for mixed boundary value problems. By solving corresponding Steklov eigenvalue problems, we derive approximations to the solutions of the Laplace equation for different boundary conditions. These approximations, based on Steklov eigenfunctions, are subsequently used to compute physical capacitances with high precision. Beyond offering accurate capacitance estimations, the Steklov expansion method also includes an error analysis grounded in Steklov eigenvalues. The presentation will feature numerical experiments that highlight the method's effectiveness and practical application.

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MS166

Averaging in a Certain Almost Hamiltonian System with Singularities

In this talk I will present an averaging theorem for a fully coupled system with singularities. Specifically, I will discuss a particular fast-slow system that arises in modeling energy transport in an open system of interacting hard-spheres. The technical part of this work addresses how to deal with singularities of the dynamics and the fact that the dynamics is fully coupled.

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MS166

Exterior Finite Energy Harmonic Functions

We introduce a *finite energy space* $E^{1,p}(U)$, where $U \subsetneq \mathbb{R}^N$ is an exterior region having compact, Lipschitz boundary ∂U, with $N \geq 3$ and $p \geq 1$. Functions in $E^{1,p}(U)$ are only required to *decay at infinity* in a broad measure-theoretic sense and be L^p-integrable of their weak gradients; moreover, mild locally integrable conditions are assumed. When $p = 2$, denote $E^1(U) = E^{1,2}(U)$, which is a real Hilbert space with respect to the gradient L^2-inner product. Note $H^1(U) \subsetneq E^1(U)$. The harmonic Dirichlet-Poisson as well as Neumann and Robin problems are well-posed in $E^1(U)$. In addition, using the exterior harmonic Steklov eigenvalues and an associated family of eigenfunctions, spectral representation of solutions of these harmonic boundary value problems is given, and the exterior Poisson's kernel is described. In addition, a reproducing kernel of the harmonic subspace $\mathscr{H}(U)$ of $E^1(U)$ as well as the capacity may be described explicitly in terms of those Steklov eigenvalues and an associated eigenfunctions. This is joint work with Professor Giles Auchmuty and partially supported by NSF-DMS11008754.

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MS167

A Risky Business: Filling Prescriptions at the Pharmacy

Pharmacists are allowed to refuse to fill a prescription. This is by design, likely to thwart drug abuse rings. How-

ever, there are instances of pharmacists who refuse to fill prescriptions connected to reproductive care and to gender-affirming care, based simply on religious or ethical reasons. This can be detrimental to people, especially in regions of the country in which there is only one pharmacy for lengthy distances. Thus, its important for people to be informed how likely a particular pharmacy is to refuse their prescription and to plan accordingly. In this presentation, I will describe the data collection my research team is undertaking in order to help share this pertinent information with the public, and the challenges involved. Moreover, I will describe the goal of the overall project.

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MS167

Data to Impact: Advancing Equity and Inclusion Through Action

Today's world recognizes that data fuels technological advancement, and artificial intelligence plays a crucial role in driving progress across various sectors, including education and economic development. However, do these advancements foster true inclusiveness and equity? The answer depends on educators and practitioners. This talk will explore how findings from the study "Gender Equality in the STEM Workforce: A Survey-Based Approach" have led to measurable actions to enhance inclusion and equity. By analyzing challenges, designing curriculum, and collaborating with industries, we can drive meaningful change to ensure broader representation in the rapidly evolving era of generative AI.

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MS168

Comparison of Structure Preserving Discretizations for the Nonlinear Schrodinger Equation with Applications to Nonlinear Optics

In this talk, we discuss a variety of efficient structure preserving numerical methods for the nonlinear Schrodinger equation (NLS) that naturally capture the inherent physical aspects of the problem under consideration. The NLS is a dispersive wave equation and its solutions satisfy properties such as mass and energy conservation. We compare a variety of classical methods such as finite difference schemes, operator splitting techniques, among others, based on whether they do or do not preserve mass and energy conservation, among other properties, in the discrete grid. We also consider the recent development of Physics Informed Neural Networks (PINNs) and in particular structure preserving PINNs for the numerical discretization of the NLS, and compare the performance of these methods to the classical numerical schemes. Finally, we consider the application of these methods and their advantages and disadvantages to the area of nonlinear optics, the branch of optics that describes the behavior of light in nonlinear media.

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MS168

Mixed Model Runge-Kutta Methods and Efficient Correction Approaches

We analyze mixed precision and mixed model Runge–Kutta additive (MP-ARK) methods that reduce the cost of the computationally expensive implicit stages in the Runge–Kutta methods by employing a cheaper low-precision or low-order model computation. The explicit stages are then performed using a high-precision or high-order model computation, providing a correction to the implicit stages. Our research focuses on several questions related to mixed model computations, including: What stability properties must the low- and high-order models satisfy for the mixed model to remain stable? How do the correction terms affect the stability of the mixed model? Can an alternative type of correction be designed to enhance the stability of the corrected mixed model method? To address these questions, we propose different correction strategies and present numerical experiments.

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MS168

Flows Through Permeable Membranes Using the Method of Regularized Stokeslets

Microscale flows through permeable membranes are ubiquitous in many biological and environmental systems, yet these types of flows are often computationally challenging to model. One approach is to use the Method of Regularized Stokeslets (MRS) to model the effect of boundary forces, and source/sink pairs to model the permeability of the boundaries that contain porous membranes. We extend this approach to handle permeable membranes for various types of fluid-structure problems. We focus on model validation, convergence analysis, selection of numerical parameters, volume conservation, and extensions to applications in three dimensions. Results will be presented in the context of flows through channels with permeable boundaries and permeable membranes under tension.

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MS168

A Novel Hybrid Low Rank Nodal Discontinuous Galerkin Method for the Boltzmann BGK Equation

The Boltzmann equation is a PDE that describes the dynamical evolution of the particle distribution function (PDF) in the six-dimensional position-velocity phase space. The equation, when solved on a grid poses immense challenges due to the curse-of-dimensionality. In this talk, we will present advances in a novel hybrid Discontinuous Galerkin (DG) and Low-Rank approximation method for the Boltzmann BGK equation. This approach aims to reduce computational costs and memory usage while maintaining solution fidelity. It leverages nodal DG discretization for the physical space variables, exploiting the method's flexibility across different geometries, and employs Low-Rank tensors for the velocity space variables to compress the PDF. We will also discuss numerical experiments that demonstrate the strengths and limitations of our solver.

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MS169

Kraus Is King: High-Order Completely Positive and Trace Preserving (cptp) Low Rank Method Open Quantum Computing Systems

We design high order accurate methods that exploit low rank structure in the density matrix while respecting the essential structure of the Lindblad equation. Our methods preserves complete positivity and are trace preserving.

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MS169

Structure-preserving High Order Low Rank Scheme for the Lindblad Quantum Master Equation

We investigate the simulation of open quantum systems governed by the time-dependent Lindblad equation, focusing on the development of accurate, efficient and structure preserving numerical methods. Specifically, we propose a low-rank framework that achieves arbitrary-order accuracy through a Nested Picard Iteration scheme. Moreover, the structure preserving (completely definiteness and unit trace) is achieved via the design of the scheme into the Kraus form. Our approach leverages the low-rank structure often present in the density matrix of open quantum systems, enabling computational savings.

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MS169

A Primer on Electronic Structure Theory

What is quantum computing useful for? The strongest case is leaning increasingly towards electronic structure theory, which is the computationally intensive part of modeling molecules, materials, and quantum devices themselves. This theory will likely play two key roles in quantum computing. First, it will be a major source of open problems for algorithmic development. Second, it can be the foundation for more accurate models of quantum devices. This talk will illustrate a few remarkable methods in electronic structure theory developed in the last century. Then I will discuss what comes out if we put one of these methods on IBM Q System ONE for 24 hours.

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MS169

Enhanced Quantum Characterization Via Entropic Optimal Transport-Driven Gibbsian Inference

In this talk, I will present a robust Bayesian-type framework for uncertainty quantification in quantum computing, designed to address the challenges posed by noisy, complex quantum systems. The proposed method integrates Gabbsian inference with a low-rank approximation of the entropic-regularized optimal transport distance, yielding a stable and computationally efficient alternative to conventional Bayesian approaches. I will highlight the methods robustness and discuss its application to characterizing uncertainty in a transmon quantum device using experimental data. Comparative results with standard Bayesian techniques will also be presented. This work is part of a larger ongoing project on quantum characterization, control, and computation, conducted in collaboration with Dr. Gabriel Huerta (Sandia National Laboratories) and PhD candidate Serafina Middleton (University of New Mexico).

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MS173

Learning Gray Swan Weather Extremes From Data: Generalization Versus Optimization Errors

AI weather models have shown remarkable skills in forecasting weather patterns, however, their skills for the rarest extreme events, the gray swans, remains unclear. In this presentation, we will first discuss some of the success and failures of AI models in forecasting gray swans. Then, we will investigate the underlying mechanisms for the success and failure, separating them into errors that stem from data imbalance (generalization error) and spectral bias (optimization error). We will specifically discuss the role of optimization error in the performance of these models.

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MS173

Generalized Aliasing Explains Double Descent and Informs Model Design

Over-parameterized models exhibit counterintuitive behaviors, such as double descent, in which models of increasing complexity exhibit decreasing generalization error. Other models may exhibit more complicated patterns of predictive error with multiple peaks and valleys. Neither double descent nor multiple descent phenomena are well explained by the traditional bias-variance decomposition. We introduce a new decomposition that we call the *generalized aliasing decomposition* (GAD) to explain the relationship between predictive performance and model complexity. The GAD decomposes the predictive error into three parts: 1.) *model insufficiency*, which dominates when the number of parameters is much smaller than the number of data points, 2.) *data insufficiency*, which dominates when the number of parameters is much greater than the number of data points, and 3.) *generalized aliasing*, which dominates between these two extremes. The GAD is helpful in diverse applications, including random feature models from machine learning, Fourier transforms from signal processing, solution methods for differential equations, and predictive formation enthalpy in materials discovery. Moreover, key components of the GAD can be explicitly without seeing any data labels, so it can answer questions related to experimental design and model selection *before* collecting data or performing experiments.

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MS173

A Unified Stability Analysis of SAM vs SGD: Role of Data Coherence and Emergence of Simplicity Bias

Understanding the dynamics of optimization algorithms in deep learning has become increasingly critical, especially as models grow in scale and complexity. Despite the empirical success of stochastic gradient descent (SGD) and its variants in finding solutions that generalize well, the precise mechanisms underlying this generalization remain poorly understood. A particularly intriguing aspect of this phenomenon is the bias of optimization algorithms towards certain types of minimaoften flatter or simplerespecially in

overparameterized regimes. While prior works have associated flatness of the loss landscape with better generalization, tools to mechanistically connect data, optimization algorithms, and the nature of the resulting minima are still limited. For instance, methods like Sharpness-Aware Minimization (SAM) have shown practical gains by explicitly promoting flatness, but lack a unified theoretical framework explaining their influence across different data structures and model architectures. In this work, we introduce a comprehensive linear stability analysis framework to dissect the behavior of optimization algorithmsSGD, random perturbations, and SAMin neural networks, focusing particularly on two-layer ReLU models. Our approach is built upon a novel coherence measure that captures the interaction between data geometry and gradient similarity, providing new insights into why and how certain solutions are favored.

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MS173

A Look at the Impact of Double Descent on Scientific Models and Practice

Phenomena like double descent have challenged widespread intuitions about the relationship between a statistical models expressivity and predictive accuracy. In the context of science, models are used in many different ways: to summarize or infer parameters from data, or as simplified representations of the processes generating those data. The use of highly complex models has accelerated scientific discovery (e.g., in the context of 3D protein folding) and enhanced scientific understanding (e.g., insights from LLMs into the mechanisms of language acquisition). Yet the use of such complex models may appear to violate the scientific principle of model parsimony (Ockhams razor). In this talk, I will discuss the ways in which phenomena like double descent have the potential to also challenge intuitions about the relationship between a scientific models expressivity and its usefulness for the scientific community. I will discuss (i) the relationship between model expressivity, model parsimony, and model misspecification, and (ii) the ways in which expressive models can be more or less interpretable, effective in guiding new research, suitable for small and noisy datasets, and in alignment with scientists assumptions about the true data-generating process(es). Most of this talk is based on the paper Marina Dubova et al. Is Ockhams razor losing its edge? doi:10.1073/pnas.2401230121.

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MS174

Extreme Focusing Events in the Semiclassical Scaled Focusing NLS Hierarchy

Talanov [Talanov, *Self focusing of wave beams in nonlinear media*, JETP Lett. 2, 138-141, 1965] discovered a class of solutions of the dispersionless limit of the focusing nonlinear Schrdinger (NLS) equation that exhibit finite-time blowup. Recently, a special solution of the dispersive focusing NLS was identified that formally regularizes these blowup solutions [Suleimanov, *Effect of small dispersion on self-focusing in a spatially one-dimensional case*, JTEP Lett. 106, 400-405, 2017] which is related to the Painlevé III hierarchy. In this talk we will discuss recent work in which we approximate the Talanov blowup data by semiclassical soliton ensembles. These are sequences of exact, reflectionless solutions of focusing NLS defined for a decreasing sequence of values of the dispersion parameter which have the property that they are increasingly accurate approximations of the Talanov initial data as the dispersion parameter $\epsilon \downarrow 0$. We show rigorously that the soliton ensembles satisfy the dispersive regularization of blowup predicted by Suleimanov. Moreover, we show how this phenomena can be extended to the full focusing NLS hierarchy. The regularization of Talanov blowup results in solutions which exhibit local growth in amplitude scaling with ϵ^{-1} which distinguishes it from the typical gradient catastrophe described by Bertola and Tovbis.

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MS174

Utilizing Special Functions in the Study of Spectral Zeta Functions

Spectral zeta functions and zeta regularized functional determinants associated with differential operators will be discussed. In particular, we will illustrate how a contour integral representation involving a characteristic function (involving special functions in explicit examples) can be utilized to analyze the spectral zeta function. The structure of spectral zeta function becomes apparent when performing the analytic continuation from this integral representation, which involves the asymptotic analysis of the associated characteristic function. Examples will be included such as the Bessel and Legendre equations. This is based on multiple joint works with Christoph Fischbacher, Guglielmo Fucci, Fritz Gesztesy, Klaus Kirsten, and Mateusz Piorkowski.

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MS174

The Ultraspherical Rectangular Collocation Method and Its Convergence

This talk concerns the ultraspherical rectangular collocation (URC) method, a collocation implementation of the sparse ultraspherical (Gegenbauer) method of Olver & Townsend for two-point boundary-value problems. The URC method is provably convergent, the implementation is simple and efficient, and the modification of collocation nodes is straightforward. The convergence theorem applies to all boundary-value problems when the coefficient functions are sufficiently smooth and when the roots of certain ultraspherical polynomials are used as collocation nodes. We also adapt a theorem of Krasnolsel'skii et al. to our setting to prove convergence for the rectangular colloca-

tion method of Driscoll & Hale for a restricted class of boundary conditions.

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MS175

A Mesoscale Model of Active Colloid Motion

Active colloids exhibit enhanced diffusion compared to regular particles of the same size and have generated much interest for biomedical and materials science applications. A variety of mechanisms exist to produce this enhanced diffusion, such as micromechanical motors of micro-organisms and the chemically induced propulsion of Janus particles. Recently, a microscopic model of an isotropic colloid has also been demonstrated to achieve enhanced diffusion. We propose a mesoscale model for the enhanced diffusion of isotropic particles in order to extend the sampling regime accessible for a high-density system of active particles.

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MS175

Best of Both Worlds: Enforcing Detailed Balance in Machine Learning Models of Transition Rates

The slow microstructural evolution of materials often plays a key role in determining material properties. When the unit steps of the evolution process are slow, direct simulation approaches such as molecular dynamics become prohibitive and Kinetic Monte-Carlo (kMC) algorithms, where the state-to-state evolution of the system is represented in terms of a continuous-time Markov chain, are instead frequently relied upon to efficiently predict long-time evolution. The accuracy of kMC simulations however relies on the complete and accurate knowledge of reaction pathways and corresponding kinetics. This requirement becomes extremely stringent in complex systems such as concentrated alloys where the astronomical number of local atomic configurations makes the a priori tabulation of all possible transitions impractical. Machine learning models of transition kinetics have been used to mitigate this problem by enabling the efficient on-the-fly prediction of kinetic parameters. In this study, we show how physics-informed ML architectures can exactly enforce the detailed balance condition, by construction. We show that such ML architectures also exhibit superior performance in terms of prediction accuracy, demonstrating that the imposition of physical constraints can facilitate the accurate learning of barriers at no increase in computational cost.

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MS175

Stochastic Norton Dynamics: An Alternative Approach for the Computation of Transport Coefficients in Dissipative Particle Dynamics

We study a novel alternative approach for the computation of transport coefficients at mesoscales. While standard nonequilibrium molecular dynamics (NEMD) approaches fix the forcing and measure the average induced flux in the system driven out of equilibrium, the so-called "stochastic Norton dynamics' instead fixes the value of the flux and measures the average magnitude of the forcing needed to induce it. We extend recent results obtained in Langevin dynamics to consider the generalisation of the stochastic Norton dynamics in the popular dissipative particle dynamics (DPD) at mesoscales, important for a wide range of complex fluids and soft matter applications. We demonstrate that the responses profiles for both the NEMD and stochastic Norton dynamics approaches coincide in both linear and nonlinear regimes, indicating that the stochastic Norton dynamics can indeed act as an alternative approach for the computation of transport coefficients, including the mobility and the shear viscosity, as the NEMD dynamics. In addition, based on the linear response of the DPD system with small perturbations, we derive a closed-form expression for the shear viscosity, and numerically validate its effectiveness with various types of external forces. Moreover, our numerical experiments demonstrate that the stochastic Norton dynamics approach clearly outperforms the NEMD dynamics in controlling the asymptotic variance, a key metric to measure the associated computational costs.

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MS176

Information Diffusion on Complex Networks: A Proportion Based Approach

When receiving new information we often are influenced by the opinions of our peers. This talk puts forward a new information diffusion model that considers the proportion of peer influence. Currently, we consider the implications of two-coloured information systems, where each node can only accept one of two colours, for example, political alignment in a two-party system, adopting a new software vs not, or choosing to believe a rumour. We discuss how the algorithm operates, how the properties of the seed nodes impact the overall outcome of the graph and how the algorithm's behaviour changes on a selection of popular complex network generation models. Particularly, we examine how the structure of the network models changes the efficiency of seed selection methods even when network properties such as size and clustering coefficient are standardized.

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MS176

A Data-Centric Approach to Pursuit-Evasion

Meyniel (1985) conjectured that the cop number of any connected graph G of order n is bounded by $O(\sqrt{n})$. In this talk, I discuss the process through which we identified key graph-theoretic properties that are most relevant to bounding the cop number such as genus, tree width, planarity, and minor-free graphs. We use computational methods alongside automated planning systems to filter out trivial Meyniel satisfiable graphs, allowing us to focus on more complex cases as we populate a database of structural graph properties. I will walk through the algorithm we developed, which processes graphs into NETWORKX objects, accumulates properties, and calculates the cop number using a PDDL planner (PLANNING DOMAIN DEFINITION LANGUAGE). Finally, I implement the back-propagation-based algorithm [Petr et. al (2022)] for computing the cop number more efficiently and compare its performance with an existing PDDL-based planner [Little (2024)]. I conclude by describing how these contributions inform our broader research direction.

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MS176

Zero-Forcing on Deterministic Complex Networks

In this talk, we explore zero forcing on deterministic complex network models. Zero forcing is a dynamic process on graphs, originally motivated by problems in quantum control and minimum rank. A currently blue node can force an adjacent node to turn blue if that node is the only adjacent non-blue node. The process begins with a set of forced nodes, called the forcing set, and iteratively experiences vertex forces. The minimum number of nodes required in an initial forcing set so that after a finite amount of time the entire graph is forced, is called the Zero Forcing number of the graph and denoted Z(G).

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MS177

On the Vems and Ifems: Spaces, Complexes and the Applications to Electromagnetic Interface Problems

Electromagnetic interface problems widely appear in a lot of engineering applications, such as electric actuators, invasive detection techniques and integrated circuit,which are typically described by Maxwell equations with discontinuous coefficients. Conventional finite element methods require a body-fitted mesh to solve interface problems, but generating a high-quality mesh for complex interface geometry is usually very expensive. Instead, using unfitted mesh finite element methods can circumvent mesh generation procedure, which greatly improves the computational efficiency. However, the low regularity of Maxwell equations makes its computation very sensitive to the conformity of the approximation spaces. This very property poses challenges on unfitted mesh finite element methods, as most of them resort to non-conforming spaces. In this talk, we will present our recent progress including several methods for this topic.

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MS177

High-order Schemes for Elliptic Interface Problem

The elliptic interface problem has piecewise smooth diffusion coefficients and source terms which are discontinuous across interface curves. Consequently, the exact solution u could be discontinuous across the interface and even if u is continuous, it has low regularity $u \in H^{1+\epsilon}(\Omega)$ with $\epsilon < 1/2$ due the second jump condition on flux. These impose challenges to traditional methods. All current known methods require complicated treatment along the interface and lack uniformly bounded condition numbers. For 2D elliptic interface problems, we first present sixth-order compact finite difference methods in rectangular or curved domains. Then we present a second-order wavelet method with proved convergence and uniformly bounded condition numbers. This talk is based on several joint work with Q. Feng, M. Michelle, P. Minev and J. Sim.

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MS177

Dispersion Correction Method for the Convected Helmholtz Equation

We are interested in solving numerically the convected Helmholtz equation

$$-\mathrm{div}(A\nabla u) - 2\imath\omega\mathbf{v}\cdot\nabla u - \omega^2 u = f \quad (1)$$

in a bounded domain $\Omega \subset \mathbb{R}^d$, $d \in \{1, 2\}$ equipped with adequate boundary conditions. It models the propagation of waves (in the time-harmonic regime) in a flow with a (normalized) velocity $\mathbf{v}$. The matrix $A := \mathrm{Id} - \mathbf{v}\mathbf{v}^T$ is then symmetric and positive definite. Discretizing such an equation suffers from dispersion errors due to the difference between the plane waves' velocities at the discretized and continuous levels (producing the pollution effect). Several studies on dispersion correction for the Helmholtz equation are available, but much fewer results are known for the convected Helmholtz equation. When the flow is constant, an idea is to use the equivalence between the classical Helmholtz equation and the convected one (due to

the Lorentz transformation) to design dispersion corrections. This surprisingly leads to a different correction than the one we get when constructing a correction directly for discretizations of equation (1). In this talk, we will first present our result in the 1D case to explain in detail the idea, and then explain the extension to the 2D case. Also, the more challenging situation of non constant flow will be discussed. The results will be illustrated with several numerical examples.

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MS177

FFT-accelerated High Order Finite Difference Methods and Their Hybridization with Neural Networks for Elliptic Interface Problems

In this talk, we will introduce an augmented matched interface and boundary (AMIB) method for solving elliptic interface problems. By effectively generating fictitious values needed in fourth order central difference approximations, the AMIB method is able to not only treat various jump conditions and boundary conditions, but also handle complicated geometries, including corner treatments. By using fictitious values to reconstruct Cartesian derivative jumps as auxiliary variables in an augmented formulation, the fast Fourier transform (FFT) algorithm will not sense the solution discontinuities, so that the discrete Laplacian can be efficiently inverted in the fourth order AMIB method. Recently, we have developed a hybrid method that integrates machine learning techniques into fast Poisson solvers for solving a simple elliptic interface problem. A neural network, trained on jump conditions, is constructed to directly predict Cartesian derivative jumps for correcting finite difference approximations. This hybrid approach extends the capabilities of AMIB methods by efficiently addressing interfaces with geometric singularities through its mesh-free neural network framework. The resulted finite difference method is not only easy to implement but also achieves fourth-order accuracy and FFT efficiency.

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MS180

Capillary-Driven Flows in Partially-Saturated Porous Materials

We examine a class of problems related to capillary rise in porous media. We focus our mathematical modeling attention on the particular case of rigid and partially-saturated porous materials. We outline a free-boundary model based on Richards' equation and show how predictions of this model compare well with experimental data for both early time dynamics and long time dynamics. We exploit these computations to understand characteristics of the capillary pressure and permeability throughout the partially-saturated region.

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MS180

Simulation of PDE-Modeled DNA Origami Signaling

DNA origami nanostructures have shown great promise in revolutionizing diagnostic testing, enabling the development of inexpensive and portable biosensors with a very low limit of detection that are capable of providing point-of-care diagnostics within minutes. Such nanostructures that contort upon binding an analyte have demonstrated unique promise, as they emit strong electrochemical signaling that may be efficiently measured in the form of capacitance. This talk will discuss the numerical approximation of the electrochemical signaling,so as to facilitate the pursuit of optimal nanostructure design and device uncertainty quantification. A set of partial differential equations that model the electro-diffusion of electrolytes together with motion of the DNA nanostructure in response to an applied field is presented. Finite difference methods are developed to solve the established model and overset grid techniques are utilized to resolve the nanostructure within the computational domain. Theoretical and numerical analysis confirm the accuracy and stability of the methods. Models inform expected capacitance time series and motivate further development.

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MS180

Mechanopathology of Esophageal Motility Disorders

Esophageal motility disorders are pathological conditions characterized by abnormally shaped deformations of the esophagus; examples include achalasia, diffuse esophageal spasm, and corkscrew esophagus. Their etiology is uncertain, but they are hypothesized to be due to the interplay of tissue hypertrophy, elastic remodeling, and muscular contraction. We use a mathematical framework based on perturbation of the equations of nonlinear solid mechanics to identify and analyze bifurcations that represent mechanical instability. Certain kinds of growth deformations and active stress patterns are found to cause buckling, which may explain the origin of the unusual shapes and help predict the onset of disease. Through our work, we uncover universal properties of instabilities in organs and tissues that could inform broader applications in tissue engineering and regenerative medicine.

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MS180

Two-Dimensional Foams and Coagulation Equations with Reaction Costs

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 several 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. Here, clusters A_n of size n obey the simple second order reaction $A_i + A_j \rightharpoonup A_{i+j}$, and under a multiplicative reaction rate cause gelation, or the creation of an infinite sized cluster. For edge rupture, we typically find the reaction $C_i + C_j \rightharpoonup C_{i+j-4}$, with C_n denoting a cell with n sides. The corresponding kinetic equations also have a collision kernel which is approximately multiplicative. In this talk, we will study generalized kinetic models for the reaction $S_i + S_j \rightharpoonup S_{i+j-\phi}$, where ϕ is a constant, positive reaction cost. Unlike Smoluchowski's model, for gelation to occur under reaction costs it must happen before a finite exhaustion time of the system. We prove necessary and sufficient conditions for gelation with reaction costs, using methods from generating functions and Laplace transforms.

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MS181

Adaptive Parameter Selection in Nudging Based Data Assimilation

Data assimilation combines (imperfect) knowledge of a flows physical laws with (noisy, time-lagged, and otherwise imperfect) observations to produce a more accurate prediction of flow statistics. Assimilation by nudging (from 1964), while non-optimal, is easy to implement and its analysis is clear and well-established. Nudgings uniform in time accuracy has even been established under conditions on the nudging parameter and the density of observational locations, , Larios et al. (2019). One remaining issue is that nudging requires the user to select a key parameter. The conditions required for this parameter, derived through priori (worst case) analysis are severe (Section 2.1 herein) and far beyond those found to be effective in computational experience. One resolution, developed herein, is self-adaptive parameter selection. This report develops, analyzes, tests, and compares two methods of self-adaptation of nudging parameters. One combines analysis and response to local flow behavior. The other is based only on response to flow behavior. The comparison finds both are easily implemented and yields effective values of the nudging parameter much smaller than those of priori analysis.

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MS181

Accelerating the Incremental Picard Yosida Iteration for the NSE Using CDA

Recent research has shown that continuous data assimilation (CDA) style nudging can accelerate and enable convergence of the Picard iteration for the steady Navier-Stokes equation, as it scales the linear convergence rate by $H^{1/2}$ where H is the characteristic spacing of the known solution data. We consider how CDA will affect a more efficient type of Picard iteration constructed using a Yosida algebraic splitting and an incremental formulation together with grad-div stabilization. We find that although the analysis was much more involved than for usual Picard, this same $H^{1/2}$ scaling of the linear convergence rate is recovered. Several numerical tests illustrate the theory.

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MS181

Advancing Nonlinear Iterative Solvers for Navier-Stokes Equations Through Data-driven Assimilation Strategies

In this talk, we investigate enhancements to nonlinear iterative solvers for the NavierStokes equations in contexts where data measurements or solution observations are available. We develop modified iterations that apply continuous data assimilation (CDA) techniques, incorporating existing data into the solvers through various nudging strategies. These approaches enable data integration through multiple mechanisms, leading to improved performance and enhanced convergence properties compared to conventional iterative nonlinear solvers.

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MS181

Model Discovery on the Fly Using Continuous Data Assimilation

We review an algorithm developed for parameter estimation within the Continuous Data Assimilation (CDA) approach. We present an alternative derivation for the algorithm presented in a paper by Carlson, Hudson, and Larios (CHL, 2021). This derivation relies on the same assumptions as the previous derivation but frames the problem as a finite dimensional root-finding problem. Within the approach we develop, the algorithm developed in (CHL, 2021) is simply a realization of Newton's method. We then consider implementing other derivative based optimization algorithms; we show that the Levenberg Maqrquardt algorithm has similar performance to the CHL algorithm in the single parameter estimation case and generalizes much better to fitting multiple parameters. We then implement these methods in three example systems: the Lorenz '63 model, the two-layer Lorenz '96 model, and the Kuramoto-Sivashinsky equation.

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MS182

On Densities of Bounded Primes for Hypergeometric Series

This talk concerns the primes that appear in denominators of various hypergeometric series. We focus on the cases of generalized hypergeometric series with rational parameters, and the case of 2F1 with quadratic irrational parameters. In the rational case we give a formula for the density of primes appearing to bounded powers in the denomina-

tors of the series. This density is one exactly when the solutions to the differential equation are algebraic functions. In the quadratic irrational case we give a lower bound on the corresponding density. Assuming the normality of p-adic digits of quadratic irrationalities, this lower bound can be shown to be an exact formula for the density of bounded primes.

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MS182

Hypergeometric Functions and Modular Forms

We will explain how certain hypergeometric series are related to modular forms, focusing on recent results of the speaker and of Allen, Grove, Long, and Tu. In particular, we will emphasize how the interplay between these two areas enables us to compute interesting values in arithmetic geometry and beyond.

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MS183

Nonlinear Spike-and-Slab Sparse Coding for Intepretable Image Encoding

Sparse coding is a popular approach to model natural images but has faced two main modelling challenges: low-level image components (e.g. edge-like structures and their occlusions) and varying pixel intensities. Traditionally, images are modelled as a sparse linear superposition of dictionary elements, where the probabilistic view of this problem is the coefficients follow a Laplace or Cauchy distribution. We present a novel probabilistic generative model, instead with spike-and-slab prior and nonlinear combination of components. The prior enables the represention of exact zeros for eg the absence of an image component, eg an edge, and a distribution over non-zero pixel intensities. The max in the data likelihood targets occlusions, ie dictionary elements correspond to image components that can occlude each other. Because these model modifications result in highly multimodal posterior distributions, parameter optimization is analytically and computationally intractable. Thus we design a Markov Chain Monte Carlo sampling approach based on the exact form of the posterior by observing that the data likelihood with the nonlinear max can be written as right and left piecewise functions, which we can apply to higher dimensional data using latent variable preselection. Results on natural and artificial occlusion-rich data with known sparse structure show our approach can successfully learn ground truth model parameters and approximate/characterize the data generation process.

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MS183

Simulations of Semi-linear Reaction-Diffusion Equations with Mixed Derivatives via Stretched Splitting Methods

This study introduces a new strategy of splitting methods for solving semi-linear reaction-diffusion partial differential equations involving mixed derivatives. Intercardinal finite difference approximations are acquired for fast and accurate simulation approximations of underlying solutions. The presentation will demonstrate that the implicit schemes obtained are numerically stable, convergent, efficient, and preservative for key physical parameters such as the solution positivity and monotonicity. Orders of accuracy of the numerical algorithms will be validated via generalized Milnes devices. Computer simulations of the intercardinal splitting methods will be presented. Related CPU and GPU oriented computational costs will be estimated and explored. Further developments of the splitting methods for ANN in particularly PINN configurations will be proposed for possible industrial applications. Exchanges of new ideas and interactions are anticipated. Students are highly welcome to this talk.

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MS183

Dubious No More: Action of the Matrix Exponential and φ-functions via Differential Equations

Exponential time integrators rely on the computation of matrix exponential and related matrix functions, generally referred to as φ functions. The computation of these φ functions contributes to the main cost of an exponential integrator. Accordingly, matrix-free strategies are popular to compute the φ functions of matrices that are large and sparse. Methods such Krylov subspaces methods have been developed for computing the linear combination of φ functions. However, their scalability in parallel computing is not ideal. In this talk, we explore the use of embedded Runge–Kutta methods to compute the linear combination of the φ functions. This method allows us to exploit the special structure of the ODE to achieve an efficient evaluation of the φ functions and provides better strong scalability compared with Krylov subspace methods.

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MS183

An Rbf-Etd Approach for High-Dimensional Black-Scholes Equations with Non-Smooth Data

The Black-Scholes equation is a bedrock in financial mathematics, widely used for pricing options and derivatives. However, its application faces major challenges, like non-smooth initial conditions, high dimensionality in multi-asset scenarios, and nonlinearities arising from factors like transaction costs or volatility dependent on option price gradients. To address these complexities, we propose an RBF-ETD scheme that combines Radial Basis Functions (RBF) for spatial approximation with Exponential Time Differencing (ETD) for efficient time integration. This approach leverages the flexibility of RBFs in solving high-dimensional PDEs and ETD's ability to handle nonlinearities and non-smooth data without iterative solvers. We validate the method by comparing it with established schemes

such as RBF with Backward Euler and RBF with Crank Nicolson to examine its comparative accuracy, stability, and computational efficiency. The proposed RBF-ETD scheme promises a robust tool for solving complex Black-Scholes models in real-world financial applications.

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MS184

Eigenvalue Properties of Gram Matrices Associated with Simplexes and Polygons

In this talk, we will discuss the eigenvalues of Gram matrices associated with simplices in Euclidean, hyperbolic, and spherical geometries. We present refined spectral properties for the Gram matrices of triangles in each setting. The analysis also includes the spectral properties of a related matrix associated with Euclidean polygons. This is a joint work with Ying Wang.

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MS184

Numerical Studies to the Chaplygin Gas Equation

In this talk, we will discuss the numerical solutions to the Riemann problem for Chaplygin gas equation, which is the Euler equations equipped with the state equation $p = -1/\rho$. The spatial discretization is performed using WENO reconstruction and time integration is achieved using TVD RK4. The numerical results confirm high order of accuracy. This is a joint work with Ling Jin.

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MS185

Modeling Infectious Disease Dynamics and Its Interaction with Human Behavior for Applications to Public Health

In many populations, vaccine refusal is replacing access as the primary barrier to ensuring high vaccine coverage. To address this problem, it has become necessary to incorporate human behaviour into epidemiological models. Coupled behaviour-disease models address this by combining a disease transmission model with a vaccinating behaviour model, creating a single, coupled nonlinear dynamical system. The literature on such models has grown significantly in recent years, but important challenges remain: existing theory is often inconsistent with real-world vaccinating behaviour, models are not validated against empirical data, and model structure needs to be enriched by accounting for population heterogeneities. In this talk I will describe interdisciplinary research dedicated to addressing these challenges, using differential equation models, network simulations, and evolutionary game theory applied to measles and COVID-19 vaccines.

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MS185

Mathematical Modeling of Nutrient-Dependent Synchronization of Neurons

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. These mathematical models describe transport across the neuronal membrane of specific ions but ignore the critical role nutrients play in keeping the neurons alive. Furthermore, since neurons are immersed in the cerebrospinal fluid, they share the same environment and thus, may compete for resources. Mathematically, the competitive LotkaVolterra model describes the dynamics of species competing for common resources. Thus, in this talk, a mathematical model for nutrient-dependent synchronization of two nearby neurons will be introduced. The competitive Lotka-Volterra model will be used to predict temporal changes in the volumes of the two neurons. This model will be further linked to the synchronized Hodgkin-Huxley model by prescribing a synchronizer function dependent on the neuronal volumes. Lastly, numerical solutions of the coupled synchronized Hodgkin-Huxley and competitive Lotka-Volterra model will be presented and discussed through the lens of clinical applications.

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MS185

A Synthetic Biology Approach to Bacteria-Mediated Cancer Therapy

Accurate targeting is a critical challenge in cancer therapy. It has been known for decades that anaerobic bacteria can cause regression of solid tumors. These bacteria are unable to germinate in healthy, well-oxygenated tissue, but can selectively colonize in the cores of solid tumors, which present low-oxygen (hypoxic) environments. But such therapeutic approaches have been unsuccessful because the bacteria are unable to impact tumor outer rim (which is relatively better oxygenated) and so cancer regrowth occurs. We are investigating the utility of genetically modifying the non-pathogenic bacterium Clostridium sporogenes for use in anti-tumor therapy. Specifically, we are introducing genes that allow for these cells to exhibit increased oxygen tolerance and for quorum-sensing triggered genetic expression. These will allow for environmentally controlled anti-tumor activity, In addition to construction and testing of these genetically engineered strains, we have developed kinetic models of population quorum-sensing activity and cellular activity in tumor micro-environments for prediction of system behaviour and as a foundation for model-based design of therapeutic interventions.

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MS185

Calcium Signaling in Oligodendrocytes: A Mathematical Theory

Myelin sheaths increase the transverse resistance of axonal fiber and support node-to-node saltatory conduction. The ability of oligodendrocyte (OG) to ensheathe multiple fibers is directly regulated by both Ca2+ signaling in these cells and by axonal activity, allowing myelin to be adaptive. This indicates that axon-myelin-OG relationships define a multivariable system with functional consequences for each variable. How they combine to elicit an integrated structural response to physiological stimuli in the nervous system is poorly understood. To investigate this system, we have recently applied computational modeling approaches to analyze ca2+ signaling on OG. This was done by developing a flux-balance model to investigate how spontaneous and evoked Ca2+ transients are regulated in these cells. By employing experimentally recorded evoked Ca2+ responses induced by ATP, glutamate, and membrane polarization, we evaluated the roles of voltage-gated Ca2+ channels, purinergic receptors, glutamatergic receptors, and Ca2+-induced Ca2+-release in governing Ca2+ transients and voltage responses. We characterized how these evoked responses affect calcium signals and analyzed their potential impact on OG function. In this talk, I will provide an overview of the results obtained focusing on two key aspects: the underlying dynamics of spontaneous and evoked Ca2+ transients in OG and their implications on myelin plasticity.

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MS186

Modelling Microrobots for Biomedical Applications

Bacteria and other microorganisms have developed effective methods of locomotion through fluids and complex environments. Microrobots can be designed to use similar propulsion systems to move around and perform functions such as targeted drug delivery, micromanipulation, and environmental remediation. Time-varying external magnetic fields are commonly used to control magnetic microrobots due to their ease of use. We model such microrobots and use numerical methods to simulate their motion in viscous fluids. After first examining the motion of axisymmetric particles that roll along a surface, we describe a microrobot design that uses helical sections to generate fluid flows that aid in capturing and transporting rod-like cargo. This design was motivated by challenges reported for previous robots used to manipulate sperm cells for assisted fertilization.

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MS186

Inverse Problems for Porous Media As a PDE Problem and As a Datacentric Problem

The theory of flow in saturated porous media is often based on Darcy's law. When coupled with an expression for the conservation of mass, this leads to a linear partial differential equation of elliptic type. In applied settings (hydrology, biomechanics) the actual behaviour observed is strongly influenced by the spatial distribution of parameters, and especially the spatial distribution of permeability. We consider two different approaches to the problem of determining a permeability distribution from measurement. In the first approach, the governing equations are re-interpreted as a first order partial differential equation for permeability. The method of characteristics is then applied to show how errors in measured pressure distributions effect estimates of permeability. The method is subsequently extended to the so-called Klinkenberg correction used when the saturating fluid is a gas. For the Klinkenberg case the governing equation is nonlinear. In either case, it is shown that there are regions for which permeability estimates are very difficult to compute. The second approach considers the problem from a data centric point of view. Using Empirical Orthogonal Functions we corroborate the predictions of the PDE-based model.

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MS186

Backscatter in Atmospheric Turbulence

The Navier-Stokes equations with parameterizations of various physical processes can be used to model turbulent flows in the atmosphere. However, the vast range of length scales in such flows presents a challenge. One solution is to apply a low-pass spatial filter to the equations of motion: motion on the large filtered scales is described by the filtered equations, while the small sub-filter scales must be modelled. Such models often use an eddy viscosity approach, in which the sub-filter-scale turbulence is assumed to influence the filtered motion much like molecular viscosity. One consequence of this approach is that sub-filter-scale turbulence is purely dissipative: the kinetic energy of the filtered flow is locally dissipated by eddy viscosity. However, local upscale transfer of kinetic energy, known as backscatter - where sub-filter-scale kinetic energy is transferred upscale to the filtered motions - is known to occur in various kinds of turbulence. In this talk, we will present numerical evidence that backscatter is also ubiquitous in atmospheric flows on different scales, including flows with buoyancy and clouds. Physical mechanisms of backscatter and implications for numerical modelling will be discussed.

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MS187

A Delayed, Stochastic Model of Prion Diseases

with Interconnectome Protein Transport

Prion diseases are rapidly fatal neurodegenerative disorders characterized by the misfolding of the endogenous Cellular Prion Protein (PrP^{C}) into a toxic variant known as Scrapie Prion Protein (PrP^{Sc}). These toxic proteins spread throughout the brain, converting PrP^{C} into more PrP^{Sc}. In this presentation, we build a model starting with heterodimer protein kinetics and incorporate three key biological elements: (i) stochasticity, to account for randomness and uncertainty in PrP^{Sc} clearance; (ii) the Unfolded Protein Response (UPR), a cellular defense mechanism that halts protein translation after a delay; and (iii) the capacity for toxic proteins to spread between different brain connectomes. Through an asymptotic limit, we establish a nonlinear, delayed, stochastic ordinary differential equation system that tracks the concentration of PrP^{Sc} within one or multiple brain regions. We demonstrate the global existence and positivity of solutions and explore qualitative outcomes, including conditions for disease persistence or extinction, as well as the emergence of Hopf bifurcations.

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MS187

Mathematical Modeling of Neurodegenerative Prion Diseases in One-Dimensional Neuronal Networks

This presentation introduces a mathematical model to simulate the progression of prion diseases in the brain. We model neurons as they interact with both normal and misfolded (scrapie) proteins. The model uses a delay differential equation to describe changes in protein concentrations and neuronal viability, with various parameters regulating protein degradation, misfolding rates, diffusion within the interstitial fluid, and the spread between interconnected neurons. Neurons are modeled in a one-dimensional space with varying connectivity distributions to mimic different types of neural networks. We visualize how neurodegenerative diseases propagate through the neuronal network over time and account for how different brain regions permit their spread.

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MS188

Dynamics in Nonlinear Discrete Lattices under a Nonlocal Coupling Configuration

The field of nonlinear photonics provides a rich platform for applications and of modeling nonlinear dynamics. An array of optical waveguides coupled by nearest neighbor interactions porvided the experimental realization of discrete solitons. Varying the topological structure of an optical array (or more generically discrete elements) , in particular through the linear coupling configuration, has lead to the emerging field of topological photonics. In this talk I will present results on the dynamics in nonlinear lattices when the linear coupling configuration is nonlocal. What modes persist and what instabilities emerge will be discussed. In particular we will point out how the long-wave (continuous) approximation leads to a fractional Nonlinear Schroedinger Equation. A model that is currently studied in many fronts.

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MS188

Global Existence of a PDE Model for Chemotaxis with Dynamic Boundary Conditions

In this talk, we will discuss a particular one-dimensional PDE model for *chemotaxis* with logarithmic sensitivity and logistic growth for the organism population density. We will present (some preliminary) results on both zero flux and time-dynamic boundary conditions on the global existence and stability of the solutions of this PDE systems.

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MS188

Thermodynamic Formalism of Special Billiard Flows

Mathematical billiards, defined by the free motion of a point particle within a domain with elastic reflections at the boundary, offer a surprisingly rich playground for exploring complex dynamical systems. While seemingly simple, billiards serve as effective models for diverse physical phenomena, ranging from the refraction of lights and lasers to the complex interactions of gas particles and even as-

pects of planetary motion. This talk will delve into the application of thermodynamic formalism, a powerful framework for analyzing the statistical properties of dynamical systems, to the study of chaotic billiards. We will demonstrate how this approach enables the computation of key dynamical invariants, providing quantitative insights into the system's chaotic behavior. Beyond a review of classical results, we will outline recent endeavors to advance the thermodynamic formalism of billiard systems.

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MS188

Data Assimilation Methods for Agent-Based Models

Digital twin technology, originally developed for engineering, is being adapted to biomedicine and healthcare. A key challenge in this process is dynamically calibrating computational models to individual patients using data collected over time. This calibration is vital for improving model-based predictions and enabling personalized medicine. Biomedical models are often complex, incorporating multiple scales of biology and both stochastic and spatially heterogeneous elements. Agent-based models, which simulate autonomous agents such as cells, are commonly used to capture how local interactions affect system-level behavior. However, no standard personalization methods exist for these models. The main challenge is bridging the gap between clinically measurable macrostates (e.g., blood pressure, heart rate) and the detailed microstate data (e.g., cellular processes) needed to run the model. In this talk, we discuss an algorithm that applies the ensemble Kalman filter, a classic data assimilation technique, at the macrostate level. We then link the Kalman update at the macrostate to corresponding updates at the microstate level, ensuring that the resulting microstates are compatible with the desired macrostates and consistent with the model's dynamics. This approach improves the personalization of complex biomedical models and enhances model-based forecasts for individual patients.

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MS189

Quantum Basics for Mathematicians and Mathematical Foundations of Quantum Algorithms

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MS189

Quantum Networks and Quantum Sensing Research Needs

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MS189

Introduction to the Quantum Intersections Convening and SIAM's Engagement on Quantum

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MT1

Self-Exciting Random Evolutions and Their Applications in Finance and Insurance

This talk is devoted to new models of random evolutions, namely, so-called self-exciting random evolutions (SEREs), and their applications. The SEREs are based on Hawkes process, i.e., they can be constructed in a similar way as, e.g., semi-Markov random evolutions (REs), but instead of semi-Markov process we have superposition of a Markov chain and Hawkes process. First, we give classifications and examples of SEREs. Then we consider limit theorems for SEREs, similar to semi-Markov REs, such as averaging, diffusion approximation, normal deviations, and rates of convergence for SEREs in the limit theorems. Some of the applications of SEREs are considered in finance, insurance, and energy markets. For example, they are self- exciting risk process, self-exciting stock price, variance-Hawkes process, etc., to name a few. The originality and novelty of the SEREs models are associated with the new features of SEREs and their many applications, such as self-exciting and clustering properties., which is not the case for previous REs, e.g.., semi-Markov REs.

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MT2

Recent and Upcoming Developments in Randomized Numerical Linear Algebra for Machine Learning

Large matrices arise in many data science applications, including as representations of datasets, graphs, model weights, first and second-order derivatives, etc. Randomized Numerical Linear Algebra (RandNLA) is an area which uses randomness to develop improved algorithms for ubiquitous matrix problems. The area has reached a certain level of maturity, and current efforts of incorporating RandNLA algorithms into core numerical libraries, as well as recent advances in Optimization, Statistics, and Random Matrix Theory, have led to new theoretical and practical challenges. This tutorial will provide a self-contained overview of RandNLA, in light of these developments.

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MT3

Building Blocks of Quantum Computing Tutorial: Implementing Quantum Gates Using Smooth Pulses with QUANTUMGATEDESIGN.JL

Quantum gates are the building blocks of quantum computing. A quantum circuits operate on quantum states by applying sequences of gates acting on local sets of qubits. Gates are implemented on quantum computers by varying the amplitudes of magnetic fields or EM radiation in time to form control pulses, which control the dynamics of the system. An optimal control problem is solved to find control pulses which implement the desired behavior of a quantum gate. In this hands-on tutorial, we explain how to set up the optimal control problem for designing a gate, and how to simulate the quantum system dynamics and solve the optimal control problem numerically using the open-source QuantumGateDesign.jl package for the Julia programming language. QuantumGateDesign.jl utilizes an arbitrarily high-order method for solving systems of ODEs based on Hermite interpolation and the discrete adjoint method for efficiently computing exact gradients to enable quasi-Newton optimization.

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MP1

Modeling the Effect of Vector Control on the Host Population in the Eradication of Malaria

Malaria remains a major health issue, particularly in sub-Saharan Africa, where it causes high morbidity and mortality. We develop a SCEIR-SCEI model emphasizing vector control, deriving the basic reproduction number, and analyzing disease-free and endemic equilibria stability. Results show that the disease-free equilibrium is stable when $R_0 < 1$, with vector control significantly more effective than human-protection measures. Numerical simulations confirm that reducing human-vector contact through vector control is critical to eradicating malaria in high-burden areas.

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MP1

Applying Acceleration to Krylov Subspace Eigenvalue Solvers

Many modern-day problems involve solving for the eigenvalues of significantly large matrices. In 2002, Golub and Ye introduced a competitive inverse-free Kyrlov subspace eigenvalue solver that focuses on large, sparse, symmetric matrices. In 2010, Quillen and Ye introduced a block generalization of the method. Recently, momentum-type acceleration has been shown effective at a low-cost to reduce the number of iterations in an iterative method, including methods for eigenvalue problems. In this poster, we will explore the effect of applying acceleration to Ye's implementations of the methods for single and block symmetric generalized eigenvalue problems.

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MP1

Oxidative Stress Management in the Liver: Elucidating Sex Differences and Disease Pathologies

Oxidative stress, a disruption in the cellular redox state, when present and high levels damages cells and contributes to conditions such as metabolic dysfunction, neurological disorders, cardiovascular disease, and aging. Interestingly, women tend to have lower levels of oxidative stress and higher concentrations of certain antioxidants than men. These differences point to the important role of sex hormones in regulating oxidative stress and its effects on the body. In this poster, I use mathematical modeling to explore how these hormonal influences shape oxidative stress dynamics and contribute to sex differences in disease progression. By connecting clinical observations with computational tools, this work provides insights into the underlying mechanisms and paves the way for sex-specific approaches to managing disease.

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MP1

Monte Carlo Simulations to Model Flux Decline in Dead-End Microfiltration Operations

Microfiltration systems use membrane filters and simple size exclusion to remove foulants, like bacteria, from feed water. Applications include wastewater treatment and biopharmaceutical product purification. A prominent concern for filtration operation is fouling of the membranes by the retained matter, which leads to a decline in the filtration flow rate and necessitates periodic backwashing to clean the fouled membrane. Through Monte Carlo simulations based on the advection-diffusion equation and classical filtration theory, we aim to model the rate and pattern of flux decline and post-backwashing recovery in dead-end, constant-pressure microfiltration. Funding: NSF CBET-2211001.

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MP1

Adaptive Parameter Selection in Nudging Based Data Assimilation

Data assimilation combines (imperfect) knowledge of a flows physical laws with (noisy, time-lagged, and otherwise imperfect) observations to produce a more accurate prediction of flow statistics. Assimilation by nudging (from 1964), while non-optimal, is easy to implement and its analysis is clear and well-established. Nudgings uniform in

time accuracy has even been established under conditions on the nudging parameter and the density of observational locations, H, Larios et al. (2019). One remaining issue is that nudging requires the user to select a key parameter. The conditions required for this parameter, derived through priori (worst case) analysis are severe (Section 2.1 herein) and far beyond those found to be effective in computational experience. One resolution, developed herein, is self-adaptive parameter selection. This report develops, analyzes, tests, and compares two methods of self-adaptation of nudging parameters. One combines analysis and response to local flow behavior. The other is based only on response to flow behavior. The comparison finds both are easily implemented and yields effective values of the nudging parameter much smaller than those of priori analysis.

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MP1

DDA: An R Package for Learning Causal Structures in Observational Data Using Direction Dependence Analysis

Understanding causal mechanisms is critical across the empirical sciences. Methods for probing causal structures of linear variable relations in observational data have received growing attention. Direction Dependence Analysis (DDA; www.ddaproject.com) provides a comprehensive framework for distinguishing between causal ($x \to y$), anti-causal ($y \to x$), and confounded ($x \leftarrow u \to y$) variable relations by leveraging non-Gaussianity information of observed variables. Although non-Gaussianity is often treated as nuisance information in traditional methods of association, DDA utilizes non-Gaussianity features to discern causal conclusions from observational data. We introduce the R package dda, which implements DDA in the R statistical programming environment. The package provides tools for model estimation, statistical testing, and visualizations for causal learning in conditional and unconditional linear models. Using real-world data from psychological research, we demonstrate the application of DDA in R to identify causal directionality and to uncover hidden confounding in complex linear variable relations. The poster highlights theoretical foundations, implementations, and applications of the dda package which provides a valuable resource for causal learning.

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MP1

Modeling Metastatic Cancer Treatment with Neoantigen Peptide Vaccine

We begin with a system of ordinary differential equations for an immunological treatment of a primary tumor by neoantigen peptide vaccines. This system is coupled with a partial differential equation of metastasis that tracks the number of metastases per time and size. Vaccine dose is taken as a control in the primary tumor ordinary differential equation to slow tumor growth and the spread of metastatic tumors. An optimal control problem is formulated to design vaccine treatment.

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MP1

The Effects of Air Pollution on Health: A Longitudinal Study of Los Angeles County Accounting for Measurement Error

This study develops a Bayesian hierarchical model to explore the effects of air pollution on respiratory and cardiovascular mortality in Los Angeles County. The model takes into account various pollutants such as PM2.5, PM10, CO, SO2, NO2 and O3, as well as a related meteorological factor: temperature. The objective is to identify the significant factors affecting selected health outcomes without including all variables in each model specification. This flexibility enables the model to capture key drivers of health risk without redundancy. To account for potential measurement error in pollution data due to imperfect monitoring or averaging, certain observed pollutant levels are treated as noise proxies for true exposure. By specifying priors for regression coefficients and measurement error parameters and estimating posterior distributions via Markov Chain Monte Carlo (MCMC) sampling, it leads to more precise and reliable estimates of the health risks associated with air pollution exposure in Los Angeles County by incorporating both the count nature of the health data and the uncertainties in pollution measurements.

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MP1

Evaluating Probabilistic and Data-driven Inference Models for Fiber-coupled NV-diamond Temperature Sensors

We evaluate the impact of inference model on uncertainties when using continuous wave Optically Detected Magnetic Resonance (ODMR) measurements to infer temperature. Our approach leverages a probabilistic feedforward inference model designed to maximize the likelihood of observed ODMR spectra through automatic differentiation. This model effectively utilizes the temperature dependence of spin Hamiltonian parameters to infer temperature from spectral features in the ODMR data. We achieve prediction uncertainty of $\pm$ 1 K across a temperature range of 243 K to 323 K. To benchmark our probabilistic model, we compare it with a non-parametric peak-finding technique and data-driven methodologies such as Principal Component

Regression (PCR) and a 1D Convolutional Neural Network (CNN). We find that when validated against out-of-sample dataset that encompasses the same temperature range as the training dataset, data driven methods can show uncertainties that are as much as 0.67 K lower without incorporating expert-level understanding of the spectroscopic-temperature relationship. However, our results show that the probabilistic model outperforms both PCR and CNN when tasked with extrapolating beyond the temperature range used in training set, indicating robustness and generalizability. In contrast, data-driven methods like PCR and CNN demonstrate up to ten times worse uncertainties when tasked with extrapolating outside their training data range.

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MP1

Joint Denoising and Sparse Identification for Nonlinear Dynamical Systems

Sparse Identification for Nonlinear Dynamical Systems (SINDy) is a technique for finding the governing equations of a dynamical system given observations of its state variables. It assumes the dynamical system is a linear combination of dictionary functions such as polynomials, sines, cosines, exponentials, etc. It also assumes the coefficients of the linear combination are mostly zeros. The coefficients are learned from the observed data by minimizing a ℓ_0 or ℓ_1 regularized objective function that quantifies how closely the observed/estimated derivatives of the state variables match those predicted by the model. In the original version of SINDy, coefficients can be approximated rapidly using Successive Thresholded Least Squares (STLS) or found exactly using Mixed Integer Optimization (MIO). However, these methods are highly sensitive to noise in the state variables and their derivatives. Denoising the data as a preprocessing step can enable good results, but typical denoising techniques have their own parameters that can require tuning. In this work, we generalize SINDy to incorporate denoising directly into the objective function that is optimized during the system identification process, improving robustness to noise. The updated objective function can be minimized by alternating between estimating denoised derivatives and identifying sparse dictionary coefficients via STLS or MIO.

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MP1

Data Assimilation with Model Errors

Nudging is a data assimilation method amenable to both analysis and implementation. It also has the (reported) advantage of being insensitive to model errors compared to other assimilation methods. However, nudging behavior in the presence of model errors is little analyzed. This report gives an analysis of nudging to correct model errors. The analysis indicates that the error contribution due to the model error decays as the nudging parameter $\chi \to \infty$ like $\mathcal{O}(\chi^{-\frac{1}{2}})$, Theorem **??**. Numerical tests verify the predicted convergence rates and validate the nudging correction to model errors.

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MP1

Mathematical Models of Ovulation: A Parameter Sensitivity Analysis

The ovulatory cycle can be disrupted through a variety of factors, including stress and associated physiological responses. Although the mechanisms are complex, these effects can be examined through mathematical modeling. This work analyzes previous mathematical models of ovulation as preliminary steps towards modeling the effects of stress on ovulation. We perform a parameter sensitivity analysis and identify a metric to quantify model outputs and important parameters that help to distinguish ovulatory phenotypes. We also discuss implications of this work for stress-related mechanisms that influence ovulatory function.

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MP1

Persistent Directed Flag Laplacian (PDFL)-Based Machine Learning for ProteinLigand Binding Affinity Prediction

Directionality in molecular and biomolecular networks plays an important role in the accurate representation of the complex, dynamic, and asymmetrical nature of interactions present in protein-ligand binding, signal transduction, and biological pathways. Most traditional techniques of topological data analysis (TDA), such as persistent homology (PH) and persistent Laplacian (PL), overlook this aspect in their standard form. To address this, we present the persistent directed flag Laplacian (PDFL), which incorporates directed flag complexes to account for edges with directionality originated from polarization, gene regulation, heterogeneous interactions, etc. This study marks the first application of PDFL, providing an in-depth analysis of spectral graph theory combined with machine learning. In addition to its superior accuracy and reliability, the PDFL model offers simplicity by requiring only raw inputs without complex data processing. We validated our multi-kernel PDFL model for its scoring power against other state-of-the-art methods on three popular benchmarks, namely PDBbind v2007, v2013, and v2016. The computational results indicate that the proposed PDFL model outperforms competitors in protein-ligand binding affinity predictions, indicating that PDFL is a promising tool for protein engineering, drug discovery, and general applications in science and engineering.

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MP3

Modeling the Role of Protein S in Blood Coagulation

Anticoagulant proteins regulate blood coagulation, protecting against unnecessary and pathological clotting. Protein S (PS) is an important anticoagulant. For instance, a type of pathological clotting known as deep vein thrombosis is associated with deficiencies in PS. Nevertheless,

much remains unknown about PS. A primary anticoagulant function of PS is to inhibit the procoagulant protein, activated factor X (E10), thereby inhibiting coagulation. We study direct inhibition of E10 by PS, as well as formation of a tripartite complex (PSC) consisting of one copy of the anticoagulant protein, tissue factor pathway inhibitor alpha (TFPI), bound to one PS and to one half activated form (E5h) of the procoagulant protein, factor V (fV). To do so, we use an established model of coagulation under flow, consisting of a system of several hundred ordinary differential equations based on mass-action kinetics with experimentally-determined parameters. To account for PS in the model, we incorporate PSC, PS, and new terms describing related interactions. Preliminary findings suggest that PSC increases TFPI concentration by anchoring TFPI to phospholipid membranes, preventing flow from washing away TFPI, decreasing coagulant activity. Findings also suggest that PS-E10 interactions significantly inhibit coagulation. However, competition for binding sites on platelets between PS and the PS in PSC, and between forms of fV and the E5h in PSC, may lessen inhibition of coagulation.

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MP3

Predicting Bleeding Phenotypes in Factor XI Deficiency using Machine Learning

Factor XI (FXI) deficiency is a rare bleeding disorder with highly variable clinical manifestations, ranging from asymptomatic cases to severe bleeding tendencies. Characterizing bleeding phenotypes in FXI-deficient patients remains a challenge due to the complex interplay between genetic, biochemical, and environmental factors. Current clinical assays fail to reliably predict bleeding risk, highlighting the need for alternative approaches. In this study, we employ machine learning techniques to develop models that identify patterns in bleeding tendencies and predict patient outcomes, aiding clinicians in risk assessment and treatment planning. These models integrate clinical data with proteomics to enhance predictive accuracy.

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MP3

Simulating Emicizumab in a Mathematical Model of Flow-mediated Coagulation

Hemophilia A is a genetic bleeding disorder characterized by deficiency of coagulation factor VIII (FVIII). FVIII normally binds to FIXa, enhancing the activation of FX, which enables generation of the enzyme thrombin that is critical for clot formation. Emicizumab is a bispecific monoclonal antibody designed to substitute for the missing activated FVIII by bridging FIXa and FX. It circumvents the limitations of traditional FVIII replacement therapy, including the short plasma half-life of FVIII and the development of autoantibodies against endogenous FVIII. We extend our previously developed ODE-based mathematical model of flow-mediated coagulation to incorporate emicizumab and its interactions with relevant factors. The model encompasses the biochemistry of the tissue factor pathway, platelet activation and deposition on the subendothelium, and flow- and diffusion-mediated transport of coagulation proteins and platelets. We simulate a range of emicizumab concentrations under varying coagulation conditions and examine its effects on thrombin generation under flow. These simulations allow us to explore the mechanisms of emicizumab in a physiologically relevant setting, provide quantitative insights into its activities in different contexts, and inform future design of hemophilia drugs.

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MP4

A Branch-and-Price Algorithm for Star Bi-Colouring of Bi-Partite Graphs

We address the star bi-coloring problem in bipartite graphs. Star bi-coloring assigns colors to vertices such that no two adjacent vertices share the same color, and any path of four vertices includes at least three distinct colors. We formulate this problem as a mixed-integer linear program and propose a branch-and-price algorithm to solve it efficiently. The algorithm integrates column generation and decomposition techniques to dynamically manage variables and utilize the graph's structure. Our implementation, built using the Coluna package in Julia, was tested on various graph types, including arrowhead matrices, sparse random graphs, complete bipartite graphs, and matrices from the HarwellBoeing collection. Results demonstrate the algorithm's ability to compute tight bounds for the minimum colors required, particularly excelling in sparse bipartite graphs. The study confirms optimality on selected test instance by systematically exploring the solution space through branch-and-bound.

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MP4

Efficient Algorithms for Evacuation Planning

There are many recent disasters such as wildfire, earthquakes, volcanic eruptions, hurricanes, and nuclear plant accidents which motivate researchers to do research on evacuation planning. For this purpose, researchers have worked the problem of locating a set of k sinks on a network that minimizes the sum of the evacuation times of all evacuees (minsum criterion). We focus on the problem of locating one sink on balanced binary tree networks

with uniform edge capacities, all while minimizing the total evacuation time for all evacuees (minsum criterion). The challenge with sink location problems is modeling congestion, which determines evacuation time during a major disaster. Designing a sub-quadratic algorithm to locate one sink on a tree network has been an open problem for about ten years. Our algorithm has a time complexity of O(n log2n), where n is the number of vertices in the network.

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MP4

Optimal Reconstruction of Sparse Jacobian

We propose a novel substitution based sparse Jacobian matrix determination method using algorithmic differentiation. With apriori known sparsity pattern for a matrix A, we employ a state-of-the-art column partitioning/coloring algorithm to generate a seed matrix S, which is used to create a compressed matrix $B = A \times S$, significantly reducing the problem's dimensionality. The sparsity pattern of the compressed matrix B is then used to construct a further reduction in problem dimensionality by recasting column reordering as Traveling Salesman Problem (TSP). Ant Colony Optimization (ACO) meta heuristic and several greedy heuristics have been employed to enable substitutable reconstruction of the Jacobian. The preliminary numerical results on a collection of standard benchmark test instances are promising, indicating the potential effectiveness of the proposed method.

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MP4

High-Performance Meta Heuristics for Agricultural Path Planning

Efficient coordination of working and tender vehicles in agricultural operationssuch as planting, spraying, and harvestingis critical for reducing downtime and increasing field productivity. This paper presents a novel application of the Simulated Annealing (SA) metaheuristic for optimizing refill planning, mission routing, and depot placement within coordinated field operations. The problem is formulated as a Multi-Depot Capacitated Vehicle Routing Problem (MD-CVRP), where agricultural fields are represented as a network of directed arcs, each corresponding to field tracks and headland passes. Constraints include vehicle capacity limits, refill timing, mission scheduling, and full coverage requirements, with objective functions minimizing non-working travel distance and time. The SA-based optimization integrates critical features such as dynamic depot selection, track assignment under capacity constraints, and adaptive traffic flow control, including controlled traffic and zone-specific access (e.g., applied/unapplied areas). Experimental results on real-world instances demonstrate that the proposed model reduces non-productive traversal time and supports effective mission planning between primary and secondary staging areas.

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PP1

Generalizing the Exponential Fréchet Algorithm

The computation of off-diagonal blocks of matrix functions $f(T)$, where T is block triangular, poses a challenging problem in scientific computing. We present a novel algorithm that exploits the structure of block triangular matrices, generalizing the algorithm of Al-Mohy and Higham [SIAM J. Matrix Anal. Appl., 30 (2009), pp. 16391657] for computing the Fréchet derivative of the matrix exponential. This work has significant applications in fields such as exponential integrators for solving systems of first-order differential equations, Hamiltonian linear systems in control theory, and option pricing in finance. Our approach introduces a linear operator that maps off-diagonal blocks of T into their counterparts in $f(T)$. By studying the algebraic properties of the operator, we establish a comprehensive computational framework, paving the way to extend existing Fréchet derivative algorithms of matrix functions to more general settings. For the matrix exponential, in particular, the algorithm employs the scaling and squaring method with diagonal Padé approximants to $\exp(x)$, with parameters chosen based on a rigorous backward error analysis, which notably does not depend on the norm of the off-diagonal blocks. The numerical experiment demonstrates that our algorithm surpasses existing algorithms in terms of accuracy and efficiency, making it highly valuable for a wide range of applications.

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PP1

On the Analytical Soliton Approximations to Fractional Forced Kortewegde Vries Equation Arising in Fluids and Plasmas Using Two Novel Techniques

The current investigation examines the fractional forced Kortewegde Vries (FF-KdV) equation, a critically significant evolution equation in various nonlinear branches of science. The equation in question and other associated equations are widely acknowledged for their broad applicability and potential for simulating a wide range of nonlinear phenomena in fluid physics, plasma physics, and various scientific domains. Consequently, the main goal of this study is to use the Yang homotopy perturbation method and the Yang transform decomposition method, along with the Caputo operator for analyzing the FF-KdV equation. The derived approximations are numerically examined and discussed. Our study will show that the two suggested methods are helpful, easy to use, and essential for looking at different nonlinear models that affect complex processes.

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PP1

Sparse Constrained Discovery of Dynamics in Epidemiological Data

We propose a methodology applying sparse regularization in parameter estimation for compartmental models. We

apply an approach inspired by SINDy (Brunton, Proctor, and Kutz) to the discovery of coefficients and model terms in specialized to compartmental models where both having conserved quantities and interpretability are important beyond fitting data in the testing regime. Some recent work (Horrocks, 2020 and Jiang, 2021) have been successful applying variations on these tools applied to epidemiological data, but many open questions remain. We present or ongoing work in tailoring these tools to the constraints of a broader class of compartment models and fitting data in various regimes.

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PP1

Computational Forays in Higher-Order Time Discretization of Maxwell's Equations

In this poster, we present our computational experiences with obtaining higher-order time discretizations of Maxwell's equations using two different strategies: *Time* and *Space*. In both, our underlying idea is to use Taylor series for expressing the time component of the solution and discretize the spatial part of the electric and magnetic fields using appropriately higher-order finite element exterior calculus (FEEC) (although other methods may also be used). In the Time Strategy, higher-order time derivatives in the Taylor series are suitably discretized with higher-order finite differencing schemes. In the Space Strategy, on the other hand, such higher-order time derivatives are translated into higher-order spatial derivatives using the Maxwell's equations themselves which are then suitably discretized spatially using FEEC. Both strategies can lead to both implicit and explicit time stepping schemes. We shall also provide instances of energy conservation in some of the methods which arise. We believe that this is one of the first instances in which these two strategies have been systematically studied and computations demonstrated. Together with some separate theoretical results which helps ground these two strategies, it is our hope that this would enable further developments in higher order time discretizations of partial differential equations.

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PP1

Topological Shape Analysis for Wing Venation Patterns

Winged insect species identification, crucial for ecological tracking and conservation efforts, generally depends on individual wing venation patterns. Traditional classification methods depend heavily on the learned skills of expert taxonomists, warranting the use of computational methods. This research introduces a novel persistent homology approach in the nascent field of topological data analysis to extract information from biological geometries over different spatial definitions of locality. Focusing on the Euler Characteristic Curve (ECC) topological summary of shape for this context, two novel transforms are introduced: the Duplicate Interpolation Transform (DIT) and the Relative Angle Variation Transform (RAVT). DIT enhances the ECC by encoding the rate of topological change, while RAVT identifies subtle 'phase transitions' indicative of significant structural shifts. These profiles potentially offer new perspectives on phylogenetic relationships as one population can be shown to be topologically similar to a controlled perturbation of another. This approach reveals unique topological profiles for hoverfly genera, and distinct co-informative sets of landmarks which are informed by the context and the spatial ranges where phase transitions occur. This methodology presents a promising avenue for automating and enhancing species characterizations and classification, as well as outlining improved general methods for interpretable engineering of geometric data.

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PP1

Using Generalized Additive Models and Multivariate Adaptive Regression Splines to Analyze Electricity Load Curves and Perform Short-Term Prediction in the Residential Sector

The widespread deployment of smart meters in the residential and tertiary sectors has made it possible to collect high-frequency electricity consumption data at the consumer level (individuals, professionals, etc.). This data is a raw material for research on the prediction of electricity consumption at this level. The majority of this research is largely aimed at meeting the needs of industry, such as applications in the context of smart homes and programs for managing and reducing consumption. The objective of this work is to deploy or implement short-term (D + 1) electrical load forecasting models at the consumer level. The complexity of the subject lies in the fact that consumption data on this scale is very volatile. Indeed, it includes a large amount of noise and depends on the consumer's lifestyle and consumption habits. We studied the influence of integrating outdoor temperature in different forms on the performance of a Generalized Additive Models (GAM) model and a Multivariate Adaptive Regression Splines (MARS) model. These two models are capable of modelling both linear relationships and non-linear interactions between influencing factors (independent variables), and were adapted to model the temperature sensitivity of load curves. The models were tested and evaluated on a large sample of disparate load curves in the residential sector. An approach was also proposed for the prediction of the most volatile load curves.

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PP1

Maximum Likelihood Estimator of Markov Processes with Censored Data for the Ehrenfest Model and Beyond

Bladt and Srensen (2005) explored likelihood maximization for discrete Markov jump processes with a finite state space, showing that the maximum likelihood estimator

(MLE) can be obtained via the EM algorithm or a Markov chain Monte Carlo method. Albert (1960) studied the estimation of the infinitesimal generator Q in continuous-time, finite-state Markov processes, proving the existence of an MLE given k independent realizations. Our work focuses on estimating Q in a finite discrete-time Markov jump process $X(t)$, where only the initial and final states $X(0)$ and $X(T)$ are known. We prove that the MLE of Q does not exist in this setting and introduce a regularized likelihood function to address this issue. We establish key analytical results proving the existence of an MLE for the regularized function. This poster presents these findings along with an example: the Ehrenfest model combined with a finite-state birth-and-death process, modeling traffic flow on a finite-block street. We develop a method to estimate Q while ensuring nonzero entries only for neighboring vertices. This connectivity constraint is encoded in the Dirac operator, restricting Q to a subspace of the algebra generated by the Dirac operator and multiplication operators.

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PP1

Proactive Short-Term Traffic Flow Prediction and Genetic AlgorithmDriven Signal Control

Traffic congestion remains a significant concern in urban areas, contributing to travel delays, increased fuel consumption, and heightened emissions. This study presents a proactive framework that couples short-term traffic flow prediction with metaheuristic-based traffic signal control. We begin by collecting high-frequency sensor datavehicle counts, Flow, and occupancyat five-minute intervals from critical intersections, forming the basis of our short-horizon forecasting model using LSTM and gradient-boosted trees. To enhance predictive accuracy, we employ systematic hyperparameter tuning, ensuring that the models parameters are optimized for the available dataset. Using these forecasts, we then apply a genetic algorithm (GA) to dynamically adjust signal phases, cycle lengths, and green splits before congestion arises. Simulation results indicate that this predictive, look-ahead approach outperforms conventional fixed-time and actuated signal strategies, yielding lower delays and smoother traffic flow. By uniting machine learningbased forecasting and a metaheuristic signal optimization algorithm, the proposed framework provides a promising pathway toward more efficient and traveler-friendly urban traffic management.

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PP1

Extending Four Bugs on a Square The Infinite Bug Chase

The classical problem of Four Bugs on a Square is often used to motivate systems of differential equations. Initially positioned at the vertices of a square, the four bugs pursue one another in a cyclic fashion and with a constant speed. The bugs converge to one another, and the asymptotic behavior of this convergence is well-understood. An extension of this problem is to initialize and constrain the bugs to a surface. With this simple modification, interesting dynamics are revealed for geometries as simple as a circle. When confined to a circle, the bugs converge to one of two stationary solutions: coalescing at a single point or assuming an infinite chase loop. Using a Monte Carlo approach, I estimate the probabilities of each outcome for a random initial condition and consider these probabilities for large numbers of bugs. Additionally, I analyze the stability of the stationary solutions. These results are verified with analytical calculations that are possible for systems with two, three, or four bugs.

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PP1

Emergence of Oscillations in a Coupled Continuous-Probabilistic Epidemic Model

In this poster, we study the dynamics of susceptible-infected-recovered epidemic model perturbed by random jumps of the disease transmission coefficient, due to external factors, such as virus mutations. To investigate the interactions between the biological dynamics of the disease spread and environmental parameters, we design an original hybrid model, obtained by coupling a continuous reaction-diffusion system, which describes the spatio-temporal dynamics of the infectious disease, with a discrete probabilistic process, that reproduces the random jumps in the transmission rate. We first establish a series of expected stability results, stating that a small perturbation of the continuous dynamics does not alter the stability of the disease-free equilibrium or of the endemic equilibrium, depending on the basic reproduction number. We then focus on the remarkable emergence of oscillations between both equilibria, under the effect of a strong perturbation. We perform various numerical simulations for illustrating our theoretical findings. This research is supported by the CoSysM3 project, Reference https://doi.org/10.54499/2022.03091.PTDC, funded by the Fundao para a Cincia e a Tecnologia (Portugal).

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PP1

Predicting General Election Outcomes from Primary Results at the Precinct Level

In the United States, polling data are collected at the state level, but election results vary substantially within states (e.g., between rural and urban areas). Unlike polls, election results are often available at the precinct level, and these fine-scale data can provide insight into how primary elections, general elections, and voter turnout are related at a granular level. Using primary and general election data at the precinct level for past presidential races, we model the relationship between the degree of partisan consensus ('entropy') in the primaries and each party's under-

or over-performance in the general election. These patterns give insight into voter turnout decisions and provide a fine-grained method for forecasting general elections.

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PP1

Scikit-Shape: Python Toolbox for Image and Shape Analysis

We introduce a Python package for image segmentation and shape analysis. Our package implements various building blocks to solve such problems, including algorithms for geometric regularization, elastic matching, adaptive discretization, and fast Newton-type minimization schemes. The package leverages the NumPy/SciPy ecosystem, making them as easy to use as Matlab, also compatible with existing Python tools. Our algorithms is freely available as an open source package for the research community at: http://scikit-shape.org

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PP1

Riemannian Trust Region Methods for Nonsmooth Multiobjective Optimization Problems

Riemannian optimization methods have received attention due to their application in machine learning. Among these methods, trust region approaches were one of the first developed and are widely used, with many variants appearing in the literature. In this work, we study a multiobjective extension of the trust region method for Riemannian optimization problems with nonsmooth objectives. Applications of this method are in a range of manifold-based machine learning problems such as the sparse PCA problem.

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PP1

Finite-Data Error Bounds for Approximating the Koopman Operator

First introduced in the 1930s, the Koopman operator framework presents an equivalent linear formulation of nonlinear systems by lifting the dynamics to an infinite-dimensional Banach space of scalar functions called observables. In the past decade the method of extended dynamic mode decomposition has emerged as a powerful computational technique to approximating the action of the Koopman operator on a finite span of functions, a dictionary, directly from data gathered from the system. The goal of this work is to further elucidate the relationship between the dictionary and the gathered data to provide explicit error bounds for the performance of the method. In particular, we show provide both analytical and empirical evidence that least squares regression techniques lead to a Monte Carlo rate of convergence in the amount of data. We can improve upon this in two ways. First, we show that growing the dictionary with the data can lead to exponentially vanishing error bounds, and second, we show that sparse regression techniques such as LASSO and basis pursuit can lead to improved accuracy and computational savings in the high-dimensional setting, where the dynamics tend to be sparser.

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PP1

Modeling and Benchmarking Geologic Hydrogen Processes with the Dusty Gas Model

As the demand for low-carbon energy solutions grows, geological hydrogen (H_2) storage emerges as a promising method for long-term energy storage. However, simulation of effective H_2 storage is challenged by the physical characteristics of hydrogen that depart from those of natural gas: light weight, low viscosity, and a small molecular cross section. Under certain circumstances in a multicomponent gas system, unique behavior including slip flow and transport up a concentration gradient can occur. Traditional subsurface transport models are unable to capture the aforementioned behavior because they assume a common solvent velocity. We present a simulator based on the dusty gas model that incorporates not only the concentration gradient driving transport, but also the relative velocities of all gases involved and their cross sections. We employ direct linear solvers to determine gas fluxes, integrating these into the PFLOTRAN parallel modeling framework. We validate the model through three test cases: steady-state transport of He and Ar, transient diffusion of a H_2-N_2-CO_2 mixture, and scalability assessments for caprock permeation in underground hydrogen storage systems. These test cases demonstrate simulation capability of upgradient diffusion and slip flow, as well as the ability to model H_2 storage processes in large geologic systems. SNL is man-

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PP1

Turing Instability and Dynamic Transitions in the GrayScott Equation

We study the dynamic bifurcation of the one and two dimensional Gray-Scott models by taking the diffusion coefficient λ of the reactor as a bifurcation parameter. We define a parameter space Σ of (k, F) for which the Turing instability may happen. Then, we show that it really occurs below the critical number λ_0 and obtain rigorous formula for the bifurcated stable patterns. When the critical eigenvalue is simple, the bifurcation leads to a continuous (resp. jump) transition if $A_m(k, F)$ is negative (resp. positive). We prove that $A_m(k, F) > 0$ when (k, F) lies near the Bogdanov-Taken point $(\frac{1}{16}, \frac{1}{16})$. When the critical eigenvalue is double, we have a subcritical bifurcation that produces an S^1-attractor $\mathcal{A}_m$. We prove that $\mathcal{A}_m$ consists of four asymptotically stable static solutions, four saddle static solutions, and orbits connecting them. We also provide numerical results that illustrate the main Theorems.

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PP1

Optimization of a Quantum Optimization Algorithm: Integration of Dynamic Adapt-Qaoa and Quclear

Quantum computing holds great promise for addressing practical challenges. However, current quantum devices suffer from noisy quantum gates, which degrade the fidelity of quantum circuits. As a result, optimizing quantum circuits is essential for achieving useful results. In this work, we explore the combination of two frameworks designed to optimize quantum circuits: QuCLEAR and Dynamic ADAPT-QAOA. First, we provide an overview of both frameworks, detailing their functions, key differences, and the individual benefits of each. Second, we present a mathematical proof that combining these two methods results in a more optimized circuit, with the order of application being inconsequential. Our empirical results for a 5-node example show that QuCLEAR reduces the CNOT gates by 43% and the RZ gates by 37.5%, while Dynamic ADAPT-QAOA achieves reductions of 36% and 39%, respectively. When combined, these methods reduce the CNOT gates by 68% and the RZ gates by 60%. Third, we compare the performance of standard QAOA with each approach individually and in tandem. Finally, we conclude with a discussion on scalability and interpretation of the results

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PP1

Exploring Polynomial Bases in Univariate Homotopy Continuation

Homotopy continuation is a numerical method for obtaining the zeros of polynomials. If a univariate polynomial has complex coefficients, it is reasonable to expect this method to find good approximations of most (perhaps all) roots of the polynomial with very small (or no) residual, and at relatively low cost in computation time and memory. However, if the polynomial has real coefficients, the algorithm may be less successful. For polynomials written in the monomial basis, this may be particularly true. We hope to show that with different interpolating bases, we can improve results of homotopy continuation for finding the zeros of a polynomial with real coefficients. That is, by improving the conditioning of the polynomial, we can reduce the number of spurious roots and have fewer false multiplicities. We will compare different interpolating basis, such as Lagrange, Hermite and some orthogonal basis, as alternatives to the standard monomial basis. Since every problem is unique, we do not expect to find one basis that offers better conditioning for all polynomials. Despite this, we wish to demonstrate some general results already known about conditioning of bases, and show how data from the homotopy paths reflect these facts and indicate error in the results in advance of analysis.

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PP1

Comparison of Methods Used to Solve the Forward Kinematics Problem for Stewart Platforms

The forward kinematics problem for Stewart platforms, a type of parallel manipulator, involves determining the position and orientation of the moving platform based on the lengths of its legs. This problem is inherently complex due to the nonlinear nature of the equations involved. Various methods have been proposed in the literature to address this challenge, which can be broadly categorized into analytical, numerical, machine learning, and sensor-based approaches, each having their own advantages and disadvantages. In this work we compare and contrast the generality, specificity, and accuracy of a diverse selection

of methods for solving the forward kinematics problem. If applicable, we compare the time and resources required for the approaches that are intended to solve the problem in real-time. Finally, we advocate for using the Lie derivative in the context of dual quaternions that represent rigid motions and twists to solve the forward kinematics problem.

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PP1

Inverse Two-Sided Laplace Transform in Quantum Many-Body Theory: Generalized Framework and Numerical Implementation

Path integral Monte Carlo (PIMC) simulations are a cornerstone method for studying quantum many-body systems, such as warm dense matter. The notoriously ill-posed inverse Laplace transform impedes extracting observables from PIMC data. Despite numerous attempts, no universally accepted approach has been identified to solve this problem and many methods remain unsatisfactory. The commonly posed optimization problem for this task is highly ill-conditioned; to address its limitations, we propose alternative formulations that improve the conditioning and introduce a more robust and physically meaningful regression approach, thereby enhancing the reliability of the solution. Specifically, we express the solution as a linear combination of kernels with induced detailed balance. In combination with prior knowledge of the shape $S(\mathbf{q}, E)$ can take, we implement regularization methods typical to this field (L^1, L^2 and MaxEnt) and implement new unexplored regularizers according to Wasserstein distance, total variation, and variance. As a key outcome, we developed the open-source Python library PyLIT (**Py**thon **L**aplace **I**nverse **T**ransform), which provides a accessible tool for reconstructing $S(\mathbf{q}, E)$ from PIMC data.

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PP1

An Automated Approach for 3D Registration of Dental Cbct and Face Scan Data

We introduce an automated method for registering dental cone-beam computed tomography (CBCT) scans with facial scan data. One of the main challenges in aligning facial scans with CBCT images lies in the difference of acquisition methods and the limited overlapping regions between the two data. Additionally, the use of machine learning for this task is hindered by the scarcity of training data, as 3D medical datasets involving radiation exposure are difficult to obtain. Our method overcomes these challenges by leveraging an existing machine-learning-based 2D landmark detection algorithm using an open-source library. We further develop a novel mathematical algorithm to identify corresponding 3D landmarks based on detected 2D landmarks. A key advantage of our approach is that it does not require annotated 3D facial landmark training data. Rather, it leverages a pre-trained facial landmark detection model that is robust and generalizes well across various 2D facial images. In other words, instead of directly detecting 3D landmarks, we simplify the problem by identifying corresponding landmarks in two 2D projection images obtained from different angles and using them. To enhance accuracy, we select 3D landmarks from sub-surfaces that exhibit minimal geometric distortion between CBCT and facial scans. Finally, for precise alignment, we apply the Iterative Closest Point (ICP) method, which refines the registration using geometric information around the detected 3D landmarks.

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PP1

A Multiscale Model on Hair Follicle Bulb Replenishment

Hair follicles (HFs) are mini-organs in skin who undergo cyclic growth. During the anagen phase, the hair shaft is produced from the bottom part of a HF, referred to as the hair bulb. Proper regulations of the HF bulb cell fate decisions are crucial to maintain an anagen HF, therefore guaranteeing the continuous production of hair. Recent experiments have provided evidence on how the HF bulb is replenished during anagen. In this work, we develop a hybrid multiscale computational model on HF bulb, integrating an agent-based submodel of cell divisions and movement, and a reaction-advection-diffusion equation submodel of diffusive signaling dynamics. Using our model, we investigate the HF bulb replenishment dynamics driven by different cell dividing strategies, showing that signaling-driven cell division may lead to efficient replenishment dynamics.

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PP1

Conditional Diffusion Models Enhanced by Continual Human Feedback Learning: Mitigating Shade Artifacts in Cbct-to-Mdct Translation

Cone Beam Computed Tomography (CBCT) is popular for its cost-effectiveness and low radiation but suffers from shade artifacts due to its narrow field of view and scattering, which motivates the development of robust CBCT-to-MDCT translation methods. While previous approaches using generative adversarial networks (GANs), such as Fidelity Embedded GANs (FEGANs), have enhanced CBCT image quality, they can also introduce additional artifacts. To address this issue, we propose a novel framework that integrates conditional diffusion models with continual human feedback learning for effective artifact mitigation and image enhancement. Specifically, we employ a denoising diffusion probabilistic model (DDPM) conditioned on initial image pairs derived from FEGAN outputs, with human feedback serving as additional conditioning to guide artifact removal. The model is iteratively refined using continual human feedback and classifier-free guidance, progres-

sively steering the generation process toward high-fidelity, artifact-free MDCT-like images. This continual learning mechanism enables the model to adapt and improve over successive iterations, ensuring stable training and robust artifact elimination. Experimental results demonstrate that our approach effectively reduces shade artifacts and reliably translates CBCT images into high-quality MDCT representations, offering a promising solution for enhanced clinical image processing and improved diagnostic accuracy.

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PP1

Improved Tail Bounds for Sums of Geometric and Binomial Random Variables: Coupon Collecting and 'The 1% Club'

Concentration inequalities play a pivotal role in probability theory, statistics, machine learning, and other fields of applied mathematics. The task of providing tail bounds for sums of random variables has been a topic that attracts interest across many diverse fields. While general results such as those established by Savanté have been extensively studied, specific cases still present opportunities for improvement. Capturing this idea, this work focuses on sums of random variables drawn from two distributions commonly used in applications involving Bernoulli trials: the geometric distribution and the binomial distribution. We present novel bounds tailored to these scenarios. For the geometric distribution, we present concentration for cases with constraints on the parameters, including the classical Coupon Collector problem and some of its generalizations. For the binomial distribution, we focus on what could be considered a "reverse" Coupon Collector problem inspired by a game show. We derive a series of theorems, each tailored to a different use case involving sums of geometric and binomial random variables. As part of our analysis, we incorporate complete homogeneous symmetric polynomials and Stirling numbers in a novel way to strengthen our results. Lastly, we provide graphical illustrations to demonstrate the effectiveness of each bound in comparison to existing results. We also highlight directions for further improvements as well as other potential use cases.

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PP1

On the Exact Solution to the Inverse Langevin Function: Asymptotically Consistent Resummation

The Langevin function (LF), a special case of the Brillouin function, is a well-defined function used in paramagnetism. Its counterpart, the inverse Langevin function (ILF), also has a myriad of applications, e.g. rubber elasticity, yet is left without an exact analytical expression. Unfortunately, due to singularities in the ILF, the Taylor series solution diverges before reaching the end of the physical domain. Thus, in lieu of "exact" numerical values, most research relies on analytical approximations of the ILF, such as Pad approximants. In this work, we create a new approximation for the ILF in the form of a resummation to the original power series that is asymptotically consistent at both ends of the physical domain, and whose maximum error is tunable to be below double precision (as additional terms are included). Additionally, we provide a new and computationally efficient method for obtaining the ILF Taylor series itself, which, in contrast to current methods, does not rely on series reversion and knowledge of the Taylor series expansion of the LF. We compare our approximation of the ILF against some of the more popular approximations used in capturing polymer chain stretch under shear and extensional deformation.

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PP1

Toward Algorithmic Foundations for Neuromorphic Computing: Discrete Methods, Mapping Strategies, and Experimental Insights

Neuromorphic computing, inspired by biological neural systems, offers energy-efficient, event-driven, and massively parallel computation. However, its non-von Neumann architecture and spike-based communication introduce significant algorithmic challenges. In this poster, we explore discrete computational problems in the context of spiking neural networks (SNNs), proposing algorithmic strategies tailored to neuromorphic architectures like Intels Loihi and IBMs TrueNorth. We make three core contributions: 1. Algorithmic Formulations for SNNs: We develop discrete optimization formulations for key problems such as graph-based pathfinding, constraint satisfaction, and local searchredesigned to leverage spiking dynamics and temporal coding. 2. Task-to-Hardware Mapping: We present heuristic algorithms that translate computational graphs to neuromorphic cores while satisfying hardware constraints like neuron/synapse limits and routing restrictions, balancing load and minimizing spike congestion. 3. Experimental Validation: Using Intel Loihi, we implement neuromorphic versions of shortest-path and satisfiability problems. Initial results show up to 3 better energy efficiency and real-time inference for dynamic inputs compared to CPU/GPU baselines. This work lays a foundation for a discrete algorithmic framework for neuromorphic systems and outlines future directions for algorithm-hardware co-design.

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PP1

Topological Analysis of a Preferential Attachment Hypergraph Model

Complex networks have been used with great success to uncover universal patterns and organizing principles in real-

world systems across diverse fields, from social networks and biological systems to technological infrastructure such as power grids and transportation networks. Motivated by the study of social networks, where new members are most likely to connect with popular members, much work has been done analyzing preferential-attachment (PA) models. To date most research has focused on graph models, while PA models on hypergraphs have only recently attracted attention. We introduce a PA hypergraph model which allows us to control how "tree-like" the hypergraph is by changing how many new and pre-existing nodes are included in a newly added hyperedge at each step. Using methods from the field of Topological Data Analysis we compute the Euler Characteristics and low-dimensional Betti numbers of the simplicial complexes formed by the downward closures of these hypergraphs. This analysis reveals structural transitions in the underlying hypergraphs as we vary both the average hyperedge size and the average proportion of new nodes in each new hyperedge. Finally, we introduce a modification of the PA hypergraph model which enforces simpliciality, a measure which describes how similar a hypergraph is to its downward closure.

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PP1

Navigating Alzheimers: Harnessing Multimodal Learning Models for Disease Classification Through PET Brain Imaging Integration

Alzheimers disease (AD) is a neurodegenerative disorder that impairs cognition and daily life. Over 50% of mild cognitive impairment (MCI) cases progress to dementia within five years, with AD being the most common outcome. Early and accurate diagnosis of cognitive decline (CD), including both AD and MCI, is essential for optimizing patient care. Developing data-efficient models could improve the feasibility of PET-based diagnostics across clinical settings. This study integrates PET imaging with quantification analysis using deep learning to enhance CD diagnosis. A multimodal model combines PET image features (PCANet, CNN) with numerical quantification data (DNN). Two data fusion approachescanonical correlation analysis and direct concatenationare explored to integrate image-based and quantification data, which are subsequently used in machine learning classifiers. The model is validated on [^{18}F]FDG PET scans from 252 subjects (118 cognitively normal and 134 with CD, including 70 MCI and 64 AD) from the Alzheimers Disease Neuroimaging Initiative dataset. In 5-fold cross-validation, DNN outperformed CNN and PCANet in accuracy. Integrating DNN and PCANet improved accuracy and reduced variability, suggesting enhanced consistency. The fusion of PET imaging and quantification data offers better diagnostic performance than single-modality approaches. This multimodal framework shows potential for improving CD classification accuracy while reducing data dependency.

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PP1

Reservoir Computing Using Force Training with Conductance-Based Neuron Models

The neuronal models previously used in reservoirs, such as the leaky integrate and fire model, produce discontinuities in the output. By using conductance-based models, which are smooth (i.e., not discontinuous), we test the hypothesis that smooth spiking reservoirs can also learn complex dynamics. We have designed closed-loop reservoirs using conductance-based neuronal models, namely the Morris-Lecar model. The reservoir consists of excitatory and inhibitory neurons sparsely connected with a random binary weight matrix and the sparsity scales inversely with the total number of neurons in the reservoir. We use FORCE training to train the reservoir on time series exhibiting various dynamics, ranging from oscillations to chaotic and hyper-chaotic dynamics. We observe that conductance-based reservoirs perform well in predicting low-dimensional temporal dynamical systems. Future work will directly compare smooth versus non-smooth neuron reservoirs in a matched parameter domain for performance differences.

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PP1

Turning Shapley into Green Values

As in the methods of hedonic modeling [Court, 1939], our objective is to estimate the green value of housing using random forests or XGBoost models by focusing on energy performance labels in order to understand how housing prices evolve when energy performance improves. We must thus extract from the RF or XGBoost models the equivalent of the coefficients estimated for these labels by the hedonic models and compare them. Unlike traditional linear models, which directly reveal the relative importance of the variables via coefficients, these complex models require alternative methods to quantify the impact of the input variables. Shapley values are often used to interpret so-called black box machine learning models, such as random forests and XGBoost, which do not provide explicit coefficients. In the context of machine learning, Shapley values are used to attribute the contribution of each input feature to the prediction of a model. Their calculation guarantees that each feature is fairly represented, taking into account all possible combinations of variables. In our case, we applied several variants of these values (SHAP, KernelSHAP and FastSHAP) to interpret the predictions given by models, by decomposing the effects of individual variables and their modalities, and we managed to propose an estimate of the green value of a housing.

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PP1

Self-Excited Oscillations in a Finite-Length Collapsible Channel Flow with a Heavy Wall

Fluid flow through a finite-length flexible-walled channel serves as a prototypical model for fluid-structure interaction in deformable conduits of the human body. Under certain conditions this fluid-structure interaction system can exhibit self-excited oscillations (SEOs) in the fluid and the wall, reminiscent of instabilities which occur as part of several physiological phenomena. We develop a cross-sectionally averaged (one-dimensional) model for laminar high Reynolds number flow through a long finite-length planar channel, where a segment of one wall is replaced by a thin membrane of finite mass that is held under longitudinal tension. Driving the flow using an imposed upstream pressure, we investigate the static and oscillatory global instabilities of the system, predicting the critical flow conditions required for the onset of SEOs. We examine the asymptotic behaviour of oscillatory normal modes in the limit where the wall mass and tension both become large (with finite leading order frequency). We elucidate a novel asymptotic structure, where the leading order wall motion is determined by a balance between wall inertia and longitudinal tension alone, which then drives flow at the following order. It emerges that this description can be rationally extended in this limit to describe the full two-dimensional flow (without cross-sectional averaging), where we construct further analytical predictions for the onset of self-excited oscillations.

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PP1

Texture Analysis of Satellite Imagery for Weather Forecasting

Weather satellites above the Earth's surface give an ever-changing view of the atmospheric events that trigger severe weather conditions like storms, flash floods, tornadoes, and hurricanes. Due to the large amount of data available today, forecasters use automated tools to correctly identify events visible in a satellite images. Such tools are often created using neural networks, which require large labeled data sets that are simply not available for many weather events. On the other hand, forecasters can reliably identify events by recognizing changes in texture. We present several texture-based methods that distinguish between convective and non-convective clouds in a set of Geostationary Operational Environmental Satellite (GOES) images. We discuss how texture-based methods can be used in tandem with machine learning methods that can then be trained on a small number of labeled samples but still identify complex weather events.

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PP1

Deep Greedy Unfolding: Sorting Out the Argsort Operator in Greedy Sparse Recovery Algorithms

Recent years have seen a growing interest in unrolled neural networks for various signal processing applications. These networks provide model-based architectures that mimic the iterations of an iterative algorithm and, when properly designed, admit recovery guarantees. However, there has been limited work on unrolling greedy and thresholding-based sparse recovery algorithms, such as Orthogonal Matching Pursuit (OMP) and Iterative Hard Thresholding (IHT), and existing efforts often lack full neural network compatibility. The primary challenge arises from the non-differentiable (discontinuous) argsort operator within their iterations, which obstructs gradient-based optimization during training. To address this issue, we approximate argsort operator by a continuous relaxation of it using a proxy called softsort. We then demonstrate, both theoretically and numerically, that the differentiable versions of OMP and IHTtermed Soft-OMP and Soft-IHTserve as reliable approximations of their original counterparts, with minimal error under suitable conditions on the softsort temperature parameter and the gap between elements in the sorted vector. Finally, implementing these algorithms on neural networks, with weights as trainable parameters, reveals that unrolled Soft-OMP and Soft-IHT effectively capture hidden structures in data, establishing a connection between our approach and weighted sparse recovery.

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PP1

- Optimizing Hyperparameters of the Glmnet Function Using Machine Learning for Accurate Solution

The glmnet is one of the most popular R packages for computing lasso solutions in linear regression. The glmnet employs the coordinate descent method, an iterative optimization technique, and the accuracy of the solution depends on hyperparameters such as the convergence threshold for coordinate descent and the number of regularization parameters. These hyperparameters are usually set to default values. However, for high-dimensional or highly correlated data, the accuracy of the solution can be significantly affected by these hyperparameters. Therefore, selecting appropriate hyperparameters is essential to get accurate solutions and achieve fast computation. We propose a machine learning-based method that automatically selects hyperparameters of the glmnet, improving accuracy while ensuring

fast computation. First, we prepare multiple datasets for solving the lasso problem. Next, we apply the lasso algorithm to the datasets and collect data on accuracy and computation time. Then, we train a neural network using this data to model the relationship among the data, the hyperparameters, and their accuracy and computation time. We select the appropriate hyperparameters by using this neural network model. We show that the proposed method effectively selects appropriate hyperparameters of the glmnet function for both real and synthetic datasets. Additionally, we have implemented the method in the R package assg, which is available at https://github.com/Shuhei-Muroya/assg.git.

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PP1

Spiraling Into Shape: Detecting Patterns with Persistent Homology

The field of topological data analysis has proven very useful for detecting structure in objects which may be missed by traditional statistical tools. Persistent homology, as the most popular tool used in topological data analysis, provides a summary of the shape captured at different resolutions. This shape is encoded using homology, which is a vector space representation of the number of holes present in the object. Persistent homology can be captured dynamically with finitely many snapshots to show the evolution of the topological features along some base space. Examples of this include the persistent homology transform (PHT), the Euler characteristic transform (ECT), and the topological vineyards, which promise to be a more wholesome summary of the shape of an object. For zero-order homology, which counts connected components, it has been observed that the PHT can detect the twists in a spiral 2-D embedded graph. This project aims to establish which types of objects exhibit this phenomenon, known as geometric monodromy, in general. It also investigates possible decomposition results for the PHTs of such objects.

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PP1

Deep Learning Approximation of Matrix Functions: From Feedforward Neural Networks to Transformers

Deep Neural Networks (DNNs) have been at the forefront of artificial intelligence (AI) over the last decade. Transformers, a type of DNN, have revolutionized Natural Language Processing (NLP) through models like ChatGPT, Llama and more recently, Deepseek. While transformers are used mostly in NLP tasks, their potential for advanced numerical computations remains largely unexplored. This presents opportunities in areas like surrogate modeling and raises fundamental questions about AI's mathematical capabilities. We investigate the use of transformers for approximating matrix functions, which are mappings that extend scalar functions to matrices. These functions are ubiquitous in scientific applications, from continuous-time Markov chains (matrix exponential) to stability analysis of dynamical systems (matrix sign function). Our work makes two main contributions. First, we prove theoretical bounds on the depth and width requirements for ReLU DNNs to approximate the matrix exponential. Second, we use transformers with encoded matrix data to approximate general matrix functions and compare their performance to feedforward DNNs. Through extensive numerical experiments, we demonstrate that the choice of matrix encoding scheme significantly impacts transformer performance. Our results show strong accuracy in approximating the matrix sign function, suggesting transformers' potential for advanced mathematical computations.

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PP1

A Transfer-Learning Pinn Framework for High-Dimensional Parametric PDEs in Subsurface Flow and Contaminant Transport

Simulating fluid flow and contaminant transport under uncertain subsurface heterogeneities poses a formidable challenge, particularly for high-dimensional parametric partial differential equations (PDEs). We present a novel transfer-learning Physics-Informed Neural Network framework that combines two complementary strategies to account for stochastic variations: (1) Function-Guided Parametric Heterogeneity, where a parametric function with random inputs generates multiple heterogeneous media realizations for sequential refinement of network parameters; and (2) Latent-Encoded Heterogeneity, which employs a pretrained generative decoder to embed complex Gaussian Random Field representations directly into the PINN. Applied to a two-dimensional Darcy flow and contaminant transport problem, this approach captures uncertainty in key parameterssuch as hydraulic conductivity, dispersivity, and sorption coefficientswhile preserving computational efficiency. The framework readily extends to other stochastic PDE scenarios, including variations in boundary conditions or contaminant source locations. Our findings underscore the benefits of transfer-learning PINNs in accelerating convergence across multiple realizations while maintaining strong physical fidelity. Ultimately, this work illustrates how integrating generative modeling, transfer learning, and physics-informed architectures can advance the modeling of uncertain subsurface systems in environmental science.

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PP1

Field-Scale Hydrogen Storage Modeling with the Dusty Gas Model

We introduce a physically accurate, massively parallel, multicomponent gas transport simulator designed for modeling hydrogen storage in geological formations at relevant conditions. We developed a geologic scale Density-based Darcian Dusty Gas model (D3G) within a parallel computing framework to represent gas flow and transport in the subsurface systems relevant to hydrogen storage, which can enhance efficiency of renewable energy sources, providing a sustainable solution in the fight against climate change. Hydrogen storage in porous media requires a cap rock and cushion gas to create a pocket to retain the hydrogen. Cushion gas is essential due to hydrogens small molecular cross-section, light weight, and low viscosity. Hydrogen often migrates up a concentration gradient, with its flow in porous media dominated by Klinkenberg slip, while the cushion gas behaves more conventionally. Traditional subsurface multiphase flow simulators, which use a combination of Darcys law for advection and Ficks law for diffusion and dispersion, cannot accurately simulate these conditions. This poster demonstrates injection and withdrawal cycles in a hypothetical hydrogen storage scenario in 3D, using millions of grids cells representing the domain. It also highlights the models scalability simulating complex interactions at the molecular level among, vapor, two gases, and the porous media. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525 SAND2025-01472A

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PP1

Simulations of Eigenvector Preferential Attachment Networks

Since the preferential attachment network [Barabsi and Albert, 1999] was popularized in the early 2000s, applications across many disciplines have appeared. A notable variant of this model is nonlinear preferential attachment, in which new vertices are attached to existing vertex v_i with probability $\frac{d_i^\gamma}{\sum_i d_i^\gamma}$ for $\gamma \in \mathbb{R}$. Adami et al. [2024] introduced eigenvector preferential attachment, wherein probability of attaching to a vertex is given by its eigenvector centrality, or its corresponding entry in the Perron-Frobenius eigenvector of the graph's adjacency matrix. We present simulations pertaining to several properties of mathematical interest, for example a condensation phenomenon with a 'superhub' dominating the graph, and sublogarithmic height, similar to that of superlinear preferential attachment. We describe directions for rigorous research into this model as well as potential challenges.

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PP1

Mathematical Analysis of Neurite Morphologies and Observation of Protein Aggregations in the Developmental Process of Human iPSC-Derived Neurons

Defining the morphological disorders of neurites causing neurodegenerative diseases such as Alzheimer's disease (AD) is an unsolved problem. In this study, we present mathematical analyses to quantify the neurite morphologies and assess the pathological state induced by AD. We first examined the neurite morphologies in the development process of iPSC-derived neurons of a healthy person and an AD patient. Their microscopic images (40X) were captured on day in vitro 3 (DIV3), DIV5, DIV7, DIV10, and DIV14 using a phase contrast microscope. From the microscopic images at each developmental stage, the neurite morphologies were analyzed based on a mathematical method (Loewner equation). For the driving force calculated from the Loewner equation, detrended fluctuation analysis (DFA) was performed, and the neurite morphologies were quantified by the fluctuation characteristics, that is, scaling exponent. The scaling exponent showed differences between healthy and AD neurites from the early stage (DIV3). Additionally, we observed the expressions of beta-amyloid and phosphorylated tau, which are known as biological factors causing AD, by immunofluorescence-staining. The results showed that the differences of their expressions between healthy and AD neurites followed the differences of the mathematically obtained quantities. Thus, the present mathematical analyses could be utilized for quickly assessing the pathological state of neurites induced by AD.

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PP1

Tensor Tv Regularization and Convolution Neural Networks Deblurring and Denoising

We consider and extend the classical Rudin-Osher-Fatemi functional for variational denoising and deblurring to tensor structured data images and videos through multi-dimensional total variation regularization. The generalization results in a minimization problem that is calculated by the fast iterative shrinkage-thresholding method for tensors. We provide several numerical experiments by applying the method to the denoising and deblurring of color images and videos. We show an analysis of how our model performs against a lightweight pre-trained Convolutional Neural Network, and how it can work in tandem with machine learning methods to supplement them without adding significant computational expense.

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PP1

Energy Based Time Stepping Methods for Phase Field Models

Phase field models (PFMs) are used to model a microstructure using continuous field variables. Given the free energy, we want to find a configuration of the field variable that will yield the lowest free energy. This can be achieved by minimizing the free energy which gives a PDE that typically combines low-order nonlinear terms with higher-order linear terms. A simple phase field model is the Cahn-Hilliard model, which gives rise to a fourth-order PDE when we minimize its free energy. We implement the scalar auxiliary variable (SAV) method which guarantees that the discrete energy decays. We compare two different adaptive time stepping schemes. A method that uses the field variable to control the error has already been developed. We developed a method that controls the error using the free energy and compared the two methods. Additionally, we develop a machine learning based adaptive time stepping method and compare it to classical methods.

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PP1

Graph Foundation Models for Flow and Transport Dataset of Discrete Fracture Network

Quantifying flow and transport through porous fractured media in the subsurface is critical in civil, industrial, and security applications, including the management of drinking water aquifers, hydrocarbon extraction, etc. The graphic data set from the computation suites Discrete Fracture Network (DFN) is employed to simulate flow and transport in such fracture media at scales ranging from millimeters to kilometers. We consider the graphical representation of DFN where nodes represent fractures which is further comprised by topological and physical attributes, and edges denote fracture intersections. One of the crucial node attributes present in the DFN graphical dataset is the physical pressure variable which is governed by Darcy flow equation. Predicting this pressure variable on all nodes for a DFN dataset based on topological and physical attributes remains a key challenge. We take advantage of graph-based foundation model that have emerged as critical components in a variety of artificial intelligence platforms that have showcased significant success in natural language processing and several other areas. We apply two graph foundation models from the class of Graph Neural Networks, which are Graph Convolutional Networks and Graph Attention Networks, to the graphical datasets of DFN. With these graph representation learning architectures, we show pressure variable predictions followed by node-level identification classification as well.

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PP1

A Reaction-Advection-Diffusion Model for Alzheimers Disease: A Preliminary Mathematical Model of Differential Susceptibility to Amyloid-?

The peptide Amyloid Beta (A) is known to play a critical role in the onset of Alzheimer's disease. It exists in a variety of conformations, including monomers, oligomers, and fibrils. Of these forms, oligomers and fibrils are of particular interest due to their varying degrees of toxicity. Factors such as production, clearance, transport, internalization, externalization, and aggregation can lead to changes in the concentrations of these species, which in turn affect neuronal health in different regions of the brain. Here, we present a mathematical model focused on differential susceptibility and key A species to describe Alzheimers progression. Model parameters are informed by published literature on A kinetics, cell viability assays, and other experiments. We focus on the hippocampus, cerebral cortex, and cerebellum, finding varying levels of accordance between our model and clinical outcomes. Additionally, we quantify the relative influence of different biological parameters in predicting the course of the disease.

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PP1

Mathematical Modeling of Ocular Tissue Deformation Due to Contact Lens Wear Accounting for Intraocular Pressure

Myopia is one of the most common ocular disorders in the world impacting approximately 28% of the global population. Orthokeratology (ortho-k) lenses are stiff contact lenses worn overnight that reshape the cornea so that corrective lenses do not need to be worn during the day. The goal of this project is to develop a mathematical model to predict the deformation of the ocular surface due to contact lenses, where the shapes of both the eye and the lens are emergent properties. We model the ocular surface as a strip of tissue, and we assume the ocular tissue is a linear elastic material deformed by intraocular pressure (IOP) and suction pressure from the contact lens. We approximate the model using finite elements in FreeFem++. To predict the stress-free reference configuration for a desired stressed ocular shape we will present an iterative algorithm and perform a convergence analysis using a simplified oc-

ular geometry. We couple the contact lens to the ocular deformation model iteratively, assuming the lens conforms to the eye due to the elastic properties of the lens. We will present results quantifying deformation to the ocular surface and the resulting stresses exerted on the ocular tissue due to the lens.

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PP1

Robust Risk Budgeting in Portfolio Management: A Manifold Optimization Perspective

The risk budgeting problem is widely considered an efficient strategy in portfolio management which allocates the total risk of a portfolio among various assets according to their contribution to the total risk. We introduce a new geometric approach for solving the robust risk budgeting problem combined with the variance risk measure under the uncertainty of the covariance matrix. We consider the uncertainty set of all positive definite matrices that are close enough to the nominal matrix estimated based on the historical data. Our approach benefits from geometric structure of the manifold of positive definite matrices for the uncertainty parameter and the manifold of Euclidean positive orthant for decision variables of the problem. Particularly, we will apply the retraction-based gradient descent ascent algorithm to solve the manifold min-max robust risk budgeting problem. Furthermore, we demonstrate the efficiency of our approach through numerical experiments.

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PP1

Modelling Plant Cortical Microtubules

The self-organization of cortical microtubule arrays within plant cells is an emergent phenomenon with important consequences for the synthesis of the cell wall, cell shape, and subsequently the structure of plants. Mathematical modelling and experiments have elucidated the underlying processes involved. However, the mechanical influence of membrane curvature on these elastic filaments has largely been ignored. We previously proposed a model to describe how the anchoring process may control the deflection of individual microtubules seeking to minimize bending on a cylindrical cell. We implement this process into a model of interacting microtubules and find the cell curvature influence should be significant: the array favours orientations parallel to the direction of elongation rather than the expected transverse direction. Even without elasticity, the geometry of large cells hinders robust microtubule organization. These results suggest the necessity of additional processes to overcome these factors. Alongside this, there has been growing interest in modelling the influence of various other processes such as nucleation and membrane tension. We present ongoing efforts in piecing together our results with others from increasingly complex models, with the goal of better understanding the bigger picture of microtubule organization.

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PP1

Analysis of Unbalanced Optimal Transport Methods for Single-Cell Gene Expression Data

In recent times Optimal Transport has been used address the problem of trajectory inference in single cell sequencing data. Existing methods, which build upon the work of [G. Schiebinger et al., Optimal-Transport Analysis of Single-Cell Gene Expression Identifies Developmental Trajectories in Reprogramming, Cell, vol. 176, no. 4, pp. 928-943.e22, Feb. 2019, doi: 10.1016/j.cell.2019.01.006.] utilise the unbalanced entropic optimal transport formulation to model the changes of the probability distributions in the gene expression space. The current method claims to incorporate biological knowledge of cell growth rates by using this as a prior knowledge upon which the transport matrix is built. Our results here show that in the feasible parameter space, the initial estimates of the model have little to no effect on the final results. We show in our work that the soft penalties on the marginal constraints, imposed by KL-Divergence are not sufficient to overcome the effect of the distance term in real world datasets .We further provide an alternative approach which better incorporates prior biological knowledge of cell growth rates and differentiation into the model.

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PP1

Efficient Leverage Score Sampling for Tensor Train Decomposition

Tensor Train (TT) decomposition is widely used in the machine learning and quantum physics communities as a popular tool to efficiently compress high-dimensional tensor data. In this paper, we propose an efficient algorithm to accelerate computing the TT decomposition with the Alternating Least Squares (ALS) algorithm relying on exact leverage scores sampling. For this purpose, we propose a data structure that allows us to efficiently sample from the tensor with time complexity logarithmic in the tensor size. Our contribution specifically leverages the canonical form of the TT decomposition. By maintaining the canonical form through each iteration of ALS, we can efficiently compute (and sample from) the leverage scores, thus achieving significant speed-up in solving each sketched least-square problem. Experiments on synthetic and real data on dense and sparse tensors demonstrate that our method outperforms SVD-based and ALS-based algorithms.

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PP1

A Time-Frequency Method for the Acoustic Wave Equation

Time-frequency methods for solving the acoustic wave equation on an exterior domain have many advantages over alternative direct-in-time approaches. However, these methods can be expensive and challenging to use in domains with trapping regions. The slow decay of the trapped waves severely reduces the region of analyticity of the solution in frequency space while simultaneously making the inverse Fourier transform integral highly oscillatory. Our approach improves analyticity properties through a complex deformation. Afterwards, the resulting oscillatory integral is handled through a fast sinc transform method. This combination results in a highly accurate and computationally efficient method for solving the wave equation, even when decay over time is slow.

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PP1

Evaluating Probabilistic and Data-Driven Inference Models for Fiber-Coupled Nv-Diamond Temperature Sensors

We evaluate the impact of inference model on uncertainties when using continuous wave Optically Detected Magnetic Resonance (ODMR) measurements to infer temperature. Our approach leverages a probabilistic feedforward inference model designed to maximize the likelihood of observed ODMR spectra through automatic differentiation. This model effectively utilizes the temperature dependence of spin Hamiltonian parameters to infer temperature from spectral features in the ODMR data. We achieve prediction uncertainty of $\pm$ 1 K across a temperature range of 243 K to 323 K. To benchmark our probabilistic model, we compare it with a non-parametric peak-finding technique and data-driven methodologies such as Principal Component Regression (PCR) and a 1D Convolutional Neural Network (CNN). We find that when validated against out-of-sample dataset that encompasses the same temperature range as the training dataset, data driven methods can show uncertainties that are as much as 0.67 K lower without incorporating expert-level understanding of the spectroscopic-temperature relationship. However, our results show that the probabilistic model outperforms both PCR and CNN when tasked with extrapolating beyond the temperature range used in training set, indicating robustness and generalizability. In contrast, data-driven methods like PCR and CNN demonstrate up to ten times worse uncertainties when tasked with extrapolating outside their training data range.

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PP1

A Discrete Phase Plane Tool

In this research work, we develop a tool in Julia to generalize the results of the paper by Sabrina H. Streipert and Gail S.K. Wolkowicz, "An augmented phase plane approach for discrete planar maps: Introducing next-iterate operators, Mathematical Biosciences 355 (2023) 108924. The purpose is to augment the phase portrait to determine the global dynamics of planar discrete systems with complex behaviors. The first generalization is to consider isoclines for any given set of directions rather than simply those associated with the coordinate directions. We show that choosing directions aligned with eigenvectors of the Jacobian at a fixed point aids in making conclusions about global dynamics. The second generalization we made was to add a curve indicating where the determinant of the Jacobian is zero and the image of that curve. This helps identify the range of the mapping, effectively reducing the space one needs to consider when determining global dynamics. This tool also allows the user to perform higher iterations, thus the reflections associated with negative eigenvalues can be eliminated by using the twice-iterated map. We determined the global stability for certain models that was indeterminable without the generalization we introduced.

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CP1

Biologically Interpretable Machine Learning Approaches for Analyzing Neural Data

Deep neural networks (DNNs) often achieve impressive classification performance, but they operate as "black boxes," making them challenging to interpret. This study explores biological neural networks (BNNs) by applying backpropagation to biophysically accurate neuron models. Using BNNs, we classify electroencephalogram (EEG) and non-EEG signals, generate EEG signals, and analyze EEG neurophysiology through model-derived parameters. Our BNNs achieve strong performance in classifying handwritten digits from the MNIST Digits Dataset and EEG recordings corresponding to alertness vs. fatigue, varying levels of consciousness, and different workload levels. They require fewer parameter adjustments while accurately capturing temporal dynamics, leading to faster learning and improved interpretability. We find similarities between these numerically efficient learning mechanisms and Hebbian learning in the brain, in terms of how weights change the loss function and how changing the weights at specific time intervals affects the loss function. Additionally, we trained our BNNs to exhibit different frequencies observed in EEG recordings and found that the variability of synaptic weights and applied currents increased with the target frequency range. Overall, applying backpropagation to accurate ordinary differential equation models for analyzing neuronal data can enhance our ability to classify and better understand neuronal activity and neural network learning.

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CP1

Entropic Learning Enables Skilful Forecasts of Enso Phase at Up to Two Years Lead Time

This paper builds on previous work in applying the entropy-optimal Sparse Probabilistic Approximation (eSPA) machine learning algorithm to the task of classifying the phase of ENSO, as determined by the Niño3.4 index (Groom et al., *Artif. Intell. Earth Syst.*, 2024). In this study, only observations and reanalyses from the satellite era are employed when training and validating the entropic learning models, and a full set of hindcasts are performed over the period from 2012 to 2022 in order to determine out-of-sample skill. The features used for prediction are the leading principal components from a delay-embedded EOF analysis of global sea surface temperature, the vertical derivative of temperature at the equator and the zonal and meridional wind stresses in the tropical Pacific. Despite the limited number of data instances available for training, eSPA is shown to avoid overfitting in this small data regime and produces categorical forecasts with comparable skill to the combined probabilistic forecasts produced from the International Research Institute for Climate and Society (IRI) ENSO prediction plume. At lead times longer than those available from the IRI plume, eSPA maintains skill out to 23 months in terms of the ranked probability skill score and $\geq$24 months in terms of the area under the ROC curve, all at a small fraction of the computational cost of running a dynamical ensemble prediction system.

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CP1

Phase Model Analysis of the Effect of Acetylcholine on the Neural Synchrony in Hippocampal Networks

Neural assemblies—transiently coordinated groups of neurons—are observed in the hippocampus and are thought to support episodic memory encoding and consolidation. Acetylcholine (ACh), a key neuromodulator, plays a crucial role in these processes. High ACh levels during active exploration and REM sleep promote encoding, while low levels during quiet waking and slow-wave sleep facilitate consolidation. We investigate how ACh modulates neural assembly formation via its impact on synchrony in the CA3 region of the hippocampus. Using a computational model of pyramidal neurons with an M-current, a slow, non-inactivating potassium current suppressed by ACh, we explore the emergence of neural assemblies, mathematically represented as cluster solutions. A phase model approximation is derived and used to analyze the existence and stability of these clusters in networks with all-to-all, symmetric distance-dependent, and nearest-neighbour coupling. Our results show that ACh can reshape network dynamics to support distinct states. Low ACh promotes global synchrony, while high ACh allows for multiple stable cluster states, enabling diverse activity patterns linked to encoding. This suggests a mechanism by which ACh modulates CA3 dynamics to regulate the different stages of memory formation.

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CP1

Rarefaction Wave Interaction and Existence of a Global Smooth Solution in the Blood Flow Model with Time-Dependent Body Force

In this talk, we introduce a simplified 1-dimensional (1D) inhomogeneous system of conservation laws governing blood flow in the cardiovascular system, and discuss how a reduced 1D model can be derived using conservation principles. We then consider the interaction of two centered rarefaction waves. First, we analyze the Riemann solutions, demonstrating that the solutions lose self-similarity due to the source term. By transforming the system into non-reducible diagonal form in Riemann-invariant coordi-

nates, we show how the interaction gives rise to a Goursat boundary value problem (GBVP). Consequently, discuss the existence and uniqueness of global C^1 solution to the GBVP using *a priori* C^1 bounds. Finally, present the results of the wave interaction, establishing that no vacuum forms within the interaction domain if the boundary data remain vacuum-free, and a vacuum emerges if the rarefaction waves fail to fully penetrate each other within finite time.

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CP1

Emergence of Multirhythmicity in Cortical Networks with Two Types of Inhibition

We study a network model composed of three interacting neuronal populations: pyramidal (Pyr) cells, parvalbumin-positive (PV) interneurons, and somatostatin-positive (SST) interneurons. Starting from a network of globally coupled quadratic integrate-and-fire (QIF) neurons with heterogeneous inputs, we reduce the full spiking network to a low-dimensional mean-field model consisting of 9 ordinary differential equations (ODEs) three for each population. This reduced system captures the essential dynamics of the network, allowing for tractable bifurcation and phase space analysis. We demonstrate the emergence of multistability, oscillatory switching, and coexisting rhythms (mixed beta states) across the populations. In particular, we find that the strength and directionality of inter-population interactions critically depend on SST-IN-mediated inhibition, which modulates transitions between distinct beta-band oscillatory states. Our results reveal how multiple subtypes of inhibitory neurons coordinate to generate and regulate complex beta dynamics, with potential implications for understanding neural mechanisms underlying motor control, cognitive function, and beta-band abnormalities observed in disorders such as Parkinsons disease.

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CP1

Using A Mathematical Model To Resolve Lassa Fever Persistence

Lassa fever (LF), caused by the Lassa virus and transmitted primarily by *Mastomys natalensis* rodents, is a severe hemorrhagic disease endemic to West Africa, with significant morbidity and mortality rates. This study develops dynamic models for LF, incorporating often overlooked factors such as vertical transmission in rodents, surface contamination, and asymptomatic human carriers. The persistence of the disease is shown analytically. Using data from Nigeria to train the models, the impact of various control and mitigation measures is assessed. The results of the study reveal that asymptomatic individuals are key drivers of LF and that including additional LF virus transmission pathways, e.g., vertical transmission and environmental contamination, increases the estimated reproduction number threefold compared to previous studies. Models incorporating rodent dynamics show the highest disease prevalence, highlighting the critical role of rodent control. In addition, a multifaceted approach, combining antiviral treatment, environmental disinfection, and personal protective equipment, significantly enhances disease control, while the introduction of a competitor rodent species can drastically reduce human and rodent infections. Ultimately, the study underscores the need for integrated, multifaceted strategies, including targeting rodents, asymptomatic cases, and comprehensive treatment and disinfection protocols, for effective LF management.

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CP2

Robust Text Decoder Using Hadamard Long Short-Term Memory with Bayesian Hyperparameter Optimization

End-to-end encryption (E2EE) is a security method that ensures communication between two parties, preventing unauthorized access to the data. However, such E2EE platforms can be used by criminals to protect their communications, hindering law enforcement efforts to investigate crimes. Thus, while E2EE provides a layer of security for legitimate users, it creates challenges for law enforcement by allowing criminals to evade detection. Here, we investigate the use of machine learningspecifically, long short-term memory (LSTM)for the task of decrypting text-based messages without prior knowledge of the encryption scheme. The study is motivated by whether a neural sequence model can learn to reverse a deterministic character-level encryption through exposure to input-output examples alone. We generate data, i.e., sentences, encrypted via a fixed and unknown substitution cipher. The model is trained to map encrypted character sequences back to their original form with cross-entropy loss. Since the sentences vary in length, the masking process is implemented using the Hadamard approach in which the loss function is computed pointwise. The trained model achieves near-perfect performance on held-out validation and test sets. The best model performance is attained by incorporating the LSTM model with Bayesian hyperparameter optimization. A key observation is that the LSTM learns the decryption mapping and linguistics, and generalizes to new sentences it has never seen.

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CP2

Spectral Finite Element Method for Linear Dispersive Metamaterials

Metamaterials exhibit unique electromagnetic properties that arise from their engineered microstructures rather than their intrinsic material composition. Their response to electromagnetic waves is governed by effective medium models such as the Drude and Lorentz models, which characterize frequency-dependent permittivity and permeability. Understanding wave propagation in dispersive metamaterials requires solving Maxwells equations with constitutive relations incorporating these models. In this study, we employ the Spectral Finite Element Method (FEM) to analyze linear dispersive metamaterials. Spectral FEM leverages high-order basis functions, offering superior ac-

curacy and computational efficiency compared to conventional finite element methods, particularly for problems with wave-like solutions. We derive the weak formulation incorporating the Drude and Lorentz models and investigate the dispersion relation of the system. The numerical approach is validated against analytical solutions, demonstrating the effectiveness of Spectral FEM in capturing wave dispersion in metamaterials. Our results highlight the advantages of spectral methods in modeling complex dispersive media and provide insights into wave behavior in engineered electromagnetic materials.

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CP2

A Conditionally Stable Partitioned Algorithm Using for Conjugate Heat Transfer Problem

In this talk, we propose a novel, provably conditionally stable weakly coupled partitioned scheme to solve the conjugate heat transfer (CHT) problem. In the monolithic approach, a single numerical solver is developed to solve for all unknowns simultaneously. In contrast, a partitioned approach applies two separate solvers in each of the sub-domains, which are sequentially solved. Monolithic solvers are computationally efficient and robust but need to be designed for each new multi-physics problem, while partitioned schemes can take advantage of existing solvers. On the other hand, many partitioned schemes may encounter stability issues. We consider a model CHT problem consisting of linear advectiondiffusion and heat equations, coupled at the interface through the continuity of temperature and heat flux. We employ high-order summation-by-parts finite-difference operators in conjunction with simultaneous-approximation-terms (SAT) in curvilinear coordinates for spatial derivatives, combined with first- and second-order time discretization, and extrapolation in time at the interface. We demonstrate that the proposed scheme is energy stable for a range of penalty parameters related to the SAT terms at the interface, along with a CFL-like relationship between the spatial and temporal grid spacings. We present numerical experiments in a 2D model problem to show effectiveness of the approach

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CP2

A Crank-Nicolson Finite Difference Scheme for Coupled $(2+1)$D Nonlinear Schrödinger Equations with a Modified Nonlinearity and Nonlinear Damping

We investigate a Crank-Nicolson finite difference scheme for a class of coupled $(2+1)$D nonlinear Schrödinger equations featuring modified nonlinearities and generalized nonlinear damping. We establish the boundedness, existence, and uniqueness of the numerical solution and demonstrate the scheme's convergence. The convergence rate achieves second order accuracy in both the time step and spatial mesh size. Extensive simulations validate the numerical scheme.

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CP2

Hadamard Deep Autoencoders with Bayesian Hyperparameter Optimization for Blind Decoding of Encrypted Texts

Encrypted communication systems are essential for protecting sensitive information across digital platforms. Yet, in adversarial contextssuch as military, intelligence, or cyber-warfarethese same systems can obscure the strategies and intentions of hostile actors. Inspired by historical cryptanalysis efforts, including the decryption of the Enigma cipher during World War II, we explore whether modern neural network architectures can learn to reverse deterministic encryption schemes without prior knowledge of their structure. Specifically, we employ autoencoders to recover plaintext from text encrypted using a fixed character-level substitution cipher. The model is trained on paired sequences of encrypted and original text, using reconstruction loss to guide learning. Since the sentences vary in length, the masking process is implemented using the Hadamard approach in which the loss function is computed pointwise. Unlike recurrent models, autoencoders offer a compressed representation of the input space, allowing the model to decompose linguisticand cipher information to directlylearn a description mapping. Through Bayesian optimization, we refine model parameters to improve generalization. Our approach achieves perfect decryption accuracy on unseen test sequences, demonstrating that even in the absence of cipher specifications, autoencoders can infer the underlying mapping.

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CP2

Recent Advances in Space-Time Spectral Methods

for PDEs in Irregular Geometry

One major drawback of classical spectral methods is their inability to handle irregularly shaped domains, which is why they have only been used sparingly in many engineering problems. Spectral element methods can handle complex geometry, but they are more difficult to implement. There have been many attempts to use classical spectral methods for elliptic PDEs in irregular domains, but there are fewer studies on spectral collocation methods for time-dependent PDEs in complex geometries. Here, we propose a numerical method to approximate the solution of time-dependent PDEs in irregular domains using space-time spectral collocation methods. The main idea is to embed the irregular domain in a regular one and extend the data from the physical domain to the larger regular domain. To achieve this, Huybrechs' method was implemented for 1D Fourier extension of the non-homogeneous term with exponential accuracy. Further, we also successfully implemented a one-dimensional non-periodic extension by modifying the Huybrechs' method. For 2D domains, a new method named 'Alternating Non-periodic Extension' was developed. This algorithm uses non-periodic extensions combined with domain embedding to achieve a practical solution methodology. Implementations for the 2D Poisson, Heat, unsteady Stokes and Navier-Stokes equations on convex and non-convex domains demonstrate spectral convergence.

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CP3

Optimal Timing for Staged Vaccination Campaigns: Insights from Scenario Tree-Based Stochastic Optimization

We develop a mathematical modeling framework to address the challenge in launching an effective staged vaccination campaign during a typical viral infection season to avoid an overwhelmed healthcare system for the entire season. Taking as an example the COVID-19 pandemic after its acute (pandemic) phase, our model takes into account the willingness of the public to receive vaccines, as well as the uncertainty of vaccination delivery and administration, to achieve the objective of optimizing the timing of the vaccine campaign and distribution subject to the global constraint that infected individuals needing hospitalization should not exceed the healthcare capacity. The integration of a dynamic transmission model coupled with scenario tree-based stochastic optimization techniques allows for the analysis of future scenarios characterized by uncertainties in vaccination rates, contact mixing, and public adherence to safety measures during different phases of the season. Identifying these future scenarios facilitates the search for strategies to dynamically adjust the timing and scale of vaccine and contact mixing during distinct phases of the viral season. Our study demonstrates that a well-timed, well-phased vaccination campaign, along with other public health interventions, can prevent overcrowding in hospitalization in a typical viral infection season.

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CP3

Density-Accuracy Tradeoffs in Real-World Graph Spanners

Graph spanners are a classical and well-studied concept in graph theory with a plethora of algorithmic applications. A spanner is a sparse spanning subgraph which preserves distances in the original graph up to some additive or multiplicative stretch. The sparsity and approximation guarantees raise a natural question: can spanners serve as (the backbone of) space-efficient data structures for approximate distance computation in real-world networks? Toward this goal, we make the first systematic study of the size and accuracy (additive error) of existing spanner construction on real-world social and information networks. Our work exhibits a number of surprising findings, which shed light on the structure of these networks, and may inspire downstream algorithm design. As it turns out, state of the art techniques using low diameter decompositions tend to produce very sparse, almost tree-like spanners in several large real-world networks. However, the real-world additive error of these spanners is suboptimal, and we show that slightly denser constructions based on the core-periphery structure may offer a more accurate alternative.

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CP3

Superfast 1-Norm Estimation

A matrix algorithm is said to be superfast (aka runs at sublinear cost) if it involves much fewer scalars and flops than an input matrix has entries. Such algorithms have been extensively studied and widely applied in modern computations for matrices with low displacement rank and more recently for low rank approximation of matrices, even though any superfast algorithm fails on worst case inputs for the latter problem. We extend this study to a new area by proposing three distinct superfast 1-norm estimators. In our extensive tests with synthetic and real word matrices all three have output 1-norm within relative error 1.5, while the outputs of two of them were consistently as accurate as LAPACK's. We point out some promising extensions of our surprisingly simple techniques. With further testing and refinement our algorithms should eventually win user's

attention.

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CP3

An Aggregated Metrics Framework for Multi-Criteria Model Validation Using Rolling Origin Evaluation

Traditional time series validation, such as Rolling Origin Evaluation (ROE), often relies on a single error metric and assumes that forecast errors are independent across series. This approach is inadequate for complex domains like banking stress testing, where models must be judged on multiple, correlated performance criteria. This paper introduces an aggregated metrics framework to extend ROE for robust multi-criteria model validation. We propose enhanced formulations of three complementary metrics: the Weighted Sum of Errors (WSA), the Weighted Aggregate Performance Metric (WAPM), and the Combined Error and Standard Deviation Metric (CESDM). Critically, our framework directly confronts the challenge of interdependent forecasts by introducing correlation-adjusted metrics, which penalize models for systemic, correlated errors. We validate the framework through a banking stress testing case study, demonstrating with numerical examples how our methodology leads to more insightful and reliable model selection compared to traditional baselines. This work provides a structured and quantifiable methodology for holistic model evaluation, better aligning the selection process with complex, multi-dimensional business objectives.

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CP3

Minimizing a Weakly Convex Function

We study the minimization of a weakly convex function that is the sum of two components: the first is convex, and the second is nonconvex. Specifically, we focus on two cases for the second function: one is weakly convex (WC), and the other is a difference-of-convex (DC) function. To solve both cases, we apply the alternating direction method of multipliers (ADMM), where the subproblems either have closed-form solutions or can be solved iteratively. To improve computational efficiency while maintaining accuracy, we incorporate an early stopping condition. We compare the proposed algorithms on two examples: the three-hump Camel function and a regularized sparse recovery problem, showing improved accuracy and efficiency compared to traditional methods.

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CP3

Superfast Low Rank Approximation

Low Rank Approximation (LRA) of a matrix are invaluable for Numerical Linear Algebra and Data Science. Some recent papers propose superfast algorithms that output LRAs with near-optimal accuracy for a large class of inputs but, as ANY superfast LRA algorithm, fail on a large class of inputs as well. To narrow the latter class we first superfast compute a crude initial LRA by applying one of these or another superfast algorithm (we specify a novel class of such algorithms). Then we recursively refine that LRA superfast by extending iterative refinement algorithms for the solution of the systems of linear and nonlinear equations and by applying the recent techniques of oversampling and compression of J. A. Tropp, A. Yurtsever, M. Udell, V. Cevher, Streaming Low-Rank Matrix Approximation with an Application to Scientific Simulation, SIAM J. on Scientific Computing, 41, pp. A2430–A2463, 2019; this enables us to control rank growth in the refinement. We analyze our algorithms and test them numerically.

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MS1

Slicing Unbalanced Optimal Transport

Optimal transport (OT) has emerged as a powerful framework to compare probability measures, a fundamental task in many statistical and machine learning problems. Substantial advances have been made over the last decade in designing OT variants which are either computationally and statistically more efficient, or more robust to the measures and datasets to compare. Among them, sliced OT distances have been extensively used to mitigate optimal transport's cubic algorithmic complexity and curse of dimensionality. In parallel, unbalanced OT was designed to allow comparisons of more general positive measures, while being more robust to outliers. In this paper, we propose to combine these two concepts, namely slicing and unbalanced OT, to develop a general framework for efficiently comparing positive measures. We propose two new loss functions based on the idea of slicing unbalanced OT, and study their induced topology and statistical properties. We then develop a fast Frank-Wolfe-type algorithm to compute these loss functions, and show that the resulting methodology is modular as it encompasses and extends prior related work. We finally conduct an empirical analysis of our loss functions and methodology on both synthetic and real datasets,

to illustrate their relevance and applicability.

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MS1

Sliced Wasserstein Kernel for Topological Descriptors

Persistence Diagrams (PDs) and Signed Barcodes (SBs) play a key role in topological data analysis (TDA), in which they are routinely used to describe topological properties of complicated shapes. Both PDs and SBs enjoy strong stability properties and have proven their utility in various learning contexts. They do not, however, live in a space naturally endowed with a Hilbert structure and are usually compared with non-Hilbertian distances, such as the bottleneck distance. In this talk, I will discuss the Sliced Wasserstein approximation of the Wasserstein distance to define a new kernel for PDs and SBs, which is provably stable, and also discriminative for PDs (with a lower bound depending on the number of PD points). We also demonstrate its practicality, by developing an approximation technique to reduce kernel computation time, and show that our proposal compares favorably to baselines on several benchmarks.

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MS1

Liouville PDE-Based Sliced Wasserstein Flows

The sliced Wasserstein flow (SWF), a nonparametric and implicit generative gradient flow, is applied to fair regression. We have improved the SWF in a few aspects. First, the stochastic diffusive term from the Fokker-Planck equation-based Monte Carlo is transformed to Liouville partial differential equation (PDE)-based transport with density estimation, however, without the diffusive term. Now, the computation of the Wasserstein barycenter is approximated by the SWF barycenter with the prescription of Kantorovich potentials for the induced gradient flow to generate its samples. These two efforts improve the convergence in training and testing SWF and SWF barycenters with reduced variance. Applying the generative SWF barycenter for fair regression demonstrates competent profiles in the accuracy-fairness Pareto curves.

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MS2

Model Discovery for Differential Algebraic Systems Using Limited Data

Differential-Algebraic Equations (DAEs) represent a broad class of differential equations that couple differential equations with algebraic relationships. These equations often represent fundamental physical principles, such as conservation laws, steady-state approximations, and system constraints. They appear across various scientific and engineering fields, including chemical engineering, power grid modeling, semiconductor physics, etc. Despite their importance, the problem of discovering models for Differential-Algebraic Equations (DAEs) is still underexplored, especially when dealing with limited and noisy data. In this talk, we will begin by discussing our recent work on SODAS (Sparse Optimization for Differential-Algebraic Systems). This framework allows for the direct identification of differential-algebraic equations (DAEs) in their original coupled form, eliminating the need to reduce them to ordinary differential equations. As time allows, we will also introduce a framework for improving the conditioning of the candidate library using orthogonalization techniques and identify the algebraic equations involved in this process.

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MS2

An Analysis of Interpretable Model Reduction for Dynamical Systems from Small and Noisy Data

Large-scale nonlinear dynamical systems often involve many interacting components. In these situations it becomes critical to identify the components that drive the coarse-scale behavior of the system. This enables a deeper understanding of the system, and the use of reduced models to accelerate simulations. The identification of these components relies on available data, which often consists of observed trajectories and measured parameters. Having sparse or noisy data can impact substantially the ability to identify these key components. In this talk, we present an analysis of IRENE2 (for Interpretable Reduction of Nonlinear Evolution Equations) in the small and noisy data regime. Our results show that the stability of the reduced models computed by IRENE2 depends substantially on the underlying dynamics, but also on the a priori decomposition of the system into elementary components. We show results in non-linear dynamical systems including chemical reaction networks.

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MS2

Interpretable Learning of Conservation Laws from Sparse Noisy Data

As data-driven learning of dynamical systems has increased in power and popularity in recent years, one challenge that has remained less widely studied is automated discovery of conserved quantities, especially in the setting of small and noisy datasets. In dynamical systems modeling, the ability to derive conserved quantities has important implications for model reduction and model accuracy, in addition to scientific understanding of underlying symmetries. However, finding conserved quantities corresponds to learning implicit equations g(x)=0 satisfied by dynamic trajectories, which is challenging to do in traditional supervised learning frameworks since it is difficult to avoid trivial solutions. This talk will discuss a new probabilistic framework for learning implicit equations from data. First, we

will explore why implicit symbolic regression is so challenging, especially in the small and noisy data setting. Then, we will derive a probabilistic framework for constructing a fitness function that resolves many of these difficulties, and is furthermore compatible with most existing symbolic regression algorithms. Finally, will show how this framework can be used to discover a complete set of independent implicit equations satisfied by the data, and how this can be utilized to recover conserved quantities from dynamic trajectories. We will conclude with a discussion of opportunities and challenges in utilizing this framework for physics-informed machine learning.

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MS2

Nonlinear Model Reduction for Hypersonic Flows

Reduced-order models (ROMs) are generally unreliable for convection-dominated problems, like those in hypersonic flows, due to the Kolmogorov barrier caused by the slow decay of Kolmogorov n-width in linear subspace approximations. To tackle this, we propose a novel landmark-based registration approach for ROMs in convection-dominated problems. Leveraging limited training data, our method applies a nonlinear data transformation using landmark-based registration with radial basis function (RBF) interpolation. In the offline phase, dominant convective features are aligned in a reference domain, yielding a rapid error decay relative to the reduced space dimension. Landmarks are created through shock detection, Monte Carlo sampling, and K-means clustering, with centroids as landmarks. Accurate correspondence is ensured by minimizing pairing distances. The online phase integrates standard ROM methods, expanding the optimization space to include domain mappings. We validate this approach on a space-time Burgers equation and hypersonic flow over a cylinder.

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MS3

Arachne: An Open-Source Interactive Graph Analytics Framework for Real-World Problems

A major data science challenge is developing interactive methods for analyzing massive, novel datasets. Bader discusses his graph algorithm development within Arkouda, an open-source NumPy replacement for interactive analysis of tens of terabytes. Massive-scale analytics combines high-performance computing with mathematical modeling to extract insights from large datasets. Data scientists face challenges with graph analytics across domains like cybersecurity and natural/social sciences. To address this, we introduce Arachne, an open-source framework enhancing accessibility in massive-scale graph analytics. Arachne offers novel algorithms including connected components, breadth-first search, triangle counting, and k-truss. The high-performance algorithms integrate into a back-end server written in Chapel language, accessible through a Python API. Arachne runs on Linux supercomputers and works with Python scripts or Jupyter notebooks-ideal for data scientists with HPC access. Bader presents algorithmic overviews and innovations his group implemented, plus improvements to graph data structures storing node labels, edge relationships, and properties. Built as an Arkouda extension, Arachne generates graphs from Arkouda dataframes. Code: https://github.com/Bears-R-Us/arkouda-njit. This work is supported in my by NSF awards CCF-2109988, OAC-2402560.

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MS3

Suitesparse:Graphblas: Graph Algorithms in the Language of Linear Algebra

SuiteSparse:GraphBLAS is a full implementation of the GraphBLAS standard, which defines a set of sparse matrix operations on an extended algebra of semirings using an almost unlimited variety of operators and types. When applied to sparse adjacency matrices, these algebraic operations are equivalent to computations on graphs. GraphBLAS provides a powerful and expressive framework for creating graph algorithms based on the elegant mathematics of sparse matrix operations on a semiring. Key features and performance of the SuiteSparse implementation of GraphBLAS package are described. In terms of performance, graph algorithms written in GraphBLAS can rival or even outperform highly-tuned specialized kernels, while being far simpler for the end user to write.

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MS3

Modeling Large-Scale Network Traffic with Anonymized Hypersparse Matrices

Global usage of the Internet is expected to exceed 5 billion people. Accordingly, the Internet is a domain as worthy of scientific exploration as land, sea, air, and space. Deepening our scientific understanding of the Internet is expected to yield correspondingly equivalent societal benefits. Observationally, the Internet can be viewed as billions (heading towards trillions) of variable sources with many mathematically interesting phenomena that are readily analyzed with high performance GraphBLAS hypersparse matrices. This talk explores these phenomena using novel anonymized AI methods designed for heavy-tailed statistical distributions of the type that are broadly seen across the Internet.

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MS3

Sparseblas: The New Interface to Sparse Linear Algebra Operations

The standardization of an interface for dense linear algebra operations in the BLAS standard enabled interoperability between linear algebra libraries, thereby boosting the success of scientific computing. Despite numerous past efforts, the community not agreed yet on a standardization for sparse linear algebra operations. Partially due to the fact that sparse linear algebra objects allow for many different storage formats needed for portable performance. This makes the definition of a Fortran interface challenging. Another problem is the size of the sparse data structure for the operation result is not always known a priori. These issues lead to many software libraries implementing sparse linear algebra routines with a custom sparse BLAS interface. At the same time, there is a demand for standardization that would improve interoperability and sustainability. Such a standard would also allow for easier integration of building blocks. In an inclusive, cross-institutional effort involving numerous academic institutions, government labs, and industrial partners, we spent over two years designing a hardware-portable interface for basic sparse linear algebra that serves the users' needs and is compatible with the interfaces currently used by vendors. In this talk, we present a C++ API for sparse linear algebra, discuss the design choices, and detail how software developers still have a lot of flexibility as to how to implement the entirety of the functional scope.

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MS4

Towards Observational Signatures of Quantum Cosmology

Cosmology stands at the frontier of physics, grappling with profound questions about the nature of the universe's origin, evolution, and composition. While quantum mechanics and general relativity individually explain fundamental aspects of reality, their unification remains one of science's greatest challenges. This research explores how quantum gravitational effects could leave measurable imprints in cosmological observations, offering new insights into dark matter, the early universe, and the nature of spacetime itself. By investigating strongly correlated quantum states, we propose novel candidates for non-classical dark matter, reshaping our understanding of cosmic structure. Additionally, quantum gravity theories - such as Loop Quantum Cosmology (LQC) - suggest that the Big Bang singularity may be replaced by a quantum bounce, fundamentally altering our perspective on the universe's past and future. Our work aims to identify observational signatures of these quantum phenomena in the Cosmic Microwave Background (CMB) and large-scale structures, bridging theory with tangible evidence.

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MS4

Quantum Computation and Information: A Theoretical Physicist's Perspective

In this talk, I will explore connections between the foundations of quantum computation and information and key ideas in quantum gravity and cosmology. I will delve into the profound role of *entanglement* in the emergence of spacetime, and striking parallels between *black hole thermodynamics* and quantum information processing, including concepts like the Ryu-Takayanagi formula for entanglement entropy ($S_A = \frac{Area(\partial A)}{4G}$). I will also discuss how quantum gravity effects might be detectable in low-energy quantum systems and the implications for understanding the universe's evolution and fate. These links offer fresh insights into the fundamental nature of the universe and suggest new avenues for *hybrid quantum-classical computing* approaches to probe cosmic mysteries.

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MS4

Quantum Annealing Advantage for Transportation Problems

Transportation optimization problems like Traveling Salesman Problem (TSP) and Vehicle Routing Problem (VRP) exhibit exponential complexity, making classical algorithms intractable for real-world logistics. We demonstrate quantum annealing's computational advantage for the Agricultural Vehicle Routing Problem (AVRP). AVRP combines minimum-overlap coverage path planning [Spekken and de Bruin, Optimized routing on agricultural fields by minimizing maneuvering and servicing time, 2013] with optimal track ordering [Bochtis and Sorensen, The vehicle routing problem in field logistics, 2009] and connector generation between tracks, constrained by machine turning radius. Track traversal ordering is equivalent to TSP, making AVRP NP-hard and requiring heuristics like ant colony optimization as track numbers grow. In this talk, we demonstrate quantum annealing's computational advantage for AVRP over classical heuristics. We formulated AVRP using SuperQ Quantum's platform with two quantum annealing approaches: D-Wave's Constrained Quantum Model (CQM) and Non-linear (NL) solvers. Experiments on 100 Saskatchewan fields compared quantum formulations against state-of-the-art ant colony algorithms [M Khan, Optimizing machine routes for agroecological criteria, FIRA World 2024]. Results demonstrate 8× and 10× speedups from CQM and NL solvers respectively, with improved solutions for 60% of instances and comparable solutions otherwise.

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MS4

Quantum Computing for Netzero Goals: The Challenges and Possible Solutions

Quantum technologies could offer new pathways for achieving net-zero goals by optimizing complex, multidimensional

challenges, such as smart grids, algorithmic materials, carbon capture, and climate modeling, primarily due to Quantum computings ability to tackle problems beyond classical computation. However, significant hurdles remain. We'll discuss hardware limitations, including qubit decoherence, noise, and the challenges of scaling to fault-tolerant levels. Additionally, energy-intensive cryogenic cooling and specialized manufacturing processes for quantum architectures raise concerns about sustainability. The talk will also explore solutions like quantum error correction, hybrid quantum-classical algorithms, and energy-efficient quantum hardware. We'll touch on the potential of quantum sensing for precise environmental monitoring. Ultimately, this presentation will examine how quantum computing can genuinely contribute to a sustainable, net-zero future, addressing both its promise and its challenges.

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MS5

Insight into the Opioid Epidemic with Mathematics and Statistics

The opioid epidemic has affected millions of people, and with the rise of fentanyl overdoses more insight is needed into the epidemic and potential strategies going forward. We are utilizing mathematical and statical modeling to study fentanyl usage and overdoses, for specific locations and behavioral dynamics, considering management options. Our collaborations include students, along with a connection to the Inland Empire Opioid Crisis Coalition (IEOCC).

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MS5

Raising Awareness About EDI in Mathematics and Beyond Through Community Building at the University of Hartford

I will talk about my efforts to popularize mathematics and to attract students in mathematics from a diverse pool of talent. Namely, I will talk about the collaboration with the library and hosting screenings of EDI related documentaries, creating the Mathematics EDI Community library and more.

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