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2024 SIAM Annual Meeting

(AN24)

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2024 SIAM Annual Meeting Online Component

July 18–20, 2024

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Abstracts appear as submitted.

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AN24 Online Abstracts begin on page 108

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IP1

Hearing the Will of the People in the Vote: Computational Challenges in Redistricting

The US political system is built on representatives chosen by geographically localized regions. This presents the government with the problem of designing these districts. Every ten years, the US census counts the population and new political districts must be drawn. The practice of harnessing this administrative process for partisan political gain is often referred to as gerrymandering. How does one identify and understand gerrymandering? Can we really recognize gerrymandering when we see it? If one party wins over 50% of the vote, is it fair that it wins less than 50% of the seats? What do we mean by fair? How can math help illuminate these questions? How does the geopolitical geometry of the state (where which groups live and the shape of the state) inform these answers? Our ability to answer these questions is still a work in progress and presents many interesting mathematical research questions. Topics include ideas from computation statistic/statistical physics, combinatorics, high dimensional probability, Markov Chain theory, and modern data science. The story thus far has been an interaction between lawyers, mathematicians, computational scientists, and policy advocates. The legal discussion has been increasingly informed by the mathematical framework. And the mathematics has been pushed to be better included the policy considerations. This back and forth has been important to finding ways to effectively inform the policymakers and courts. The problem of understanding gerrymandering has also prompted the development of a number of new computational algorithms that come with new mathematical questions. The next round of redistricting analysis will necessarily need to be more refined and nuanced. The methods use a mixture of advanced sampling and mathematical modeling ideas; mixing ideas from computational chemistry, Bayesian Sampling and computational statistical mechanics. There is also the opportunity to be less reactive. There are opportunities to try to influence the process by which new maps are drawn before turning to the courts. There is also the possibility to direct the conversation by showing the effect more fully considering factors such as communities of interest, incumbency or proposed procedural elements of laws. For me, these questions began with an undergraduate research program project in 2013 and have led me to testify in a number of cases: Common Cause v. Rucho (that went to the US Supreme Court), Common Cause v. Lewis, Harper v. Lewis, and Harper v. Hall/Moore. Related ideas have central in a number of cases including testimony by a collection of computational scientists. I will endeavor to both recount the policy and court room successes and challenges as well as the computational and mathematical challenges.

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IP2

Case Studies on the Role of Loss Landscape in Neural Network Generalization

Many behaviors observed in deep neural networks lack satisfactory explanation. Consider a core question: When do overparameterized neural networks avoid overfitting and generalize to unseen data? Empirical evidence suggests that the shape of the training loss function near the solution matters: the minima where the loss is flatter tend to lead to better generalization. Yet quantifying flatness and its rigorous analysis, even in simple models, has remained elusive. In this talk, we focus on a class of nonconvex models arising in low-rank matrix recovery as test cases, and show that for many well-known models under standard statistical assumptions (e.g., matrix sensing, matrix completion, robust PCA, and two-layer neural networks), flat minima (those with smallest local average curvature) provably generalize. These algorithm-agnostic results suggest a theoretical basis for favoring methods that bias iterates towards flat solutions and help inform the design of better training algorithms.

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IP3

Gradient Flows, Non-smooth Kernels and Generative Models for Posterior Sampling in Inverse Problems

This talk is concerned with inverse problems in imaging from a Bayesian point of view, i.e. we want to sample from the posterior given noisy measurement. We tackle the problem by studying gradient flows of particles in high dimensions. More precisely, we analyze Wasserstein gradient flows of maximum mean discrepancies defined with respect to different kernels, including non-smooth ones. In high dimensions, we propose the efficient flow computation via Radon transform (slicing) and subsequent sorting or Fourier transform at nonequispaced knots. Special attention is paid to non-smooth Riesz kernels. We will see that Wasserstein gradient flows of corresponding maximum mean discrepancies have a rich structure. In particular, singular measures can become absolutely continuous ones and conversely. Finally, we approximate our particle flows by conditional generative neural networks and apply them for conditional image generation and in inverse image restoration problems like computerized tomography and superresolution. This is joint work with Johannes Hertrich (UCL) and Paul Hagemann, Fabian Altekruger, Robert Beinert, Jannis Chemseddine, Manuel Graf, Christian Wald (TU Berlin).

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IP4

Formulating Effective Models, Methods, and Conceptual Frameworks for the Geosciences

Can waves transport significant amounts of ocean heat and tracers great distances, thus affecting Earths climate? This question was the basis for a project which culminated in the wave-driven circulation model and a concrete answer to how this process takes place. Moreover, the project also showed that wave-generated transport was most intense in the nearshore, leading to an examination of the impact of wave-generated transport on important nearshore processes, such as movement of ocean pollution and nutrients in coastal areas. In my talk, I will describe how the vortex-force conceptualization led to the formulation of the model and a theoretical basis for how waves and currents interact at scales larger than the wave scales. The ever-present noise in natural processes and in the instruments used to measure them motivated me to create computational methods that could combine models, such as the wave circulation model and models for climate and weather, and observations in a probabilistic framework to make better predictions. While optimal estimate methods for linear problems existed, the focus of my work was instead on developing algorithms that could handle the more common noisy nonlinear processes in the geosciences. I will detail some of the strategies I used to create methods and algorithms that assimilate observations, rational models, and machine-learned data-driven constructs to improve forecasts in time-dependent problems, arising in the geosciences and beyond. Finally, I will discuss my more recent work, which employs mathematical arguments to guide in quantifying and understanding resilience in the context of a changing climate and biological systems response via adaptation to stresses.

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IP5

Data-Driven Modeling of Nonlinear Dynamical Systems via Spectral Submanifolds

I discuss a recent dynamical-systems-based alternative to machine learning in the data-driven reduced-order modeling of nonlinear phenomena. Specifically, spectral submanifolds (SSMs) represent very low-dimensional attractors in a large family of physical problems that range from wing oscillations to transitions in pipe flows. A data-driven identification of the reduced dynamics on these SSMs gives a mathematically rigorous way to construct simple, accurate and predictive reduced-order models for solids, fluids, and controls without the use of governing equations. I illustrate this on problems that include accelerated finite-element simulations of large structures, prediction of transitions in pipe flows, reduced-order modeling of fluid sloshing in a tank, and model-predictive control of soft robots.

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IP7

The Mathematics of Nurturing a Digital Twin

With the invention of digital computers in the mid 1940's, John von Neumann envisioned numerical weather prediction (NWP) as a revolutionising application of this technology and famously stated in a talk at Princeton in 1950: "All processes that are stable we shall predict. All processes that are unstable we shall control." In today's language, von Neumann had sown the seeds for the modern concept of NWP as a digital twin (DT) of actual weather processes in the atmosphere, its physical twin (PT). Since the days of von Neumann, DTs have found ground breaking applications in science and engineering. Still many challenges remain when considering highly complex multi-scale processes arising from, e.g., aeronautics, cognition, ecology, and pharmacology. Mathematically speaking, a DT can often be described as a partially observed Markov decision process (POMDP). Solving POMDPs computationally constitutes one of the most challenging problems around. Still, tremendous progress has been made in closely related fields such as data assimilation, uncertainty quantification, control and optimisation, and model reduction. A key emerging questions is thus how we can successfully synthesise these advances into a tool broadly applicable to DT. In my talk, I will map out one possible roadway.

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IP8

Applied Mathematics, Clouds and Storm Dynamics

This talk describes a model-hierarchy approach to characterize and model atmospheric flows with clouds, rain, and storm dynamics. As a minimum requirement, it is necessary to incorporate phase changes of water into the fluid equations describing conservation of mass, momentum, and energy. The presence of moving phase interfaces leads to richer mathematical and physical frameworks within which to explore fundamental mechanisms for the formation and evolution of features associated with precipitation events, which are becoming increasingly more extreme. The model hierarchy provides new insights regarding discontinuous front-like solutions, separation of fast and slow dynamics, conservation of moist potential vorticity, and coherent structures in flows with clouds and rain.

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IP9

Critical Transitions in Complex Systems: Theory and Applications to Climate and Ecosystem Dynamics

Many systems in nature are characterized by the coexistence of different stable states for a given set of environmental parameters and external forcing. Examples for such behavior can be found in different fields of science ranging from mechanical or chemical systems to ecosystem and climate dynamics. As a consequence of the coexistence of a multitude of stable states, the final state of the system depends strongly on the initial condition. Perturbations, applied to those natural systems can lead to a critical transition from one stable state to another. Those transitions are called tipping phenomena in climate science, regime shifts in ecology or phase transitions in physics. Such critical transitions can happen in various ways: (1) due to bifurcations, i.e. changes in the dynamics when external forcing or parameters are varied extremely slow (2) due to fluctuations which are always inevitable in natural systems, (3) due to rate-induced transitions, i.e. when external forcing changes on characteristic time scale comparable to the time scale of the considered dynamical system and (4) due to shocks or extreme events. We discuss these critical transitions and their characteristics and illustrate them with various examples from climate and ecosystem dynamics.

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IP10

Sampling and Generative Modeling Using Dynamical Representations of Transport

Drawing samples from a probability distribution is a central task in applied mathematics, statistics, and machine learning—with applications ranging from Bayesian computation to computational chemistry and generative modeling. Many powerful tools for sampling employ transportation of measure, where the essential idea is to couple the target probability distribution with a simple, tractable "reference' distribution, and to use this coupling (which may be deterministic or stochastic) to generate new samples. Within this broad area, an emerging class of methods use *dynamics* to define a transport incrementally, e.g., via the flow map induced by trajectories of an ODE or the stochastic mapping induced by sample paths of an SDE. These methods have shown great empirical success, but their consistency and convergence properties, and the ways in which they can exploit structure in the underlying distributions, are less well understood. We will discuss properties and theoretical underpinnings of these new dynamical approaches to transport. In particular, we will discuss the statistical convergence of generative models based on neural ODEs and flow matching. We will also present two new, contrasting, dynamical constructions of transport: a gradient-free method that avoids complex training procedures by instead evolving an interacting particle system that approximates a Fisher–Rao gradient flow; and a discrete-time dynamical system based on an infinite-dimensional Newton iteration, which involves successively solving linear PDEs. We will attempt to illuminate the relative advantages and pitfalls of these dynamical methods.

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IP11

Learning the Solution Operators of Forward and Inverse Problems for PDEs

Given the very high computational cost of numerically simulating PDEs, there is an increasing interest in learning the underlying PDE solution operator from data. We review the emerging field of operator learning by laying out its mathematical foundations and discussing different architectures ranging from neural operators to transformers. Both mathematical results and extensive numerical experiments will presented in the talk to compare different operator learning models. Downstream applications to Inverse Problems for PDEs will also be presented.

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SP1

W. T. and Idalia Reid Prize Lecture: 100 Years of Traffic Models: From Road Tolls to Autonomy

In 1924, on The Quarterly Journal of Economics, Frank H. Knight debated on social costs using an example of two roads, which was the base of the Wardrops principle. The author suggested the use of road tolls and it was probably the first traffic model ever. Few other milestones of a long history include the traffic measurements by Greenshields in 1934, the Lighthill-Whitham-Richards model in late 1950s and follow-the-leader microscopic models. After describing some of these milestones, we will turn to modern theory of conservation laws on topological graphs with application to traffic monitoring. The theory required advance mathematics such BV spaces and Finsler-type metrics on L1. In late 2000s, this theory was combined with Kalman filtering to deal with traffic monitoring using data from cell phones and other devices. Then we will turn to measure-theoretic approaches for multi-agent system, which encompass follow-the-leader-type models. Tools from optimal transport allows to deal with the mean-field limit of controlled equations, representing the action of autonomous vehicles. We will conclude discussing how autonomy can dissipate traffic waves and reduce fuel consumption, then illustrating the results of a 2022 experiment with 100 autonomous vehicles on an open highway in Nashville.

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SP2

John von Neumann Lecture: Exploring the Mysteries of Deep Neural Network Optimization

In 1961, Minsky perceived a fundamental flaw within the burgeoning field of artificial neural networks. He doubted that such a nonlinear system could be effectively trained using gradient methods, because unless the structure of the search space is special, the optimization may do more harm than good. Fast forward to today, and we observe deep neural networks far more complex than those envisioned at the field's inception being successfully trained with methods akin to gradient descent. It has, indeed, become evident that the objective function displays a highly benign structure that we are only starting to comprehend. In this lecture, I aim to summarize our current understanding of this enigmatic optimization process. I will explore a diverse array of themes, including intrinsic dimensionality, the optimization landscape, and implicit regularization, and I will highlight key open questions, all within the context of residual networks and generative models.

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SP3

AWM-SIAM Sonia Kovalevsky Lecture: Mathematics for Bioartificial Organ Design

The future of bioartificial organ design is poised with tremendous promise. Achieving success in this field necessitates collaborative efforts among experts spanning diverse domains such as biology, medicine, engineering, materials science, and mathematics. This presentation aims to illuminate the pivotal role played by recent advancements in mathematical analysis and numerical method development in studying the interplay between fluids and poroelastic media (fluid-poroelastic structure interaction), and how these innovations have significantly contributed to the design of a bioartificial pancreas for the treatment of Type 1 and Type 2 diabetes. Collaborators: Yifan Wang, Jeffrey Kuan, Justin Webster, Boris Muha, Martina Bukac, Lorena Bociu, Shuvo Roy

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SP4

Past President's Address: Finite Element Methods

for Least-Squares Problems

Finite dimensional linear and nonlinear least-squares problems appear in data fitting and the solution of nonlinear equations. In this talk I will present some recent results for the infinite dimensional analogs of such problems. They include (i) a general framework for solving distributed elliptic optimal control problems with pointwise state constraints by finite element methods originally designed for fourth order elliptic boundary value problems, (ii) a multiscale finite element method for solving distributed elliptic optimal control problems with rough coefficients and pointwise control constraints, and (iii) a convexity enforcing nonlinear least-squares finite element method for solving the Monge-Ampere equation.

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SP5

I. E. Block Community Lecture: Go Boldly Where No Math Has Gone Before

The role of mathematics in the worlds greatest discoveries and inventions is often overlooked or unappreciated by the general public. What we remember about maths in school might amount to prime numbers or finding the length of hypotenuse, both of which may appear to have no relevance to our everyday lives. How many of us will recall words like polynomial and integral and appreciate the applications of these fundamental mathematical concepts? Can we easily name the many mathematicians who have pioneered world-changing scientific breakthroughs? This talk aims to change all of that. I will bring you on a journey of mathematical progress and share with you the reasons why I believe that maths is important, exciting and innovative. You will learn about the multitude of ways that maths has helped to solve the worlds greatest challenges, and the scientists who championed these innovations. The journey will continue into modern times, where maths is being used to tackle important unsolved issues affecting us now and dictating our future. The final stop will bring us to space where I will describe my role as a mathematician taking on the future of space sustainability.

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SP6

Theodore von Krmn Prize Lecture: From Reduced-Order Modeling to Scientific Machine Learning

Reduced-order models play a critical role in achieving design, control and uncertainty quantification for complex systems. They are also a key enabling technology for predictive digital twins. Our Operator Inference approach combines classical theory of projection-based reduced-order modeling with a modern algorithmic perspective from data-driven scientific machine learning. The result is a scalable, non-intrusive, physics-informed approach to deriving surrogate models that embed structure dictated by the underlying physics. An attractive property of the approach is its flexibility in expressing the reduced-order model in a linear subspace or a nonlinear (polynomial) manifold. Operator Inference is shown to be successful in achieving predictive reduced-order models for challenging engineering problems where training data are sparse and expensive to acquire.

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JP1

Joint Plenary with the SIAM Conference on Discrete Mathematics (DM24): New Frontiers in Structure Vs Randomness with Applications to Combinatorics, Complexity, Algorithms

In 1936, Erdos and Turan asked the following: Suppose you have a set S of integers from $1, 2, \ldots, N$ that contains at least N / C elements. Then, for large enough N, must S have three equally spaced numbers (i.e., a 3-term arithmetic progression)? In 1946, Behrend showed that C can be at most $exp(\sqrt{(\log N)})$. Since then, the problem has been a cornerstone of the area of additive combinatorics, with the best bound being $C = (\log N)^{(1+c)}$ for some constant $c > 0$. Recent work obtained an exponential improvement showing that C can be as big as $exp((\log N)^{0.09})$, thus getting closer to Behrend's construction. In this talk, I will describe this result and the main ingredient, a new variant of the "structure vs. randomness" paradigm. The latter is an old technique with many applications in complexity theory, algorithm design, and number theory, and the new variant can potentially lead to further progress. I will highlight two such applications: 1. Communication complexity: explicit separations between randomized and deterministic multi-party protocols. 2. Algorithm design: fast combinatorial algorithms for Boolean matrix multiplication, detecting triangles in graphs. Based on works with Amir Abboud, Nick Fischer, Zander Kelley, Shachar Lovett.

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JP2

Joint Plenary with the SIAM Conference on Applied Mathematics Education (ED24): Signals of a Critical Transition in Inclusive Stem Education

In the last few years, we have experienced several external shocks to our educational system, such as COVID-19 and renewed critical conversations about racism in higher education. How is the mathematics community responding? I will highlight a few efforts across the math institutes and in classrooms to confront inequity and rehumanize mathematics education. I will also explore how complex systems theory and computational approaches can be used to understand how our educational system is changing. In a recent study, we conducted a computational text analysis of educational journal articles in postsecondary biology education to understand how attention to topics in social justice, equity, diversity and inclusion have evolved over time. We found a rapid shift in attention to inclusive teaching occurs between 2018 and 2019, marked by an increase in section length, increased use of inclusive teaching keywords, and an increase in complexity of ideas in the semantic network. Some effect is associated with structured authoring resources and support. However, this alone is not enough to explain the observed shift, suggesting that many other structures, conversations, and investments are already providing the fertile ground that is advancing educational equity in STEM education.

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JP3

AN24/AMS Joint Plenary: Hydrodynamic Quantum Analogs

Since Yves Couders discovery in 2005 that droplets may self-propel along the surface of a vibrating liquid bath, numerous studies have shown that these walking droplets exhibit features previously thought to be exclusive to the microscopic, quantum realm. The walking droplet system represents a macroscopic realization of wave-particle duality, and of a pilot-wave dynamics of the form proposed for microscopic quantum particles by Louis de Broglie in the 1920s. Experimental and theoretical results allow us to explore its potential and limitations as a quantum analog, and so redefine the boundary between classical and quantum. Theoretical descriptions of the hydrodynamic system allow us to forge links with existing quantum pilot-wave theories. Fledgling, trajectory-based descriptions of quantum dynamics, informed by the hydrodynamic system, are explored. Particular attention is given to illustrating how the non-Markovian droplet dynamics may give rise to features that are taken as evidence of quantum nonlocality in their microscopic counterparts.

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CP1

AI Education: Pioneering Initiatives in Algeria and the UAE

As Artificial Intelligence (AI) becomes increasingly pivotal across industries, the necessity of preparing a skilled workforce capable of harnessing its potential becomes paramount. This research paper delves into the importance of designing and developing education and training systems that incorporate AI and machine learning (ML), with a particular focus on the initiatives undertaken by Algeria and the United Arab Emirates (UAE). The contribution explores the establishment of specialized universities and schools for AI, such as the Mohamed Bin Zayed University of Artificial Intelligence (MBZUAI) in the UAE and the cole nationale suprieure d'intelligence artificielle (ENSIA) in Algeria. These institutions offer comprehensive bachelor, master, or engineer's degree (integrated bachelor-master) programs, reflecting a proactive approach in recognizing the profound impact of AI on the future of technology and industry. The lecture discusses the global landscape of AI education, the importance of AI education for the workforce, and the benefits of specialized AI education. Additionally, it addresses challenges in implementing AI education programs and considers future implications, emphasizing the transformative role these initiatives play in shaping the local and global AI landscape. Through case studies and analyses, this research contributes to the discourse on the integration of AI into education and training and its implications for the evolving workforce.

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CP1

Integrating Black History and Algebra Concepts: Creating Inclusive Learning Spaces in Mathematics Education

In this dynamic and engaging session, Dr. Kendall Ware, a distinguished Doctor of Education specializing in mathematics education, will share his innovative approach to creating inclusive learning spaces in mathematics classrooms. The session will focus on Dr. Ware's groundbreaking series of mathematics textbooks, specifically tailored for Algebra 1, which seamlessly integrates Black History with algebra concepts. This unique instructional practice not only enhances students' mathematical understanding but also fosters an environment where diversity is celebrated, and every student feels seen, heard, and valued.

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CP2

Recovering Superconvergence of SEM on Curved Domains Using ApSEM (AES-FEM post-processed SEM)

Due to their potential to deliver superior accuracy and superconvergence, spectral element methods (SEM) are a powerful tool for solving PDEs in engineering. Their superconvergence relies on well-shaped tensor product elements. When applied to complex geometries, the accuracy of SEM often degrades because of geometric inaccuracies near curved boundaries and the use of simplicial or non-tensor-product elements. In this poster, we present a method to recover superconvergence on domains with curved boundaries. To improve geometric accuracy near curved boundaries, we propose using h- and p-geometric refinement, which refines the mesh near high-curvature regions and increases the degree of geometric basis functions, respectively. We utilize mixed-element meshes with simplicial elements near curved boundaries and rectangular tensor-product elements elsewhere. To address the loss of superconvergence due to the use of simplicial elements, we introduce ApSEM, which uses the adaptive extended stencil finite element method (AES-FEM) as a postprocessing technique of SEM on mixed-element meshes to recovered high-order accuracy near the curved boundaries. We present results from solving the convection-diffusion equation in 2D and 3D, which show up to two orders of magnitude of improvement in the solution accuracy. We also demonstrate the efficiency of ApSEM in that it can recover superconvergence of the nodal solutions without significantly increasing the computational cost.

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CP2

On the Convergence of a Numerical Method for Helmholtz Equation

In this work, we consider the development and analysis of a compact higher-order finite difference method for solving a Helmholtz Equation, which rises from a variety of applications, particularly in geophysics. Despite the simple form, the multi-dimensional Helmholtz equation is difficult to solve numerically with high accuracy and efficiency, mainly due to the fact that the discretized linear system is indefinite, which makes most iterative methods fail to converge or converge very slowly. On the other hand, a direct solution to such a large-scale linear system is not realistic due to the high requirements for computing resources. In this work, we combine the combined compact scheme with the operator splitting technique to develop a higher-order compact finite difference scheme. Taking advantage of operator splitting and converting the multi-dimensional problem into a sequence of locally one-dimensional problems, thus, high efficiency can be archived while a high order of accuracy will be obtained by adopting the compact finite difference discretization. Except for the analysis of the convergence, several preliminary numerical examples are solved to demonstrate the accuracy and efficiency of the new method.

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CP2

A Residual-Based Approach to Boundary Value Problems for Multiple-Obstacle Acoustic Scattering

We propose an efficient iterative method for solving multiple acoustic scattering problems in two and three dimensions. The idea of this algorithm consists of separating the obstacles using artificial boundaries around each obstacle, and at that boundary, to use high-order local absorbing boundary conditions (ABC). These boundary conditions are derived from the exact form of the outgoing wave, specifically using the Karp and Wilcox farfield expansions. A residual-based method, inspired by the Generalized Minimal Residual (GMRES) algorithm, is introduced as an efficient method for computing the scattered wave inside the computational domain. This method allows the multiple-scattering problem to be decomposed into a set of single-scattering problems which can be solved using the information from the other scatterers at the previous step. We examine the convergence of this method, and present multiple numerical examples demonstrating its accuracy and efficiency.

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CP2

Fast Iterative Methods for Variable Coefficient Diffusion Equations on a Disk

A fast and efficient iterative method to solve steady variable coefficient diffusion equations on a disc is first introduced. We then use this method in combination with numerical techniques for integration in time to solve unsteady variable coefficient diffusion equations and the Ginzburg-Landau equation with variable coefficient. These methods make use of a change of variable that transforms the original problems to Helmholtz problems which are then numerically solved by iterating Poisson problems using an FFTRR-based fast Poisson solver introduced in Borges and Daripa [L. Borges and P. Daripa. A fast parallel algorithm for the Poisson equation on a disk. J. Comput. Phys., 169(1):151192, 2001]. The performance of these methods is investigated using several numerical examples. In the method proposed here on the unit disc, no polar coordinates are involved. Hence the usual problems with the singularity of polar coordinates are avoided.

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CP2

On The Numerical Integration of One Nonlinear Parabolic Equation

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

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

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

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

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

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CP2

A Fourth Order Exponential Time Differencing Scheme with Dimensional Splitting for Simulating

Nonsmooth Reaction Diffusion Systems

An L-stable, fourth-order exponential time differencing (ETD) Runge-Kutta scheme with dimensional splitting is developed to solve nonsmooth, multidimensional, nonlinear systems of reaction-diffusion equations (RDE). 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 RDEs with mismatched initial and boundary data as well as those with discontinuous initial data.

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CP3

Transverse Spectral Instabilities in Rotation-Modified Kadomtsev-Petviashvili Equation and Related Models

The rotation-modified Kadomtsev-Petviashvili equation which is also known as the KadomtsevPetviashviliOstrovsky equation, describes the gradual wave field diffusion in the transverse direction to the direction of the propagation of the wave in a rotating frame of reference. This equation is a generalization of the Ostrovsky equation additionally having weak transverse effects. We investigate transverse instability and stability of small periodic traveling waves of the Ostrovsky equation with respect to either periodic or square-integrable perturbations in the direction of wave propagation and periodic perturbations in the transverse direction of motion in the rotation-modified Kadomtsev-Petviashvili equation. We also study transverse stability or instability in generalized rotation-modified KP equation by taking dispersion term as general and quadratic and cubic nonlinearity. As a consequence, we obtain transverse stability or instability in two dimensional generalization of RMBO eqution, Ostrovsky-Gardner equation, Ostrovsky-fKdV equation, Ostrovsky-mKdV equation, Ostrovsky-ILW equation, Ostrovsky-Whitham etc.

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CP3

Global-in-time Physical Vacuum Solutions to the Compressible Navier-Stokes Equations with Density-dependent Viscosities and Stability for the Spherically Symmetric System

Expansion can give rise to global-in-time solutions in the free boundary setting through the stability of so-called affine motions which expand into vacuum. By perturbing a new class of expanding affine motions, we prove global existence for the physical vacuum free boundary compressible Navier-Stokes equations with density-dependent viscosities under the assumption of spherical symmetry. Moreover, viscosity independent estimates are established.

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CP3

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

We expand upon the study of propagating poroacoustic waves conducted in [P.M. Jordan, Poroacoustic Solitary Waves Under he Unidirectional Darcy-Jordan Model, Wave Motion, 94 (2020)], emphasizing moments of “gradient-catastrophe” or wave overturning. Our numerical method, with the reliability of bisection and a speed comparable to a finite-difference method, solves the 1D, unidirectional Darcy-Jordan model as a Cauchy problem. The hyperbolic and nonlinear nature of this PDE results in a physical shock and a multi-valued solution profile, where our method maintains accuracy without knowledge of an analytical solution. We display the efficacy of this root-finding method by computing solutions at each point in the space-time grid for different initial conditions with physical significance.

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CP3

Dynamics of a Multi-Layer Fluid System in Cylinder Geometry

A long-wave asymptotic model is used to analyze the linear stability of the Navier-Stokes equations for a falling multi-layer fluid system in cylinder geometry. The impact of different parameters on the linear growth of the interfacial disturbances is investigated, when disturbances are small. The growth rate of the disturbances is computed and used to determine where the system is unstable to small amplitude disturbances. Nonlinear evolution equations are also derived to investigate the dynamics when the disturbances are not small.

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CP3

Spectral Methods for Capillary Surfaces

Capillary surfaces satisfy the equation that the mean curvature of the surface is proportional to the height of the surface at each point. These surfaces model the equilibrium shapes of liquid interfaces and the usual boundary conditions encode the wetting properties of that fluid with the container with the nonlinear natural boundary conditions. We present spectral methods for computing capillary surfaces. We consider radially symmetric configurations as well as the general PDE problem. In the course of developing these methods for the full PDE problem we will also present spectral methods for the Plateau problem for minimal surfaces as well as problems for constant mean curvature surfaces.

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CP4

Eigenfrequencies and Eigenmodes Analysis of Axially Loaded Beam Supported by One Parametric Foundation

This study aims to analyze the eigenfrequencies and eigenmodes of the fundamental structures of a continuous system, namely beam structure. Axially loaded beams over elastic foundations with non-classical boundary conditions frequently appear in structural design, and modal analysis of those structures is significant and fundamental in engineering structures. This research examines the eigenmodes and eigenfrequencies of the beams with and without elastic foundations attached to rotational springs using analytic and numerical methods. Using the separation of variables, frequency and mode shape equations are initially developed and further roots of algebraic equation for frequency determination will be extracted by applying the root-finding technique. A built-in program that calculates eigenfrequencies and eigenmodes of free vibration of beams over elastic foundation is employed using the finite element method. Comparative numerical and analytic analyses are presented, as well as eigenmodes are depicted to illustrate the excellent agreement. Effects of rotational spring stiffness are also observed. It is also analyzed how the elastic foundation constant affects the eigenfrequencies of the structure. Investigation of the vibrating beam on elastic foundation with non-classical boundary conditions has an incredible interest in an assortment of practicalcases.

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CP4

A Novel Relationship Between Normalized Laplacian Energy and Well-known Indices: Sombor and Zagreb Indices

Graph descriptors such as normalized Laplacian energy, Somber index, and Zagreb index are often employed in various scientific contexts. Based on spectral graph theory, the Normalized Laplacian energy sheds light on the structure and connectivity of networks in the social, communication, and biological domains. The Somber index is essential in chemical graph theory because it provides insights into molecule stability and reactivity by analyzing the distribution of atom degrees and distances. By measuring molecular graph topology, the Zagreb indices are vital tools in mathematical chemistry that help predict molecules' physical and chemical characteristics. Let χ_n^k be the set of all n-vertex graphs with exact chromatic number k. Das and Shang characterized graphs achieving the maximum Sombor index of graphs in χ_n^k in terms of chromatic number. This paper extends the characterized graphs, achieving the minimum Sombor of graphs in χ_n^k in terms of chromatic number. Furthermore, by employing Rayleigh's quotient principle, we present a first-ever comparison between the normalized Laplacian energy and the Sombor and first Zagreb indices in terms of eigenvalues. To extend our results, we suggest some open problems to contribute in the direction of extremal graph theory.

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CP4

Tridiagonal and Single-Pair Matrices and the Inverse Sum of Two Single-Pair Matrices

A novel factorization for the sum of two single-pair matrices is established as product of lower-triangular, tridiagonal, and upper-triangular matrices, leading to semi-closed-form formulas for tridiagonal matrix inversion. Subsequent factorizations are established, leading to semi-closed-form formulas for the inverse sum of two single-pair matrices. An application to derive the symbolic inverse of a particular Gram matrix is presented. A single-pair matrix, also known as one-pair matrix, Green's matrix, "matrice factorisable", and generator-representable semiseparable matrix, has the symmetric form

$$\mathbf{A} = \left(a_{\min(i,j)} b_{\max(i,j)}\right) = \begin{pmatrix} a_1b_1 & a_1b_2 & \cdots & a_1b_n \\ a_1b_2 & a_2b_2 & \cdots & a_2b_n \\ \vdots & \vdots & \ddots & \vdots \\ a_1b_n & a_2b_n & \cdots & a_nb_n \end{pmatrix}$$

where $(a_i), (b_i)$ is a pair of n nonzero real or complex numbers. Single-pair matrices may arise in a variety of applications, including tridiagonal matrix inversion, oscillatory mechanics, and Gram matrices. The inverse of a single-pair matrix, if it exists, is known in closed form as a symmetric tridiagonal matrix.

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CP4

Automatic Complexity and Quantum Logic over Finite Fields

The automatic complexity of finite words was introduced by Shallit and Wang (2001). It measures the complexity of a word x as the minimum number of states of a finite automaton that uniquely accepts x. Here, an automaton M uniquely accepts a word x if x is the only word of length $|x|$ accepted by M. Via the digraph representation of automata we can view the computation of this number of states as a problem of extremal graph theory. A quantum version of automatic complexity was studied by Kjos-Hanssen (2017). We explore a finite field analogue of quantum automatic complexity, with particular attention to the subspace structure of the automata and the associated quantum logic. We define an EZ-Hilbert space and discuss its limitations for the study of quantum automatic complexity.

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CP4
Density Separation with Tensor Factorization

The nonnegative tensor factorization is used to separate mixtures of probably densities. A kernel density estimation transforms raw samples into compressed and discretized densities. An implementation of a specialized block coordinate descent algorithm that enforces the required simplex constraints is guaranteed to converged to Nash equilibria. Numerical experiments on real geological and spatial transcriptomics data, using our open source Julia implementation, illustrate the model's effectiveness at separating the density mixtures.

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CP4
Data Assimilation for Quantum Nv Diamond Spectroscopy

Nitrogen-vacancy (NV) defect centers in diamond have generated much interest for their uses in quantum information and sensing. Despite the rapid NV applications development, our grasp of basic NV properties is incomplete, which is important to understand to fully exploit potential uses. In this work we construct a statistical model for NV spectroscopy and use it in synthetic experiments to solve inverse problems. Our principal application is to develop a primary sensor based on the NV diamond quantum optical properties. This is a significant challenge because the NV diamond structure is sensitive to temperature and pressure as well as magnetic and electric fields, including electromagnetic fields of nearby atoms and molecules. First, using the Hamiltonian for the effects of local strain and the environmental variables, we identify the observable components based on the invertibility of various observation systems. Next, we observe the influence of temperature and pressure on the NV center by solving the Schrdinger Equation and computing the theoretical spectroscopy curve. We assume that the observed photon counts are Poisson random variables with rates proportional to the theoretical spectroscopy. Then, using the Maximum Likelihood Estimation we find the parameter values that maximize the likelihood. Last but not the least we determine the robustness of the model using sensitivity analysis

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CP5
Studying Disease Reinfection Rates, Vaccine Efficacy and the Timing of Vaccine Rollout in the Context of Infectious Diseases

The global landscape, characterized by distinct COVID-19 waves and variants, introduces complexities to the pandemic. This research investigates vaccine efficacy and emphasizes the critical role of timely vaccination. Departing from conventional modeling, we introduce two models that account for the impact of vaccines on infections, reinfections, and deaths. Recognizing the intricacy of these models, we use the Bayesian framework and specifically utilize the Metropolis-Hastings Sampler for estimation of model parameters. The study conducts scenario analyses, quantifying the duration during which the healthcare system in Qatar could have potentially been overwhelmed by an influx of new COVID-19 cases surpassing the available hospital beds. Additionally, the research explores similarities in predictive probability distributions of cumulative infections, reinfections, and deaths, employing the Hellinger distance metric. Comparative analysis, employing the Bayes factor, underscores the plausibility of a model assuming a different susceptibility rate to reinfection, as opposed to assuming the same susceptibility rate for both infections and reinfections. Results highlight the importance of early vaccination in reducing infections, reinfections, and deaths. This study offers crucial insights for evidence-based public health interventions, advocating early vaccination as a key strategy against future pandemics.

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CP5
Modeling the Heterogenous Nfκb Dynamics of Single Immune Cells

Macrophages function as immune sentinel cells, initiating appropriate and specialized immune responses to various pathogens. The transcription factor NFκB controls macrophage gene expression responses and its temporal dynamics enable stimulus-specificity of these responses. Our laboratory generated extensive single-cell NFκB dynamic data using a fluorescent reporter mouse. Here, we employed a non-linear mix effects model (NLME) coupled with the mechanistic model to infer the parameter variation within the signaling network, capturing the stimulus-specific but highly cell-to-cell heterogeneous NFκB dynamics. Parameter distributions were inferred through the Stochastic Approximation Expectation Maximization (SAEM) approach and then fit the individual cell data using maximum a posteriori (MAP) estimation. Qualitative and quantitative assessments demonstrated an excellent concordance between simulations and experimental data. The model allowed identifying biochemical reactions that cause heterogeneity in NFκB dynamics; investigating the dose response behavior of each ligand; discerning the information leakage across the signaling network; and exploring how different ligand responses combine in combinatorial ligand stimulation conditions. Each of these led to new insights that were experimentally tested and validated. Our work presents a new computational research tool for studying NFκB dynamics in single immune cells.

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CP6

Discover Climate Change via Optimal Transport

Climate change is an essential topic in climate science, and the accessibility of accurate, high-resolution datasets in recent years facilitates the extraction of more insights from big data resources. Nonetheless, prevailing research has predominantly focused on mean value changes and largely overlooks other changes in the probability distribution. By using optimal transport, a novel method called Wasserstein Stability Analysis (WSA) is developed to identify probability distribution changes, especially the extreme events in climate change. WSA is applied to 21st-century warming slowdown period and is compared with traditional mean-value trend analysis. The result indicates that despite no significant trend, the central-eastern Pacific experienced a decline in hot extremes and an increase in cold extremes, indicating a La Nina-like temperature shift. Further analysis at two Arctic locations suggests sea ice severely restricts the hot extremes of surface air temperature. This impact is diminishing as sea ice melts. By detecting distribution changes, WSA is a powerful tool to examine climate change dynamics, providing enhanced data-driven insights for understanding climate evolution.

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CP6

Exploring the Accuracy of Sars-CoV-2 Antibody Escape Predictions by Using Large-Scale Data

The emergence of SARS-CoV-2 has emphasized the urgent need for global preparedness against evolving pathogens. One critical area of focus is the study of neutralizing antibodies to combat viral diseases. However, the rapid evolution of viruses allows them to develop resistant mutations to these antibodies, effectively evading the immune system's ability to recognize and neutralize the threat. Predicting these escape mutations is crucial for detecting threats early and developing effective countermeasures. In this study, we applied our previously developed MD+FoldX approach, a 3-D structure-based approach that harnesses the power of Molecular Dynamics (MD) for structural ensemble generation and FoldX for high-throughput estimation of binding energy scores. To evaluate the accuracy of MD+FoldX in predicting escape mutations, we have leveraged extensive deep mutational scanning experimental data, focusing on the SARS-CoV-2 receptor binding domain. We fine-tuned the cutoff that distinguishes between predicted escape and non-escape mutations, resulting in an optimized cutoff that consistently aligns with or falls below our previously established cutoff for most of the systems. Our findings demonstrate promising performance, with accuracy ranging from 23% to 78% across a diverse array of systems. This suggests the methods may be suitable for identifying clinically relevant mutations, including those present in prominent variants of concern.

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CP6

Dynamical Simulation of the Syrian Refugee Crisis: Quantifying the Driving Factors of Forced Migration

With over 30 million refugees worldwide at the end of 2023, forced migration across national borders has become a global reality and a major international policy issue. Here, we propose a dynamical model based on the Syrian Refugee Crisis to quantify the factors that influence a refugees decision to migrate and their destination choice. The model simulates refugee migrations in space and time, from the moment they flee their country of origin until they are granted asylum in a host country or lose refugee status by attrition or repatriation. Migration is driven by comparative attractiveness scores based on differences in quality of life, political stability, societal violence, cultural familiarity, and distance between countries, while accounting for risk aversion and psychological inertia. By comparing simulation results to United Nations High Commissioner for Refugees (UNHCR) data, we determine weight parameters that quantify the relative importance of each attribute in inducing a migration flow. The model is a computationally efficient forecasting and ex-post analysis tool, providing insight into the dynamics of refugee flow and effect of immigration policies.

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CP6

Invariant Solutions of Nonlinear Mathemaical Modeling of Natural Phenomena

The main objective is to demonstrate the advantages of the invariance method in obtaining new exact analytic solutions expressed in terms of elementary functions for various physical phenomena. One application of the invariance method will be the mathematical modeling of oceanic and atmospheric whirlpools causing weather instabilities and, possibly, linked with climate change. As another particular example, it will be demonstrated that the invariance method allows to obtain the exact solutions of fully nonlinear Navier-Stokes equations within a thin rotating atmospheric shell that serves as a simple mathematical description of an atmospheric circulation caused by the temperature difference between the equator and the poles with included equatorial flows modeling heat waves, known as Kelvin Waves. Special attention will be given to analyzing and visualizing the conserved densities associated with obtained exact solutions. As another modeling scenario, the exact solution of the shallow water equations simulating equatorial atmospheric waves of planetary scales will be analyzed and visualized. The presentation focuses mainly on the physical meaning and visualization of the invariant solution rather than on mathematical derivations.

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CP6

Asymptotic Solution of Electromagnetic Heating of Skin Tissue with Lateral Heat Conduction

We study the thermal effect of an electromagnetic beam of millimeter wavelength on a three-dimensional skin tissue. As the electromagnetic wave propagating into the skin tissue, it is absorbed with the length scale of penetration depth determined by the skin absorption coefficient. The absorbed energy becomes the heat. The temperature evolution is governed by the absorbed electromagnetic energy and heat conduction in the depth and in the lateral directions. For a beam of 94 GHz frequency, the penetration depth is sub-millimeter. The length scale in the lateral directions is the beam radius. In many applications, the beam radius is significantly larger than the penetration depth. The leading term approximation of temperature distribution is obtained by neglecting the lateral heat conduction and has separable dependence on depth and lateral coordinates. In this study, we formulate a two-term approximation in which each term has separable dependence on depth and lateral coordinates. We derive analytical expressions of the two terms. The two-term asymptotic approximation provides a practical and accurate way for predicting the temperature distribution of the skin tissue. This approximation is especially important in cases where the beam size is moderately larger than the penetration depth. For those cases, the effect of lateral heat conduction is not negligible but is well captured in the two-term asymptotic solution.

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CP6

Shape Studies of 3 and 4 Substituted Diarylamide Quasiracemates

This study compared the shape space of pairs of quasienantiomers using a computer based model to quantify the differences in molecular shape and provide a diagnostic tool for quasiracemate prediction. One aspect of this tool is a novel approach to finding approximations of molecular volume which is then compared to molecular volume data from two previously reported studies.

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CP7

High-Order Rogue Wave Formation in Discrete and Continuous Nonlinear Schrdinger-Type Equations

We provide numerical evidence of high-order rogue wave formation in the focusing nonlinear Schrdinger equation from Thomas-Fermi-like initial conditions. The initial conditions are ground states of the defocusing Gross-Pitaevskii equation with a harmonic trap making the preparation of such waveforms feasible in an experimental setting. We confirm the persistence of rogue wave formation in higher dimensions through numerical studies of the non-polynomial Schrdinger equation and the full three-dimensional case. Additionally, we find that a similar phenomenology holds for the Ablowitz-Ladik model.

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CP7

Impact of Foundation Type on Natural Frequencies of Various Beam Models with Non-Classical Boundary Conditions

This consideration investigates the modal behavior of elastically constrained beams with different types of foundations and provides insights into the effects of various factors on the eigenfrequencies of beams. The Galerkin finite element method and variable separations are employed to determine the eigenfrequencies and mode shapes that are used in different beam theories while taking into account non-classical boundary conditions. The impact of factors such as flexural rigidity, transverse modulus, and Winkler foundation constant on the natural frequencies of different beam models is analyzed. The proposed method efficiently converges to the exact solution without shear locking in the stiffness element. The results reveal that the natural frequencies of the beam increase due to the shear layer, flexural rigidity, and foundation constant. Moreover, the elastic foundation parameters influence the natural frequency of the beam, depending on the relative values of beam stiffness and foundation stiffness. Furthermore, incorporating both shear deformation and rotary inertia has a more significant effect on the eigenfrequencies of Euler-Bernoulli beams than incorporating only one of these effects. The findings of this work provide valuable insights into the behavior of beams under different foundation conditions and have potential applications in the design and optimization of structures involving beams, thus improving our understanding of beam analysis.

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CP7

On Evolving Network Models and Their Influence on Opinion Formation

We will discuss a model for continuous-time opinion dynamics on an evolving network, in which the opinion formation process is coupled to a network evolving through a system of ordinary differential equations for the edge weights. We interpret each edge weight as the strength of the relationship between a pair of individuals, with edges increasing in weight if pairs continually listen to each others opinions and decreasing if not. We investigate the impact of various edge dynamics at different timescales on the opinion dynamics itself. This is done partly through analytic results and partly through extensive simulation of two case studies: one using bounded confidence interaction dynamics (as in the classical Hegselmann-Krause model) and one using an exponentially decaying interaction function. We find that the dynamic edge weights can have a significant impact on the opinion formation process; they may help a population reach consensus but can also reinforce polarisation. We also describe how and when consensus can be achieved at a particular target opinion by controlling weight dynamics. Overall, the proposed modelling approach allows us to quantify and investigate how the network and opinion dynamics influence each other, and how one can influence the dynamics externally.

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CP7

Multivariate Technique for Detecting Variations in High-Dimensional Imagery

The field of immunology requires refined techniques to identify detailed cellular variance in high-dimensional images. Current methods mainly capture general immune cell proportion variations and often overlook specific deviations in individual patient samples from group baseline. We introduce a simple technique that integrates the Multivariate Shewhart Control Chart (MSCC) with random projection (RP) methods, specifically designed to identify changes in immune cell composition in high-dimensional images. Uniquely, our method provides deeper insights into individual patient samples, allowing for a clearer understanding of group differences. We assess the efficacy of MSCC across various RPs: Achlioptas (AP), plus-minus one (PM), Li, and normal projections (NP), considering shift size, dimension reduction, and image dimensions. Simulations reveal variable detection performances across RPs, with PM outperforming and Li lagging. Practical tests using single-cell images of basophils (BAS) and promyelocytes (PMO) emphasise their utility for individualised detection. Our approach elevates high-dimensional image data analysis, particularly for identifying shifts in immune cell composition. This breakthrough potentially transforms healthcare practitioners cellular interpretation of the immune landscape, promoting personalised patient care, and reshaping the discernment of diverse patient immune cell samples.

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CP8

Exploring Cyclic Competition Using Clustering Indexes

We discuss the clustering index of pattern formation of a cyclic competition game. In the lattice simulation, the state changes when four nearby neighbors differ from the central species. Based on this finding, we construct a ”clustering index” by counting the number of different neighbor species. We observe that the points with high index values are at the boundaries of each species, and as the mobility increases, the index increases, just as the spiral wave increases when the three species coexist. However, when they go extinct, they have a high index value for some time and then it goes to zero. Therefore, we average the indexes over time and find the correlation between index, extinction probability, and mobility, which is known to play a critical role in the coexistence of the three species in the simulation. We also estimate extinction using the clustering index and machine learning tools.

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CP8

A Dynamical Systems Approach to Neurodegenerative Diseases

Neurodegenerative diseases include Alzheimers (AD), Parkinsons, as well as other rarer conditions. In the USA, one in three seniors dies with AD or another dementia. Despite massive efforts and investments, there is still no disease-modifying treatment for neurodegeneration even if recent drug developments allow for slowing the disease progression. However, since about 2008, the medical community has publicly released large and comprehensive datasets, starting with the AD neuroimaging initiative cohort, opening the way to the computational study of neurodegenerative diseases. The datasets are very rich and complex. They contain 100 to 10,000 subjects, often several visits, one to twenty per subject, spanning up to twenty years. The data included clinical and historical medical records, protein concentrations, brain Magnetic Resonance Imaging both raw and pre-processed with volumes, thickness, and shape measurements, functional imaging functional MRI and molecular imaging, multiple cognitive tests, as well as genetic data. We learn nonparametric ODEs for modeling disease progression using subsets of this data. While the vector field is common to all subjects up to a few covariates, the initial conditions are subject-dependent. We present experiments and results for AD as well as for Multiple Sclerosis.

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CP8

A Comparative Analysis of Host-Parasitoid Models Considering the Sequence of Density-Dependence and Parasitism

We present a comparison of two sets of discrete-time, host–parasitoid models. The first set was previously analyzed by Marcinko and Kot (2020) and assumed that density-dependence precedes parasitism in the life-cycle of the host. In this talk, we present our analysis of a parallel set of models, now specifying that parasitism precedes density-dependence. Each of the four models in this second set includes a particular combination of standard functional forms for density-dependent growth of the host species and for parasitism. We focus on comparing the two sets of models to gain insight into the impacts of the order of events in the host species' life-cycle. We include consideration of bifurcations, as well as comparing equilibria and other stable attractors.

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CP8

Using Dynamic Thresholds to Explain Neural Responses to Time-Varying Inputs

While much theoretical attention has been devoted to the spontaneous activity of neurons, less is known about the dynamic mechanisms shaping their responses to time-dependent inputs, although such inputs may be of significant physiological relevance. We use dynamical systems methods to analyze the origin of three response phenomena associated with certain neurons: post-inhibitory facilitation, in which an otherwise subthreshold excitatory input can induce a spike if it is applied with proper timing after an inhibitory pulse; slope detection, in which a neuron spikes to a transient input only when the inputs rate of change is in a specific, bounded range; and phase-locking, in which neuronal responses to noisy periodic inputs only occur during a narrow band of phases. As a key aspect of our analysis, we provide a geometric characterization of thresholds associated with all of these phenomena, including non-standard dynamic, or time-dependent, thresholds.

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CP8

The Effect of “fear’ on Two Species Competition

Input your abstract, including TeX commands, here. The abstract should be no longer than 1500 characters, including spaces. Only input the abstract text. Don't include title or author information here.

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CP8

Cardiac Tissue Chaos and Periodic Orbits: Experiments and Control

Many cellular cardiac voltage models exhibit chaotic dynamics suggesting that the irregular heart rhythms of cardiac disease may also be chaotic and have a nonlinear mechanism of control. However, little experimental evidence has documented the chaotic behavior of excitations in living cardiac tissue. This study aims to quantify and qualify the chaotic nature of cardiac tissue with voltage measurements from both single-cell and multicellular experiments. Single cardiomyocytes of bullfrogs were paced with constant, high-frequency forcing. Leading Lyapunov Exponents were estimated from action potential duration (APD) time series yielding negative exponents for frequencies near period-doubling cascades and positive exponents for arrhythmic behavior. Additionally, stable period-three orbits and unstable periodic orbit shadowing was found in the arrhythmic response. Further, biphasic perturbation to the forcing frequency appeared to be able to stabilize an unstable periodic orbit of the arrhythmic response. On a multicellular scale, unstable periodic behavior is also observed in the ventricle fibrillation of pigs, rabbits, and humans in isolated regions across the heart. These findings indicate cardiac tissue is partly governed by chaotic factors and nonlinear control can be employed to terminate arrhythmias.

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CP9

An Energy Conserving Higher Order Method for Maxwell's Equations

In this presentation, we propose an implicit leapfrog scheme that is energy conserving for a system of Maxwell's equations. Our main contribution is in devising this time discretization scheme, and showing that the fully discrete error for our proposed method with spatial discretization using a sequence of higher order finite element spaces that form a de Rham complex is convergent. We use a formulation of the Maxwell's equations as a system consisting of an electric scalar variable p alongside electric field and magnetic flux variables, E and H, respectively. The scalar p allows for a spatial discretization that can enable E to be divergence free discretely. We first demonstrate well posedness for a variational formulation of this Maxwell's system. We then show stability, energy conservation and error convergence with our proposed temporal semi-discretization. Finally, we show that the error for the full discretization of this Maxwell's system converges quadratically in the step size of the time discretization, and as an appropriate polynomial power of the mesh parameter for the spatial discretization. We provide computational results with higher order finite elements to validate our theoretical claims for some model problems in two and three spatial dimensions.

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CP9

Exponential Time Differencing Schemes for Fractional Oscillation Models

Fractional evolution equations of oscillatory type provide an effective tool to model some anomalous oscillatory behaviors. Typically, the solutions of these equations display oscillatory patterns, occasionally demonstrating unpredictable behavior. Hence, creating effective numerical techniques that accurately capture the oscillations in these solutions can pose a challenge. In this talk, we present an efficient novel second-order numerical scheme based on the exponential time differencing technique, special approximations of Mittag-Leffler function, and the non-uniform mesh. The Convergence and the stability properties are examined and confirmed through numerical experiments.

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CP9

Algebraic Inverse Fast Multipole Method: A Fast Direct Solver

Integral equation-based methods are one of the most sought-after methods for solving PDEs. The discretization of the integral equations gives rise to a dense linear system. Solving this linear system is what it takes to solve the underlying PDE. Naive methods are highly prohibitive as they scale as $\mathcal{O}(N^3)$. In this talk, we describe the Algebraic Inverse Fast Multipole Method (AIFMM), a fast direct solver that scales as $\mathcal{O}(N)$. It is built on the idea of hierarchical matrices that exploit the rank structuredness of the underlying matrix. An extended sparse system is constructed from the hierarchical matrix representation, which is then solved by elimination and back substitution. The main highlights of AIFMM are that i) It is completely algebraic, which makes it suitable for any kernel function. We use our new nested cross approximation to construct low-rank approximations ii) Some of the fill-ins encountered in the elimination phase of the solver are low-rank, so they can be efficiently compressed iii) It is faster than HODLR-based fast direct solver iv) It is more efficient than the existing Inverse Fast Multipole Methods. We substantiate the accuracy, and computational complexity of AIFMM by solving problems from computational electromagnetics. We will further compare the performance of AIFMM with HODLR and GMRES.

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CP9

New Analysis of Overlapping Schwarz Methods for Vector Field Problems with Generally Shaped Domains

In this presentation, we suggest a new approach to analyzing overlapping Schwarz methods for problems posed in H(curl) and H(div) in 3D with generally shaped domains. The theory is based on new discrete Helmholtz type decompositions that are robust to the topological properties of the domain.

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CP9

Applications of the Generalized Minimal Residual (GMREs) Algorithm on the Exact Solution of Multiple Acoustic Scattering Problems

An exact solution to multiple acoustic scattering problems from circular cylindrical obstacles in two-dimensions can be represented in terms of eigenfunction expansions for each scatterer. An infinite linear system for the coefficients of these expansions results after applying obstacle boundary conditions. Due to the poor conditioning of this coupled system, direct solution methods applied to it have not successfully handled configurations with large numbers of obstacles, or those with obstacles that are relatively close together. We propose a residual-based iterative algorithm, inspired by the Generalized Minimal Residual (GMRES), to efficiently solve the resulting linear system. This algorithm effectively decouples the problem by iteratively solving for the coefficients of one obstacle assuming that the coefficients of the other obstacles are known from a previous iteration step, then successively iterates on the residuals of the proposed solution, while aiming to eliminate the residuals entirely. We display results comparing the performance of this algorithm to a direct solver and to a finite-difference approximation of the associated multiple scattering boundary value problem.

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CP10

Stochastic Immunology Model and Its Analysis

We present a stochastic model in immunology describing the evolution of influenza A disease in the human organism. Euler-Maruyama simulation algorithm is used to analyze the stochastic model. Numerical simulations explore the dynamic behavior of the system of reproduction in vitro in the absence of any immune component. There are two absorbing states for the dynamics of our system: extinction of virus cells and extinction of host cells. The mean times of absorption and probabilities of absorption depending on the parameters of the system are also investigated in the simulations.

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CP10

Scalable Time-Stepping for Nonlinear PDEs Through Krylov Subspace Spectral Methods

Exponential integrators provide an efficient approach to solving large stiff systems of ODEs derived from PDEs, compared to standard time-stepping schemes. However, the bulk of the computational effort in these methods is due to products of matrix functions and vectors, which can become very costly at high resolution due to an increase in the number of Krylov projection steps needed to maintain accuracy. In this talk, exponential integrators are modified by using Krylov subspace spectral (KSS) methods, instead of Krylov projection methods, to compute products of matrix functions and vectors. Numerical experiments, featuring diffusion equations and wave propagation problems, show that this modification causes the number of Krylov projection steps to become bounded independently of the grid size, thus dramatically improving efficiency and scalability. Finally, it is shown how a similar approach can be used to derive multistep methods of both Adams and BDF type that also realize these benefits.

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CP10

On Numerical Differentiation of Chaos

Computing the linear response, or the derivative of long-time-averaged observables with respect to system parameters, is a central problem for statistics and engineering. Conventionally, there are three straight-forward formulas for the linear response: the pathwise perturbation, the divergence, and the kernel differentiation formula. We shall explain why none works for the general case, which is typically chaotic, high-dimensional, and small-noise. We present the fast response formula, which is an ergodic-theorem type of formula for the linear response of hyperbolic chaos. It is the average of some function of u-many vectors over an orbit, where u is the unstable dimension, and those vectors can be computed recursively. Then we discuss how to further incorporate the kernel differentiation trick to overcome non-hyperbolicity.

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CP10

A Class of Robust, Fast Direct Solvers Based on Hodlr2d

Solving systems of linear equations is often a challenge in science and engineering. Naive direct solvers are expensive for large system sizes, since the computational cost scales cubically in the underlying number of unknowns. In this work, we propose a new fast direct solver, whose computational cost scales almost linearly in the underlying number of unknowns. Our new fast direct solver leverages the fact that most of the linear systems arising out of N-body problems possess an exploitable rank structure. The time and space complexity for our new fast direct solvers scales almost linearly with the system size N, which makes them particularly useful for linear systems of equations arising out of large-scale scientific applications.

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CP10

Convergence Remedies for Option Pricing on Sparse Grids

The curse of dimensionality refers to the fundamental challenge that in the numerical solution of multidimensional partial differential equations (PDEs), the number of unknowns increases exponentially with dimension, leading to computational intractability of even moderate dimension problems. On an isotropic grid with d dimensions and n unknowns in each dimension, the number of unknowns is $\mathcal{O}(n^d)$. We use the sparse grid combination method [Griebel et al, 1992] to alleviate the curse of dimensionality; resulting in $\mathcal{O}(n(\log n)^{d-1})$ unknowns instead. However, the use of the sparse grid combination method for parabolic PDEs comes at a cost of requiring smooth initial conditions. We demonstrate potential convergence issues that arise from the nonsmooth/discontinuous initial conditions, typical of computational finance problems. We present remedies that restore convergence, emphasizing on appropriate use of coordinate transformation, appropriate application of one-dimensional grid-alignment, as well as on more general techniques. We consider multidimensional American option pricing problems, and problems with digital and/or complex payoffs. We obtain second-order accurate solutions and Greeks.

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CP11

Modeling Stochastic Disease Transmission from Within-Host Dynamics to Between-Host Spread

This research used a stochastic multiscale modeling approach to unravel the complex dynamics of infectious disease transmission. At the within-host scale, we used a mathematical model of viral particle replication and immune responses, specifically T-cell and antibody dynamics. Our case study focused on a mathematical within-host model for COVID-19 developed in a previous paper. The probability of infection was modeled by linking viral dynamics and immune response on a sigmoidal probability function, where infection depends on the day of contact between a susceptible and an infected individual. Within a linear contact network with varying encounter frequencies, our investigation revealed that the timing of host encounters is a more critical factor in disease spread than the number of encounters. Furthermore, we found that antibody dynamics play a critical role in reinfection cases, underscoring the importance of well-timed vaccination of previously infected nodes. Our numerical results highlight the importance of intra-host dynamics in influencing infectiousness and emphasize the critical role of well-timed encounters in disease spread.

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CP11

Identifiability Analysis and Model Reduction Approaches for Mechanistic Models of Biological Soft Tissues

The accurate estimation, interpretation, and reduction of parameters in mechanistic models depends on the structure of the model with respect to its parameters and the responses for which data is available. For many models of biological tissues, data is available for only a limited number of responses, relative to the overall size of the model. This leads to non-identifiability of model parameters; these parameters cannot be uniquely estimated from the data or are noninfluential in affecting a particular model response. Conversely, determining subsets of identifiable parameters can enable model reduction by fixing non-identifiable parameters or through emulation using non-mechanistic models. Techniques for local sensitivity-based identifiability analysis, model reduction and emulation will be presented for mechanistic models of biological soft tissues with applications to wound healing, cardiovascular biomechanics and orthopedic biomechanics. The tailoring of techniques will be discussed for each application, including approaches in the presence or absence of data.

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CP11

Modeling Covid-19 Disease with Deterministic and Data-Driven Models Using Daily Empirical Data in the United Kingdom: Influence of the Vaccination

In this work, we propose an overview of the COVID-19 situation in the UK using both mathematical (a nonlinear differential equation model) and statistical (time series modeling on a moving window) models on the transmission dynamics of the COVID-19 virus. This is done by integrating a hybrid model and daily empirical case and death data from the UK. We partition this dataset into before and after vaccination has started in the UK to understand the influence of vaccination on disease dynamics. We used the mathematical model to present some mathematical analyses and the calculation of the basic reproduction number (R_0). Also, the model was fitted to the data from the UK to validate the mathematical model. The Homotopy Perturbation Method was used for the numerical simulation to demonstrate the dynamics of the disease with varying parameters and the importance of vaccination. Furthermore, we used statistical modeling to validate our model by performing principal component analysis to predict the evolution of the disease outbreak in the United Kingdom on some statistical predictor indicators from time series modeling on a 14-day moving window for detecting which of these indicators capture the dynamics of the disease spread across the epidemic curve. The results of the PCA, the index of dispersion, the fitted mathematical model, and the mathematical model simulation are all in agreement with the dynamics of the disease in the UK before and after vaccination started.

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CP11

An Extension to a Lumped-Parameter Model for Kidney Pressure During Stone Removal

Previous work has derived mathematical models to predict relationships between irrigation flowrates and pressures during ureteroscopy (URS) [Williams, J.G. et al., A lumped-parameter model for kidney pressure during stone removal]. This foundational work assumes sufficiently low flowrates through the ureteroscope such that flow is laminar, and the relationship between the pressure drop along the length of the scope and the flowrate through it is linear. Here, we reconsider this assumption, and determine ureteroscopy conditions under which flows through the scope are no longer laminar, and relationships between flows and pressures are nonlinear. The novel extension to the model uses the empirical Blasius correlation to relate the pressure drop across the scope to the flowrate through it. With this incorporated into our mathematical modeling framework, we can more accurately predict flowrates and intrarenal pressures (IRPs) across the full operating space, and we validate the mathematical model with data from bench-top experiments. Mathematical modeling of ureteroscopy irrigation has enormous potential to guide ureteroscopic device design, and to aid in understanding the impact of different operating setups on flowrates and IRPs. The work here is part of a continued effort to improve the fidelity of this modeling framework while maintaining computational simplicity to ensure efficient and accurate in-silico predictions.

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CP11

Efficient Models of the Cortex via Coarse-Grained Interactions and Local Response Functions

Modeling the human cortex is challenging due to its structural and dynamic complexity. Spiking network models can incorporate many details of cortical circuits but are computationally costly and difficult to scale up, limiting their scope to small patches of cortex and restricting the range of phenomena that can be studied. Alternatively, one can use simpler and phenomenological models. They are easier to build and run, but more difficult to compare directly to experimental data. This talk presents an efficient modeling strategy that aims to strike a balance between biological realism and computational efficiency. The proposed modeling strategy combines coarse-grained (CG) representations of local circuits with steady-state local responses. A crucial observation is that potential local responses can be computed independently of dynamics on the coarse-grained level, as a consequence of anatomical structures and the nature of neuronal interactions. We first *precompute a library of steady-state local responses driven by possible lateral and external input. Then, the steady states of the modeled cortical area come naturally from the fixed point of the CG model. They can be computed by an iterative scheme combined with fast library lookup. Our approach is tested on a biologically detailed model of primate primary visual cortex (V1). Our CG model successfully produces similar activities as the biologically detailed model at* $\sim \frac{1}{1600}$ *of the computational cost.*

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CP11

Novel Travel Time Aware Metapopulation Models: A Combination with Multi-Level Waning Immunity to Assess Late-Phase Epidemic and Endemic Scenarios

In the field of infectious disease modeling, precise modeling of transmission dynamics is crucial. We present a novel metapopulation model approach that incorporates travel time to better assess disease spread influenced by mobility. This model surpasses traditional compartmental models by factoring in transmission during travel, a component present in agent-based models but often overlooked in metapopulation approaches. Our model uses a hybrid Graph-ODE framework, which is adaptable to any ODE-based model, to capture the complex relationship between mobility and infection spread, essential for analyzing densely connected regions. Our findings indicate that incorporating mobility data significantly alters outbreak patterns, offering a more nuanced tool for predicting epidemic trajectories and evaluating mobility-related interventions. This model aids in informed decision-making for intervention implementation or removal, like mandatory masks in public transport, balancing the preservation of mobility as a social good with minimizing travel-driven disease spread.

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CP12

Maxwell's Equations and Hmm

Meta-materials have unique electromagnetic properties and possess transformative potential for optics. Electromagnetic waves are governed by a set of partial differential equations called Maxwell's equations. The material response to electromagnetic waves is modeled by constitutive laws. Accurate simulations of Maxwell's equations with dispersive constitutive laws can aid the design of such materials. However, materials with such unique electromagnetic properties often have nano-scale structures that pose a challenge in solving Maxwell's equations numerically due to the resulting high computational cost. We describe a novel numerical method enabled by Heterogeneous Multiscale Methods (HMM), designed to simulate Maxwells equations coupled with the constitutive laws efficiently. We also present an energy analysis and error analysis for this numerical method.

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CP12

Enhancing Dynamical System Analysis Through Quantum Recurrent Neural Networks

We investigate the application of Quantum Long Short-Term Memory and Quantum Gated Recurrent Unit models, integrated with Variational Quantum Circuits, in modeling complex dynamical systems, including the Van der Pol oscillator, coupled oscillators, and the Lorenz system. Implementing these advanced quantum computing techniques, we compare their performance with traditional Long Short-Term Memory and Gated Recurrent Unit models. Our findings indicate that the quantum computing-based Quantum Long Short-Term Memory and Quantum Gated Recurrent Unit models demonstrate enhanced accuracy. The study concludes that these quantum models are effective and provide performance that is on par with or exceeds that of conventional Long Short-Term Memory and Gated Recurrent Unit models approaches in the field.

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CP12

Modeling Hypothermia and Frostbite with Coupled Hydrological and Thermal Models.

We present a multiscale computational model simulating body temperature in extremities subject to extreme cold (hypothermia). Blood flow in tissue is modeled as (1) Darcy flow in a continuum representing microvasculature, with sources/sinks provided by (2) a network flow model representing large arteries and veins. Flow is coupled to the Pennes bioheat transfer equation, which models temperature in the tissue, with flow in microvasculature dictating the coefficient for heat exchange, and flow in arteries serving as an additional energy source. The body responds to hypothermia by vasoconstriction. To simulate this response, we augment with a constrained ODE representing the bodys metabolic and vasoconstrictive responses. This talk will present both models and analysis.

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CP12

Numerical Computation of Generalized Rosenau-RLW Equation Via B-spline Over BFRK Approach

In this work, a septic B-spline scheme has been used to simplify the process of solving an approximate solution of the generalized Rosenau-regularized long-wave equation (GR-RLWE) with initial boundary conditions. The resulting system of first-order ODEs has been dealt with Butcher's fifth-order Runge-Kutta (BFRK) approach without using finite difference techniques for discretizing the time-dependent variables at each time level. Here no transformation or any kind of linearization technique is employed to tackle the nonlinearity of the equation. Two test problems have been selected for numerical justifications and comparisons with other researchers on the basis of efficiency, accuracy, and results of the two invariants M_I (mass) and E_I (energy) of some motion that has been used to test the conservative properties of the proposed scheme.

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CP12

Adaptive Radial Basis Function Methods for Data Reduction

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, polynomial tail, and RBF-type are selected adaptively for each RBF. We defined a machine learning problem in which these properties are learned to minimize the data reduction error. We demonstrate the method for applications of scattered data reduction on the sphere.

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CP12

Machine Learning-Based Solver Selection for Simulation of Multiphysics Processes in Porous Media

Porous media processes involve various physical phenomena such as mechanical deformation, transport, and fluid flow. The strong couplings between them must be captured by accurate simulations. Choosing an efficient solver for these simulations usually consists of decoupling into subproblems related to separate physical phenomena. Then, the suitable solvers for each subproblem and the outer iteration scheme must be chosen. The wide range of options for them makes it difficult to find the optimum. To make matters more complicated, solvers come with numerical parameters that need to be optimized. Furthermore, different solvers perform best when different processes dominate in the model, for example, the transport process can switch between advection and diffusion dominance. Switching solvers with respect to the dominant process can be beneficial, but the boundaries of when to switch solvers are unclear and complicated to analyze. We have addressed this challenge by developing a machine learning framework that automatically searches for the optimal solver for a given simulation setup, based on statistical data from previously solved problems. For a series of problems, such as time steps in a time-dependent simulation, the framework updates and improves its decision model online during the simulation. We will show how it outperforms preselected state-of-the-art solvers for our test problem setups, which include linear Biot poroelasticity and non-isothermal fluid flow.

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CP13

Learning Topological Properties on Graphs Using Continuous-Time Message Passing Via the Heat and Wave Equations

Graph Neural Networks (GNNs), while transformative, face challenges in capturing the full essence of graph structures due to their reliance on discrete-time message passing. This conventional approach, despite ensuring permutation equivariance, struggles with oversmoothing, underreaching, and computational bottlenecks, thus limiting its effectiveness in capturing graph structure. In this talk, I will introduce Continuous-time Message PASSing Network (COMPASS), a method designed to overcome these limitations by incorporating continuous-time dynamics derived from the heat and wave equations. Based on a solid theoretical foundation, COMPASS distinguishes itself in complex tasks such as the prediction of geometrical and topological features such as Ricci curvature, persistent homology, and the generating parameters of random graphs. Additionally, COMPASS can accurately predict topological attributes of molecular graphs, such as total polar surface area and ring counts, marking a significant improvement over existing discrete-time message passing networks.

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CP13

Fast Multivariate Newton Interpolation for Downward Closed Polynomial Spaces.

We introduce a fast Newton interpolation algorithm of runtime complexity $\mathcal{O}(Nn)$, where N denotes the dimension of the underlying downward closed polynomial space and n its l_p-degree, $p > 1$. We demonstrate the algorithm to reach the optimal geometric approximation rate for analytic Bos-Levenberg-Trefethen functions in the hypercube, in which case the Euclidean degree, $p = 2$, turns out to be the pivotal choice for resisting the curse of dimensionality. The spectral differentiation matrices in Newton basis are sparse, which enables realizing fast pseudo-spectral mehtods on flat spaces, polygonal domains, and regular manifolds. In particular, we discuss applications for high-dimensional PDEs and reaction diffusion systems on surfaces.

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CP13

A Fully Lagrangian Particle Level-Set Method for Solving PDEs on Deforming Surfaces

Numerical simulations of real-world systems often involve complex and dynamic geometries as boundaries or phase interfaces. Discretizing dynamic non-parametric geometries uses either meshes or point clouds. Meshfree methods enable Lagrangian simulations where the surface points move with the deforming geometry. Accurately approximating differential-geometric quantities, such as surface normals and curvatures, however, is challenging in meshfree Lagrangian approaches. So far, in Lagrangian particle methods, colorfield approaches have been popular due to their simplicity. However, their binary indicator function limits the overall accuracy of the computed surface normals and curvatures. Higher-order approaches mostly use level-set methods to implicitly describe geometries. However, most level-set methods rely on a regular Cartesian mesh, requiring particle-mesh interpolation, which, as we show, again limits the overall accuracy. Here, we propose a Lagrangian particle level-set method that performs well on irregular point clouds in a narrow band. Our method is based on high-degree regression using Newton-Lagrange polynomials on unisolvent nodes. We show high-order convergence for basic shapes and highlight the robustness of the method on a spiraling vortex. Finally, we show results for a simulation of reaction-diffusion systems on deforming, dynamic surfaces embedded in a fluid, demonstrating how the method enables computing surface differential operators in complex problems.

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CP13

Efficient Parameter Estimation of Spatiotemporal Random Fields Using the Debiased Whittle Likelihood

Physical surfaces, from the microscopic to the planetary scale, exhibit a range of morphologies that evolve under the action of differential operators. The statistical description of a surface as a spatial random field characterized by a covariance or spectral density is flexibly parameterized by the Matern form. Surface-modifying differential operators depend on properties intrinsic to the medium. We address the problem of recovering the statistical parameters of spatial random fields, the deterministic parameters that govern their evolution, and their relationship, from fields observed as finite samples with irregular boundaries, random deletions, or non-uniform structures. Our solution relies on the “debiased Whittle likelihood’, which measures the discrepancy between the empirical periodogram and its expectation under the Matern form. The Whittle likelihood is constructed by projecting observations using the discrete Fourier transform, which approximately diagonalizes the covariance matrix. We develop a robust workflow and accessible software for simulating and estimating large datasets. We formulate parameter search initialization strategies, compare optimization methods, and study trade-offs between efficiency and robustness in estimating the three-parameter Matern form and reduced, two-parameter cases. We explore how modeling evolving random fields leads to time-dependent parameter trajectories that may be uniquely diagnostic of processes within the natural sciences.

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CP13

Computational Topology and Machine Learning: Discovering Sars-CoV-2 Evolution and Transmission

In the fight against SARS-CoV-2, the rapid evolution of the virus presents a significant challenge for vaccine and antibody drug development. Frequent mutations across the virus's genome necessitate a swift and accurate understanding of their impacts, a task that proves both time-intensive and costly for traditional wet lab approaches. This talk delves into the innovative use of Computational Topology and Machine Learning as powerful tools in this battle. Specifically, I will explore their role in predicting the binding free energy (BFE) changes caused by mutations in the interaction between the virus's Spike protein and the human ACE2 receptor or antibodies. Such computational methods offer a faster, cost-effective alternative to traditional methods, enabling a deeper understanding of mutation-induced changes in infectivity and the effectiveness of antibody treatments. This research opens new pathways for the design of more precise and potent vaccines and antibody treatments, offering a glimpse into a future where technology and biology converge to combat viral threats more effectively.

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CP14

Langevin Equation with Dry Friction for Active Brownian Motion

Brownian motion with some persistence in the direction of motion, commonly known as active Brownian motion, has been used to model many crucial active transport processes like the pursuit of foreign particles in the bloodstream by white blood cells, the transmission of impulses in a neuron, and the secretion of hormones by endocrine glands. Many chemically powered nanoparticles also exhibit active Brownian motion. Such transport of matter and information in nature has been observed to show properties of transient super diffusion, ephemeral non-Gaussian displacement distribution, non-monotonic evolution of Non-Gaussian Parameter (NGP), and tempered power-law distributed displacement steps. Here, we present a Langevin equation, initially proposed to mimic animal foraging dynamics, that can manifest these key features. The equation can be solved numerically using the Euler- Maruyama method. The correspondence of the process with the stochastic Telegraph process will also be discussed.

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CP14

Multi Level Monte Carlo for Multi-Modal Distributions Arising in Computational Chemistry

Multi Level Monte Carlo (MLMC) is a technique that allows numerical estimation of an expected value with significantly less computation than traditional Monte Carlo sampling. Multi modality of the distribution, typically arising in physical chemistry application, is addressed with a specific transformation of the probability space, which otherwise challenges the stability of MLMC. Rather than using a very accurate, yet expensive estimator, it uses stepwise refinement of estimators with increasing levels of accuracy to compute the expectation. This talk presents an application of MLMC to the estimation of free energies driving chemical reactions. For atomistic problems, we show how the transformation of the probability space in MLMC leads to stability with respect to time-step refinement which is fundamental to the multilevel nature of the technique in applications with steep energy gradients at particle-particle collisions, and long-time diffusive motions. We compare the computational performance of MLMC to bootstrap and standard Monte Carlo estimators, providing insights into the essential challenges of adaptive time step schemes and opening new possibilities for applications computing energies for chemical processes and phase transformations.

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CP14

A Representative Interest of Pi and Its Simple Digital Summation

This paper is concerned with the relationship between classical bounds and real digits of Pi. The qualitative part of this research proposes an additional bound (pairing) in fractions to attain accuracy of ten decimal digits on both sides of the formula. In the quantitative part, the key digital data sets of Pi and the paired fractions are investigated similarly according to elementary statistical methods.

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CP15

Real Time Application Of Deep Learning Based Flare Smoke Detection

Effectively addressing the energy transition challenge

involves curbing hydrocarbon emissions from energy-intensive industries. Manual monitoring is inconsistent and expensive. Plans for an automated smoke detection system are underway, utilizing an in-house deep learning model. The current model has false positives from steam, prompting the objective to enhance it, reducing false positives for real-time smoke detection in an efficient closed-loop system. At the core is a computer vision model developed with a dataset of over 40,000 flare images from 22 flares across 7 locations, employing an 80:20 split for training and validation. The training dataset included steam images without smoke labels to mitigate false positives and minimal smoke images to enhance sensitivity to light smoke. External testing on unseen datasets ensured robustness and generalizability. An internally developed smoke detection model is enhanced to provide an end-to-end flare smoke detection, alerting, and DCS control solution using existing CCTV cameras. The false positives from steam images are reduced by 70%, slightly increasing false negatives but significantly improving precision in alerts. The real-time performance is enhanced, reducing CPU inference time from 0.586 to 0.381 seconds on average. This novel approach enables real time identification of smoke in flare images, using semantic segmentation and compact vision transformers, contributing to more effective and sustainable monitoring.

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CP15

Symbolic Regression Via Neural Networks

Identifying governing equations for a dynamical system is a topic of critical interest across an array of disciplines, from mathematics to engineering to biology. Machine learning - specifically deep learning - techniques have shown their capabilities in approximating dynamics from data, but a shortcoming of traditional deep learning is that there is little insight into the underlying mapping beyond its numerical output for a given input. This limits their utility in analysis beyond simple prediction. Simultaneously, a number of strategies exist which identify models based on a fixed dictionary of basis functions, but most either require some intuition or insight about the system, or are susceptible to overfitting or a lack of parsimony. Here, we present a novel approach that combines the flexibility and accuracy of deep learning approaches with the utility of symbolic solutions: a deep neural network that generates a symbolic expression for the governing equations. We first describe the architecture for our model and then show the accuracy of our algorithm across a range of classical dynamical systems. This talk is based on the paper "Symbolic Regression Via Neural Networks", Chaos 33:083150, 2023.

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CP15

Esacl: An Efficient Continual Learning Algorithm

A key challenge in the continual learning setting is to efficiently learn a sequence of tasks without forgetting how to perform previously learned tasks. Many existing approaches to this problem work by either retraining the model on previous tasks or by expanding the model to accommodate new tasks. However, these approaches typically suffer from increased storage and computational requirements, a problem that is worsened in the case of sparse models due to need for expensive re-training after sparsification. To address this challenge, we propose a new method for efficient continual learning of sparse models (EsaCL) that can automatically prune redundant parameters without adversely impacting the model's predictive power, and circumvent the need of retraining. We conduct a theoretical analysis of loss landscapes with parameter pruning, and design a directional pruning (SDP) strategy that is informed by the sharpness of the loss function with respect to the model parameters. SDP ensures model with minimal loss of predictive accuracy, accelerating the learning of sparse models at each stage. To accelerate model update, we introduce an intelligent data selection (IDS) strategy that can identify critical instances for estimating loss landscape, yielding substantially improved data efficiency. The results of our experiments show that EsaCL achieves performance that is competitive with the state-of-the-art methods.

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CP15

Can Publically Available Large Language Models Write C++ Code Using Kokkos?

Since late 2021, large language models (LLMs) have seen an explosion of attention in the popular press. Besides the oft mentioned chatbot applications, the issue of code generation, summarization and translation has also attracted a non-trivial amount of attention. Since a substantial amount of the code-specific models have been focused specifically on Python, one might wonder how effective LLMs are for writing high-performance computing (HPC) ready C++ code. We evaluate a number of publicly available LLMs on a dataset of human-generated query-response pairs using Kokkos and consider the effectiveness of retrieval-augmented generation (RAG) and fine-tuning on improving said models.

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CP16

Vertex Clustering in Dynamic Networks

In this talk, we introduce spatiotemporal graph k-means (STGkM), a novel, unsupervised method to cluster vertices within a dynamic network. Drawing inspiration from traditional k-means, STGkM finds both short-term dynamic clusters and a "long-lived' partitioning of vertices within a network whose topology is evolving over time. We provide an exposition of the algorithm, illuminate its operation on synthetic data, and provide results on a diverse set of applications. We will also briefly outline our theoretical results, in both deterministic and stochastic settings. One of the main advantages of STGkM is that it has only one required parameter, namely k; we therefore include an analysis of the range of this parameter and guidance on selecting its optimal value. This talk is based on a conference paper and a forthcoming journal paper.

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CP16

Invariant Kernels in Riemannian Symmetric Spaces

Kernel methods are powerful tools in machine learning. Classical kernel methods are based on positive-definite kernels, which map data spaces into reproducing kernel Hilbert spaces (RKHS). For non-Euclidean data spaces, positive-definite kernels can be difficult to construct. In the first part of this lecture, we present a rigorous analysis of the positive-definiteness of the Gaussian kernel when defined on a non-Euclidean symmetric space using the L^p-Godement theorems (where $p = 1, 2$), which provide verifiable necessary and sufficient conditions for a kernel defined on a symmetric space of non-compact type to be positive-definite. Beyond the connection with the Gaussian kernel, the new results in this work lay out a blueprint for the study of invariant kernels on symmetric spaces, bringing forth specific harmonic analysis tools that suggest many future applications. In the second part of the lecture, we propose the use of reproducing kernel Krein space (RKKS) based methods, which require only kernels that admit a positive decomposition. We show that one does not need to access this decomposition to learn in RKKS. We then investigate the conditions under which a kernel is positively decomposable. We show that invariant kernels admit a positive decomposition on homogeneous spaces under tractable regularity assumptions. This makes them much easier to construct than positive-definite kernels, providing a route for learning with kernels for non-Euclidean data.

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CP16

Multi-Objective Optimization Via Wasserstein-Fisher-Rao Gradient Flow

Multi-objective optimization (MOO) aims to optimize multiple, possibly conflicting objectives with widespread applications. We introduce a novel interacting particle method for MOO inspired by molecular dynamics simulations. Our approach combines overdamped Langevin and birth-death dynamics, incorporating a "dominance potential' to steer particles toward global Pareto optimality. In contrast to previous methods, our method is able to relocate dominated particles, making it particularly adept at managing Pareto fronts of complicated geometries. Our method is also theoretically grounded as a Wasserstein-Fisher-Rao gradient flow with convergence guarantees. Extensive experiments confirm that our approach outperforms state-of-the-art methods on challenging synthetic and real-world datasets.

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CP16

Learning High Dimensional Nonlinear Odes

We present a technique for learning high dimensional nonlinear dynamical systems. This technique uses a weak formulation to extend and generalize occupation kernels from previous work done by Dr. Joel A Rosenfeld, and applies them in a Vector Valued Reproducing Kernel Hilbert Space. We demonstrate linear scaling of the algorithm complexity with the dimensionality of the dynamical system. We bench-marked this technique against a collection of state of the art methods on simulated and real datasets. We observe competitive performance on all the tested datasets. We also present theoretical guarantees for the method.

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CP16

Stochastic Occupation Kernels for Learning Stochastic Differential Equations

Occupation kernels have been successfully used to learn dynamical systems. We propose a method to learn dynamical systems with a random component. That is, we learn stochastic differential equations (SDEs). Given snapshots of trajectories, we first learn the drift of an SDE, and subsequently learn the diffusion-squared given the drift. The method relies heavily on occupation kernels derived from bounded linear functionals. While learning the diffusion-squared, we solve a semi-definite program derived from a constrained optimization problem. We present examples and simulations.

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CP16

Interpretable and Extrapolative Model Reduction of Complex Dynamical Systems

Complex dynamical systems such as the large-scale chemical reaction networks in combustion, atmospheric chemistry or materials chemistry can involve hundreds of species engaging in thousands of reactions. Model reduction is thus desirable for both interpreting complex dynamics by identifying key reactions in the network, as well as enabling accelerated simulations. In this talk, we will focus on interpretable model reduction, and describe a data-driven method we developed utilizing L1-regularization for interpretably reducing nonlinear dynamics. Our method requires minimal parameterization, has polynomial-time complexity, and exhibits good predictive power when used to extrapolate in both time and state space compared to traditional methods. When applied in practice for systems ranging from combustion chemistry to microstructure evolution in shocked materials, the availability of training data is a persistent challenge. We will discuss how our method can be used in the small dataset regime to extrapolate learned dynamics to different conditions such as temperature and shock velocity.

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CP17

Heterogeneous Multi-Output Gaussian Process for Noisy Computer Models

Computer models, or simulators, are an indispensable tool in the study of physical systems. However, modern computer models generally require substantial computational resources and may produce noisy high-dimensional outputs. To calibrate these models efficiently, we employ fast surrogate models built upon limited simulation outputs. This talk introduces the Latent Component Gaussian process. This method utilizes a basis representation of the output, modeling each latent component as a separate Gaussian process. Unlike previous works that assume a homogeneous error variance across outputs, our formulation accommodates a general error covariance matrix for the noise. With an appropriate linear transformation of the output, this method provides exact inference in its prediction without incurring significant additional computational costs. The efficacy of this method is demonstrated through a series of numerical experiments and a case study. The case study focuses on the emulation of a viscous anisotropic hydrodynamics model used in heavy-ion collision simulations.

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CP17

Spiral Waves and Transient Structures in a Model of Interacting Moving Oscillators

Spiral waves have been observed in the aggregation of the slime mold Dictyostelia Discoideum. There are well studied excitable-media models that incorporate the diffusive signaling molecule cyclic AMP (cAMP) in addition to cells. cAMP mediates the interplay of its intracellular production and cell motion. We present a minimal model of cells with internal oscillators that foregoes modeling any additional signaling molecules. Their net effects enters the model via the interaction of the oscillators. This model is a Lattice Gas Cellular Automaton model on a hexagonal lattice. The cells have an adhesive phase in their internal oscillator. While in the adhesive phase, the cells are more likely to stick together. The interaction of the oscillators of the cells, is modeled via the Kuramoto model with the introduction of a delay. In this model, the spatial and synchronization components are tightly connected. The particles movement is determined by the oscillators phases with some random bias. We show that this model can generate spiral waves in both the movement of the particles and in the particles oscillators as well as other complex structures. The criteria and conditions needed to generate spiral waves is also discussed.

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CP17

Kinetic Approach to Modeling Transport of Active Matter in Confined Domains

Many biological and biomimetic micro-swimmers can be effectively described as active rods, that is, they have an elongated shape and transduce energy into persistent autonomous motion while swimming. As opposed to their passive counterparts, active rods under an imposed flow with confinements exhibit intriguing phenomena such as boundary accumulation and upstream swimming. These phenomena significantly determine how active rods are transported through micro-channels. First, a basic agent-based model for active rods will be introduced in this talk. Next, this model will be applied to study transport properties of active rods in micro-channels of various geometry. Finally, I will discuss a kinetic approach allowing for direct computation of the probability distribution function of the active rods location and orientation. The distinguishing feature of the approach to be presented is that it takes into account wall accumulation of rods and has two probability distribution functions: one for rods in the bulk and the other one for accumulated rods. This is a joint work with Shawn D. Ryan (Cleveland State University).

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CP17

Tikhonov Regularization As a Nonparametric Method for Uncertainty Quantification under Moment Constraints

Computational models are widely used to predict the behavior of systems arising in science and engineering. They usually depend on parameters whose values must be estimated from data. Thus, to realize their predictive power, it is critical to perform parameter estimation and uncertainty quantification. In some applications, only observations about an ensemble of systems are available, where each one evolves according to the same model but for different parameter values. In these cases, one can estimate some moments of the unknown probability density for the parameters. In this talk, we propose a Bayesian model for which the maximum a posteriori (MAP) estimate for the density corresponds to Tikhonov regularization for moment constraints on the density. We show that the infinite-dimensional problem characterizing the MAP can be reformulated equivalently as a finite-dimensional problem. In several cases of interest, this problem is convex, unconstrained, and the objective function is smooth. Therefore, it can be solved using algorithms with optimal convergence rates. Although the trade-off is that the objective is defined by a possibly high-dimensional integral, our results characterize the regularity of the integrand, allowing the use of tailored numerical schemes to approximate it. Furthermore, our theoretical results characterize the form of the optimal density, whereas our numerical results illustrate the performance of our method and confirm our theoretical findings.

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Delay Induced Swarm Pattern Bifurcations in Mixed Reality Experiments

Our work provides a model for swarming behavior of coupled mobile agents with communication-time delay which exhibits multiple dynamic patterns in space, which depend on interaction strength and communication delay. The model is created based on statistical mechanics principles so it applies to large numbers of networked agents. A thorough bifurcation analysis has been carried out to explore parameter regions where various patterns occur. We extend this work to robotics applications by introducing a mixed-reality framework in which real and simulated robots communicate in real time creating the self-organized states predicted by the theory. Mixed reality retains the key features of physical experiments that are hard to capture through simulation alone. The proposed swarm controller was tested on two different robotic platforms: NRLs autonomous air vehicles and UPENNs micro-autonomous surface vehicles on water. A careful bifurcation picture of the swarm dynamic patterns is compared between theory and experiment as a function of attraction strength and delay. Our experimental results led to further development of the theory in order to explain observed experimental behaviors such as bi-stability of swarm patterns, not predicted by the mean-field model.

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CP17

Numerical Approach for Age Dependent Compartment Modeling

Use of age-dependent coefficients in compartment models allow can allow for more efficient modeling of dynamical systems with large spatial domains. However, the structure of the equations are now partial differential equations with integral boundary conditions. Here we propose a numerical approach and demonstrate the results on a three-compartment cycle for a variety of age functions that model (exactly): exponential decay, advection, and advection-dispersion. We then demonstrate that we can apply this method to a delayed contagiousness SEIR model and a reaction-diffusion system involving a porous biofilm. Some analysis on the convergence will be provided.

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CP18

Exploring Collateral Sensitivity: A Mathematical Framework for Understanding Antibiotic Resistance Evolution

Sequential exposure of pathogens to antibiotics has been shown to induce changes in sensitivity to other previously used drugs, a phenomenon known as collateral sensitivity. This finding suggests that proper management of available drugs could prevent the development of resistance. In this study, we have developed a mathematical framework based on the theory of dynamic systems control to investigate the significance of collateral sensitivity in the context of bacterial resistance evolution. Using a linear dynamical model, we describe the qualitative effect of antibiotic interactions (collateral sensitivity or cross-resistance) on the population dynamics of bacteria, which continuously evolve towards resistance under antibiotic pressure. We analyze these variables through the concept of invariant control sets, which describe the regions of the state space in which we can feasibly maintain the system states. Through the concept of invariant control sets, we assess the success or failure of sequential drug therapies. Our results indicate that collateral sensitivity could be used to prevent bacterial resistance development. However, intelligent sequential strategies are required, as the clinical recommended cyclic sequences may not be sufficient in all cases.

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CP18

The Iterated Geometric Mean and Complex Arguments

It is known that the Marcus-Lopes, defined for a set of N positive real arguments, can be employed to effect an iterated mean that generalizes the well-known Arithmetic-Harmonic Mean (AHM). Like the AHM, it returns the geometric mean of those n arguments; hence, this generalized AHM effects an iterated geometric mean, or IGM. This paper illuminates properties of the Marcus-Lopes means and the IGM, before establishing that the Marcus-Lopes means can be expressed as linear combinations of their arguments, using positive real coefficients. We use this property to establish the convergence of the IGM for sets of complex arguments, as long as those arguments reside within some cone having vertex at the origin and angular extent less than p.

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CP18

Data-Driven Evaluation of ML/DL Performance for Timely and Precise Fault Identification in Cyber-Physical Systems

Multivariate time series classification (TSC) plays a crucial role in diverse real-world applications, from finance to vehicle diagnostics. In automotive diagnostics, TSC can be used for fault detection—a critical component of modern automotive diagnostic frameworks, where accurate and timely identification of anomalies is paramount. This study introduces a supervised learning benchmark for fault detection in automotive systems using Controller Area Network (CAN) data, leveraging the first publicly available dataset of its kind containing simulated faults. We employ a data-driven approach to capture the complex temporal dependencies inherent in high-dimensional CAN data. The proposed benchmark provides a robust analytical basis for model comparison among traditional ML/DL techniques, highlighting the effectiveness of each technique in discerning subtle system faults and demonstrating their capability for rapid and precise fault identification (exceeding 98% accuracy). We delve into the nuances of algorithmic performance under the data-driven paradigm, highlighting strengths and limitations of each approach by evaluating model robustness against the complexities inherent in TSC and analyze advanced performance metrics providing a comprehensive evaluation of model capabilities. Unveiling the potential of ML/DL methods in diverse diagnostic scenarios, this study paves the way for reliable system monitoring across cyber-physical systems.

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CP18

Tradeoffs Between Koopman Model Approximation and Data-Driven Stabilizing Control

Koopman system identification techniques can identify nonlinear dynamics by learning a linear model that is higher dimensional than the data used to train the model. The resulting model has two components: the *model approximation component* and the *subspace closure component*. The model approximation component captures the evolution of the measurements in time. The subspace closure component handles the remaining dynamics in the Koopman model. These two components can be clearly seen when the dictionary of the Koopman model is state-inclusive. When designing controllers for a state-inclusive Koopman model of an unknown system, the parameters in the model approximation component are key in the design of the controller. They should be fixed and untouched. However, we demonstrate several control design strategies under different data-driven problem formulations that tell a different story about the parameters of the subspace closure component. In each case we show that the parameters in the subspace closure component can be used as degrees of freedom to facilitate the controller design. When control is the objective, the subspace closure component of the Koopman model becomes secondary and subject to the control design process. This implies that certain scenarios merit data-driven control strategies distinct from system identification strategies that prioritize best fit.

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CP18

Airy Beams Interaction at the Interface of Nonlinear Optical Media

We studied a computationally intensive problem of airy beam interaction at a dielectric interface. The beam dynamics is simulated by the beam propagation method and the particle theory is applied to understand the problem analytically. The numerical simulations agree with the results of the analytical model. Airy beams are beneficial for delivering optical power in various optical settings. We found that the trapped beam at the interface acts as a power-controllable switch to reflect or transmit the incident beam at the interface.

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CP19

Prescriptive Analytics and Data-Driven Optimization Paradigms for Enhanced Operations

In the first part of the talk, we present prescriptive analytics paradigms for data-driven decision-making for complex systems and environments. Conventional data-driven decision-making methods assume access to plentiful, well-structured data to generate a prediction model, and subsequently, an optimization model is used to create a decision. However, real data can be incomplete (sparse, missing), partially observable, time-varying, and unstructured. We present joint learning and optimization frameworks to tackle emerging challenges in services and operations caused by the complexity and limitations of data and difficulties inherent in data-system integration. Our approaches are based on amalgams of machine learning, distributionally robust/stochastic optimization, and combinatorial optimization. In the second part of the talk, we discuss the application of data-driven optimization to kidney exchange.

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CP19

Sequential subspace methods on Stiefel manifold optimization problems

We study the minimization of a quadratic over Stiefel manifolds (the set of all orthogonal r-frames in R^n), which has applications in high-dimensional semi-supervised classification tasks. To reduce the computational complexity, sequential subspace methods(SSM) are employed to convert the high-dimensional minimization problems to low-dimensional ones. In this paper, we are interested in attaining an optimal solution of good quality, i.e., a "qualified" critical point. Qualified critical points are those critical points, at which the associated multiplier matrix meets some upper bound condition. These critical points enjoy the global optimality in special quadratic problems. For a general quadratic, SSM computes a sequence of "qualified critical points" in its low-dimensional "surrogate regularized models". The convergence to a qualified critical point is ensured, whenever each SSM subspace is constructed by the following vectors: (i) a set of orthogonal unit vectors associated with the current iterate, (ii) a set of vectors corresponding to the gradient of the objective, and (iii) a set of eigenvectors associated with the smallest r eigenvalues of the system matrix. In addition, when Newton direction vectors are included in subspaces, the convergence of SSM can be accelerated significantly. This is one joint work with Chung-Kuan Cheng and Chester Holtz.

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CP19

CQnet: Convex-Geometric Interpretation and Constraining Neural-Network Trajectories

We introduce CQnet, a neural network with origins in the CQ algorithm for solving convex split-feasibility problems and forward-backward splitting. This work presents a novel interpretation of a neural network's internal operation and provides practical ways to incorporate constraints on the trajectories or network output. CQnet's trajectories are interpretable as particles that are tracking a changing constraint set via its point-to-set distance function while being elements of another constraint set at every layer. More than just a convex-geometric interpretation, CQnet accommodates learned and deterministic constraints that may be sample or data-specific. The constraints may be satisfied at every network layer and the output, or the constraints can be a target towards which the states progress. We provide proof of stability with minimal assumptions. The combination of constraint handling and stability put forward CQnet as a candidate for various tasks where prior knowledge exists on the network states or output.

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CP19

An Exact and Efficient Algorithm for Basis Pursuit Denoising Via Differential Inclusions

Basis Pursuit Denoising (BPDN) is a cornerstone of compressive sensing, statistics and machine learning. Its applicability to high-dimensional signal reconstruction, feature selection, and regression problems has motivated much research and effort to develop algorithms for performing BPDN effectively, yielding state-of-the-art algorithms via first-order optimization, coordinate descent, or homotopy methods. Recent work, however, has questioned the stability, accuracy and efficiency of these state-of-the-art algorithms for BPDN. For example, the glmnet package for BPDN, which is state-of-the-art due to its claimed efficiency, suffers from instability and can yield inaccurate solutions that lead to many so-called false discoveries. Another example is existing homotopy methods for BPDN; most require technical assumptions that may not hold in practice to compute exact solution paths. Without a stable, exact, and fast algorithm, these shortcomings will continue to hinder BPDN for high-dimensional applications. In this talk, we present a novel homotopy algorithm based on differential inclusions that is stable and performs BPDN exactly (numerically, up to machine precision). We will present some numerical experiments to illustrate the efficiency of our algorithm and discuss various theoretical implications of our algorithm.

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CP19

Non-Linear Particle Swarm Optimization Algorithm for Non-Linear Fixed-Charge Transportation Problems

The non-linear fixed-charge transportation problems are one of the challenging NP-hard problems. Hence, a new non-linear particle swarm optimization algorithm (NPSO) with new inertia weight and acceleration coefficients have been introduced that not only explores the search space but also maintains the feasibility condition of the transportation problem. The performance of the proposed NPSO is compared with its existing variants. Also, some benchmarks problems from the literature have been solved and the results are compared.

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CP19

Geometry of the Space of Generalised Networks

Interactions and relations between objects may be pairwise or higher-order in nature, and so network-valued data are ubiquitous in the real world. The space of networks, however, has a complex structure that cannot be adequately described using conventional statistical tools. We intro-

duce a measure-theoretic framework for generalised networks and propose a metric that extends the Gromov-Wasserstein distance between graphs. We characterise the geometry of this space, thereby providing a unified theoretical treatment of generalised networks that encompasses the cases of pairwise, as well as higher-order, relations. In particular, we show that our generalised network metric is equivalent to the Gromov-Wasserstein and co-optimal transport metrics when restricted to the subspaces of measure networks (pairwise relations) and measure hypernetworks (higher-order relations), respectively. We extend our analysis to the setting where vertices and hyperedges have additional label information, and derive efficient computational schemes to use in practice. Equipped with these theoretical and computational tools, we demonstrate the utility of our framework in a suite of applications, including hypergraph alignment, clustering and dictionary learning from ensemble data, multi-omics alignment, as well as multiscale network alignment.

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CP20

Novel Numerical Reconstruction and Isolation of Different Nonlinear Dynamics in Videos Via Deep Learning and Applications to Dynamic Mri

Isolating different types of dynamics in video data is a highly relevant problem in video analysis particularly in dynamic medical imaging where contrast, respiratory and patient motion poses a great challenge. The analysis and further processing of the dynamics of interest is often complicated by additional unwanted dynamics. This work proposes a novel nonlinear approach for the reconstruction and separation of different types of nonlinear dynamics in a video data via deep learning. The dynamic images are represented as the forward mapping of a sequence of latent space variables via an unsupervised generator neural network with no pre-training. The latent variables are structured so that temporal variations in the data are represented in the dynamic latent space, which is independent from the general structure of the frames characterized in the static latent space. Different kinds of dynamics are also characterized independently from each other via latent space disentanglement using one dimensional prior information, called triggers. Leveraging the triggers, the method better reconstruct a video containing different dynamics, freeze any selection of dynamics and obtain accurate independent representations of the other dynamics of interest. The method subsequently figures out if one of the dynamic trigger is unknown by optimizing the latent code that detects the dynamical changes over time. This is a significant outcome of the method. The method is applied to MRI.

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CP20

Descriptor Hybridization for Cervical Cancer Colposcopy Image Classification

Cervical cancer stands as a predominant cause of female mortality, under-scoring the need for regular screenings to enable early diagnosis and preemptive treatment of precancerous conditions. The transformation zone in the cervix, where cellular differentiation occurs, plays a critical role in the detection of abnormalities. Colposcopy has emerged as a pivotal tool in cervical cancer prevention since it provides a meticulous examination of cervical abnormalities. However, challenges in visual evaluation necessitate the development of Computer Aided Diagnosis systems. Our study introduces a novel descriptor hybridized approach with feature reduction for classification of cervical cancer colposcopy images. Our approach combines conventional descriptors that capture edges and textures with contemporary deep-learning descriptors for color, outperforming the existing state-of-the- art methods. Our approach achieves exceptional performance in the range of 99%-100% for both normal-abnormal and type classification on the IARC dataset provided by WHO.

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CP20

Fast and Interpretable Support Vector Classification Based on the Truncated ANOVA Decomposition

Support Vector Machines (SVMs) are an important tool for performing classification on scattered data, where one usually has to deal with many data points in high-dimensional spaces. We propose solving SVMs in primal form using feature maps based on trigonometric functions or wavelets. In small dimensional settings the Fast Fourier Transform (FFT) and related methods are a powerful tool in order to deal with the considered basis functions. For growing dimensions classical FFT-based methods become inefficient due to the curse of dimensionality. Therefore, we restrict ourselves to multivariate basis functions, each one of them depends only on a small number of dimensions. This is motivated by the well-known sparsity of effects and recent results regarding the reconstruction of functions from scattered data in terms of truncated analysis of variance (ANOVA) decomposition, which makes the resulting model

even interpretable in terms of importance of the features as well as their couplings. The usage of small superposition dimensions has the consequence that the computational effort no longer grows exponentially but only polynomially with respect to the dimension. In order to enforce sparsity regarding the basis coefficients, we use the frequently applied ℓ_2-norm and, in addition, ℓ_1-norm regularization. The found classifying function, which is a linear combination of basis functions, and its variance can then be analyzed in terms of the classical ANOVA decomposition.

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CP20

Second-Order Adjoint-Based Data Sensitivity and Impact Analysis for Neural Network Applications

Evaluation of the sensitivity of a validation functional to data used in a neural network training process is considered as a feasible tool for assessing the impact of individual data components in determining the networks performance. An analytic derivation of the data sensitivity equations is presented together with a practical implementation based on second-order derivative information. The methodology is formulated in the context of model-constrained optimization and relies on the development of a second-order adjoint model to evaluate the Hessian-vector product and estimation of the data sensitivity through the iterative solution of a large-scale linear system. The practical ability to assess all-at-once the performance impact associated with various data components is illustrated for a binary classification problem. In this context, performance impact estimates derived a priori from data sensitivity computations are validated a posteriori through data removal experiments.

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CP20

The Occupation Kernel Method for Learning Vector Fields with Constraints

The occupation kernel method (OCK) has proven itself as a robust and efficient method for learning nonparametric systems of ordinary differential equations from trajectories in arbitrary dimensions. Using an implicit formulation provided by vector-valued reproducing kernel Hilbert spaces, we aim to show how the OCK method can be adapted to learn vector fields satisfying various physical constraints. In particular, by choosing an appropriate kernel, we can ensure that the learned vector fields analytically satisfy either solenoidal (divergence-free) and irrotational (curl-free) properties. We validate the proposed method through experiments on a variety of simulated and real datasets. It is shown that the added constraints often lead to better approximations in these application specific problems.

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CP20

The Bregman-Tweedie Classification Model

This work proposes the Bregman-Tweedie classification model and analyzes the domain structure of the extended exponential function, an extension of the classic generalized exponential function with additional scaling parameter, and related high-level mathematical structures, such as the Bregman-Tweedie loss function and the Bregman-Tweedie divergence. The base function of this divergence is the convex function of Legendre type induced from the extended exponential function. The Bregman-Tweedie loss function of the proposed classification model is the regular Legendre transformation of the Bregman-Tweedie divergence. This loss function is a polynomial parameterized function between unhinge loss and the logistic loss function. Actually, we have two sub-models of the Bregman-Tweedie classification model; H-Bregman with hinge-like loss function and L-Bregman with logistic-like loss function. Although the proposed classification model is nonconvex and unbounded, empirically, we have observed that the H-Bregman and L-Bregman outperform, in terms of the Friedman ranking, logistic regression and SVM and show reasonable performance in terms of the classification accuracy in the category of the binary linear classification problem.

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CP21

Enhancing the Efficiency of Multivariate Control Charts in the Presence of Missing Values With Machine Learning Techniques

Multivariate control charts have gained popularity as a tool for tracking and enhancing the performance of processes with several variables. The efficacy of control chart analyses, however, may be compromised by the substantial alteration caused by missing data in these multivariate datasets. Therefore, to ensure appropriate process monitoring, it is essential to address missing values in the control chart before estimating phase I parameters. There are two popular approaches to dealing with missing values: either deleting all cases with missing values or imputing the missing values with plausible estimates. In this paper, we examine how various techniques of missing value imputation such as regression, kNN, random forest (missForest), and multiple imputation by chained equation (MICE) affects the performance of multivariate control charts. Ultimately, this will guide engineers to make well-informed

choices when applying and analyzing multivariate control charts with missing values. We evaluated the effectiveness of these techniques by conducting a simulation study with different sample sizes and missing value percentages. Our simulation results show that, of all competing techniques, imputing missing values by machine learning methods perform the best.

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CP21

The McCormick Martingale Optimal Transport

Martingale optimal transport (MOT) often yields broad price bounds for options, constraining their practical applicability. In this study, we extend MOT by incorporating causality constraints among assets, inspired by the nonanticipativity condition of stochastic processes. However, this introduces a computationally challenging bilinear program. To tackle this issue, we propose McCormick relaxations to ease the bicausal formulation and refer to it as McCormick MOT. The primal attainment and strong duality of McCormick MOT are established under standard assumptions. Empirically, McCormick MOT demonstrates the capability to narrow price bounds, achieving an average reduction of 1% or 4%. The degree of improvement depends on the payoffs of the options and the liquidity of the relevant vanilla options. This is a joint work with Prof. Erhan Bayraktar and Prof. Dominykas Norgilas. The preprint is at https://arxiv.org/abs/2401.15552

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CP21

Physics Informed Quantum Long Short-Term Memory for Dynamical Systems

We present an approach to solving dynamical systems using a physics informed quantum long short-term memory neural network, showcasing a novel quantum machine learning model that outperforms traditional numerical methods in both speed and accuracy. Focused on dynamic systems modeling, our study leverages the computational power of quantum computing and the interconnectivity of neural networks for efficiently solving ordinary differential equations, a fundamental challenge in many scientific and engineering applications. By implementing this model on quantum hardware and comparing its performance with classical numerical methods, we demonstrate the hybrid model's superior computational efficiency and precision in solving complex dynamical systems. Our results indicate that the hybrid model not only provides faster solutions to ordinary differential equations but also maintains a high accuracy. This efficiency gain is attributed to the inherent advantages of quantum computing, including entanglement and superposition.

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CP21

Optimization of Drilling Parameters Using Nonlinear Regression and Hybrid Deep Learning, A Comparative Study

In this paper, we propose to use Drilling Specific Energy (DSE) technique to minimize the cost of drilling operations by minimizing the rig operation time. DSE is the modified version of Mechanical Specific Energy (MSE) which introduced the bit hydraulics to MSE. Introducing bit hydraulics will improve the ROP significantly. The first part of this work will involve the development of a correlation between rate of penetration (ROP) and the affecting parameters such as (WOB, RPM, Torque, and bit hydraulics). In fact, it is very possible; that some parameters that increase the ROP such as increasing the WOB may cause the bit foundering looking to reduction in the (ROP). Thus, the problem becomes optimization of drilling parameters to improve (ROP). Design variables to be considered include the weight on bit (WOB), the rotary speed (RPM), equivalent circulating density (ECD), and the pump circulation rate. The objectives to consider include the increasing the rate of penetration. Constraints during drilling will include differential pressure constraints (necessary to stay within a safe operating window). Nonlinear Multiple Regression (NMR) models are first performed then followed by Extreme learning Machine (ELM) with adjusted parameters. First simulation results show that the ELMs outperform the multiple regression models

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CP22

Fast Phase Retrieval: An Algorithm for Deterministically Solving a Class of Non-Convex Quadratic Programs in Polynomial Time.

Phase retrieval problems lie at the heart of many fields including crystallography, quantum tomography, biological imaging, and more. These non-convex quadratic programs arise from magnitude measurements of linear operators. We introduce an algorithm for solving a large class of multi-dimensional phase retrieval problems robustly and efficiently. Our algorithm is based on combining a modified solution to the Schwarz problem (a classical analysis problem) with a local search. We show this method is guaranteed to converge to the global minimizer for problem data that is bounded sufficiently far away from zero. We demonstrate that our method serves as a vast generalization of the traditional Hilbert transform approach to phase retrieval.

We further show that our algorithm is robust against noise and takes at most O(N Log N) operations.

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CP22

A Variant of Harsanyi's Linear Tracing Procedure to Select a Proper Equilibrium

The linear tracing procedure plays an essential role in Harsanyi and Selten's (1988) equilibrium selection theory. The concept of proper equilibrium was formulated by Myerson (1978), which can eliminate some counterintuitive perfect equilibria. Nonetheless, it remains a challenging problem to have a linear tracing procedure for selecting a proper equilibrium. To tackle this problem, this paper develops a variant of the linear tracing procedure by constituting a perturbed game in which each player maximizes her payoff against a linear convex combination between a prior belief profile and a given mixed strategy profile, where the combination coefficient for each player is a function given by an extra variable to the power of the number of pure strategies for the player. Applying the optimality conditions to the integration of the perturbed game and a convex-quadratic-penalty game, we acquire from the equilibrium condition and transformations on variables a smooth path that starts from an arbitrary strategy profile and ends at a proper equilibrium. As an alternative scheme for equilibrium selection, we present a variant of Harsanyi's logarithmic tracing procedure to select a proper equilibrium. Moreover, we give a variant of Harsanyi's linear tracing procedure and a variant of Harsanyi's logarithmic tracing procedure for selecting a perfect d-proper equilibrium.

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CP22

Sparse Data Regulation on Recurrent Neural Network for Time-Dependent Pdes

Deep learning method has emerged as an alternative approach for solving partial differential equations. Deep neural networks are integrated into physical systems governed by partial differential equations and trained by minimizing a loss function. When only sparse data is available, the partial differential equations constraints are posed as penalty terms in the loss function. However, this loss function may face gradient pathologies, which are characterized by the stiffness of gradients in the residuals originating from both boundary and initial conditions, consequently resulting in unsatisfactory outcomes. In this article, we utilize the Gated Recurrent Units network to solve the time-dependent partial differential equations without using boundary conditions. We also make the initial condition the initial state to reduce the computational cost. The time iteration scheme is approximated by the Gated Recurrent Units network. Then, we incorporate the prior knowledge of governing equations into the iteration scheme. After that, the implicit method is implemented on these iteration schemes to estimate the new time iteration scheme. The sparsely observed data also are added as the regulator to achieve the desired accuracy. The effectiveness of the algorithm is demonstrated by applying it to several numerical experiments, including Burgers, Allen-Cahn, nonlinear Schrodinger equations, and coupled two-dimensional Burgers equations.

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CP22

An Interpretable Graph Neural Network for Disease Classification on High-Dimensional Data

Omics data play crucial roles in exploring disease pathways, forecasting clinical outcomes, and gaining insights for disease classification. However, the significant challenge of dealing with a relatively small number of samples and a large number of features complicates the development of predictive models for omics data analysis, with inherent sparsity in biological networks and the presence of unknown feature interactions adding further complexities. The advent of Graph Neural Networks (GNN) helps alleviate these challenges by incorporating known functional relationships over a graph. However, many existing GNN models utilize graphs either from existing networks or the generated ones alone, which limits model effectiveness. To overcome this restriction, we proposed an innovative GNN model that integrates information from both externally and internally generated feature graphs. We extensively tested the model through simulations and real data applications, confirming its superior performance in classification tasks compared to existing state-of-the-art baseline models. Furthermore, our GNN model can select features with meaningful interpretations in the biomedical context.

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CP23

Young-Laplace Approach to Measuring Spatially Distributed Forces.

Measuring spatially distributed forces is crucial for studying how organisms move at various scales and remains a significant challenge. Piezo or capacitive pressure mats are readily available for animals like humans, but measuring forces in small animals (¡100g) remains outside the scope of current methods. Photoelasticity measuring tools have been previously developed, but their success has been limited by factors such as substrate size and the obstruction of light by the animal's body. Traction force microscopy is a widely used force probing technology at the cellular scale, but it does not scale up to faster measurement rates that are needed for animal locomotion. We present a new sensor to measure spatially distributed in-vivo loads in normal and tangential directions. This sensor utilizes the deformation of a thin sheet to back-calculate the applied traction; reminiscent of traction force microscopy, but with some notable differences. The substrate is a pre-stressed thin sheet that behaves more like a membrane than a shell, allowing normal and tangential load approximation via simplified membrane elasticity equations. We demonstrate the viability of this approach through numerical studies and propose an experimental realization with a non-contact digital image correlation system. Additionally, design criteria have been developed to satisfy users needs, such as spatial resolution, minimum load detection thresholds, and animal comfort.

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CP23

Application of a Neural Network to Computing the Stress Distribution of a Bridge Cross-Section

The accurate prediction of stress distribution in bridges is crucial for their design, maintenance, and safety. Unfortunately, solving for stress in bridge cross-sections can be computationally intensive and time-consuming, especially if the resolution is high. This is because we typically examine the stress at steady-state, which requires the use of implicit methods involving many iterations over large matrices. To optimize the bridge design process, we need a more efficient approach than that afforded by implicit methods. This paper introduces a novel approach utilizing tensorized Fourier Neural Operators (TFNOs) to predict the Airy stress, tension, and compression inside diverse bridge cross-sections. TFNOs rely on spectral convolutions, meaning they can learn solution spaces more efficiently than CNNs or GANs which rely on localized spatial convolutions. Given that stress fields represent solution spaces, we anticipate that TFNOs can achieve good predictions using a fraction of the training data as the aforementioned alternative architectures. After training our TFNOs using 508 data points of resolution 128 x 128, we found that the TFNOs did well predicting the Airy stress and normal stress within randomly shaped bridge cross sections. TFNOs demonstrate promise in capturing the nuanced stress distributions within bridges, aiding in identifying potential failure points, optimizing material usage, and ensuring safe load-bearing capacities.

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CP23

Strategies for Active Electromagnetic Field Control

In this presentation we will introduce the general mathematical formulation of the main problem of active control of electromagnetic fields in general environments and present several theoretical results to address it. Then we will showcase several important sub problems together with relevant numerical simulations with applications to enhanced communication modalities, energy focusing schemes, radar invisibility strategies or decoy strategies.

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CP23

Steady Vibration Problems in the Theory of Moore-Gibson-Thompson Thermoporoelasticity

In this talk, the linear model of Moore-Gibson-Thompson (MGT) thermoelasticity for porous materials is introduced in which the coupled phenomenon of the deformation of material, the concept of Darcy's law and the MGT law of heat conduction is presented. The basic boundary value problems (BVP) of steady vibrations of this model are investigated. Indeed, the fundamental solution of the system of steady vibration equations is constructed explicitly. Green's identities are obtained and the uniqueness theorems for the classical solutions of the BVPs are proved. The surface and volume potentials are constructed and their basic properties are given. The BVPs are reduced to the always solvable singular integral equations for which Noether's theorems are valid. Finally, the existence theorems for classical solutions of the internal and external BVPs are proved by means of the potential method and the theory of singular integral equations. Acknowledgements: This work was supported by Shota Rustaveli National Science Foundation of Georgia (SRNSFG) [Grant # FR-23-4905].

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CP23

L^p-Estimate for Time-Harmonic Maxwell's Equations in Heterogeneous Materials

Uniform estimate for the time-harmonic Maxwell's equations in heterogeneous materials is concerned. The heterogeneous materials are periodic and consist of two types of isotropic constituents. One type of high-conductivity and low magnetic permeability constituent of small size is compactly embedded in each period so that this constituent is disconnected. The other type of normal conductivity and magnetic permeability constituent contains the rest of the material. The contrast ratios of the conductivity and the magnetic permeability in one constituent to those in the other can be very large. In this work, L^p-estimates uniform in the contrast ratios and the periodic size for the electromagnetic fields and their rotations are derived.

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CP24

Imex-Mri-Gark: Flexible and Efficient High-Order Methods for Time Dependent Multiphysics Problems

Multiphysics processes, such as those found in plasma dynamics, climate dynamics, or chemical kinetics, often exhibit multiple time scales. Moreover, spatial discretizations may yield ODE systems with both stiff and non-stiff components, thereby numerically demonstrating multiple time

scales. To efficiently address these complexities, time integration schemes employing two or more time-step sizes, commonly referred to as multirate time integrators, are used. Here, we introduce a class of multirate time integrators known as Implicit-Explicit Multirate Infinitesimal Generalized-Structure Additive Runge-Kutta (IMEX-MRI-GARK) methods. The novelty of these methods lies in their mixed treatment of the slow time scale using an IMEX scheme, coupled with a flexible choice of integrators for the fast time scale, all while achieving high-order accuracy. IMEX-MRI-GARK methods leverage the order condition theory of GARK methods and infinitesimal time integrators to develop methods with orders up to four. This presentation will highlight the performance of these methods compared to typically employed legacy integrators and other multirate approaches

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CP24

Multiscale Motion and Deformation of Bumps in Stochastic Neural Fields with Dynamic Connectivity

Persistent neural activity in the cortex can represent estimates of parametric variables during delays of working memory tasks. Organizing activity patterns according to cell feature preference reveals activity bumps that stochastically wander in ways that predict errors in delayed estimates. Continuum neural field models support such bump solutions and can be analyzed to reveal relationships between neural architecture and the extent of wandering, providing neuromechanistic theories of response errors. Models often ignore the distinct dynamics of bumps in both excitatory/inhibitory population activity, but recent neural recordings suggest both play a role in delayed estimate encodings and responses. In past work, we maintained separate excitatory/inhibitory neural population activity and leveraged asymptotic analysis to understand how network architecture shapes stochastic bump movement. We extended this analysis to incorporate effects of short term plasticity that dynamically modifies connectivity at a slower timescale. Facilitation (depression), which strengthens (weakens) synaptic connectivity originating from active neurons, tends to increase (decrease) stability of bumps when acting on excitatory synapses. The relationship is inverted when plasticity acts on inhibitory synapses.

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CP24

A Generalized Cur Decomposition for Matrix Pairs

A CUR factorization is a type of low-rank matrix decomposition that approximates a given matrix using a small subset of its rows and columns. Unlike traditional low-rank decompositions, which use orthonormal bases, a CUR factorization offers advantages such as preserving sparsity and non-negativity, improved data interpretation, and reduced storage requirements. A standard CUR factorization is designed to handle one data matrix at a time. However, various practical applications involve multiple data matrices, in which one is tasked with extracting the most discriminative information of one data set relative to others. In this work, we generalize a CUR decomposition to the setting where we have two data sets. Given matrices A and B having the same number of columns, such a decomposition provides low-rank approximations of both matrices simultaneously in terms of a subset of their rows and columns. Two key applications we discussed include data perturbation problems where a matrix is perturbed with non-white noise and one is interested in recovering the unperturbed matrix. Another application is in a setting where we have two matrices and the goal is to find a low-rank representation of one relative to the other.

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CP24

Parametrized Fokker-Planck Equation on the Generative Model

In this research, we develop and analyze a numerical method for the Fokker-Planck equations by leveraging the generative model from deep learning. We formulate the Fokker-Planck equation as a system of ordinary differential equations (ODEs) on finite-dimensional parameter space with the parameters inherited from the generative model, such as normalizing flows. The fact that the Fokker-Planck equation can be viewed as the L2-Wasserstein gradient flow of the Kullback-Leibler (KL) divergence allows us to derive the ODEs as an analogous gradient flow on the submanifold of probability densities generated by the neural networks. We design numerical schemes for the time discretization of the proposed ODE. Our algorithms are sampling-based and can readily handle computations in higher-dimensional spaces. Moreover, we provide upper bounds for the asymptotic convergence and error analysis for our method. Some follow-up research on general Wasserstein geometric flows will also be briefly discussed.

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CP24

Interpretable Approximation of High-Dimensional Data Based on the Analysis of Variance Decomposition

When we consider the approximation of a high-dimensional function, the most fundamental issue is the curse of dimensionality. We need an exponentially increasing amount of data per dimension to achieve reasonable accuracy. However, there is a significant class of functions where the sparsity-of-effects principle applies, i.e., we have only or mostly low-dimensional interactions between the dimensions. The Analysis of Variance (ANOVA) decomposition is an important tool in the analysis of dimension interactions of multivariate, high-dimensional functions. We exploit sparsity in the ANOVA decomposition in a setting with complete orthonormal systems to obtain an approximation framework for high-dimensional functions where the sparsity-of-effects principle applies. The framework is also based on fast Fourier methods such as the NFFT. In addition, we can use the properties of the ANOVA decomposition and global sensitivity analysis to infer from the approximation which dimensions and dimension interactions are important. We can relate this to supervised learning, where we have labeled data available for training a model that is able to predict the labels on future data. Here, we have a close relationship to approximation theory since we may assume that an unknown underlying function maps each data point to its label. It is this function that we want to learn or approximate.

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CP25

Scattering Characteristics of a Wave-Bearing Shell Connected to Rigid and Flexible Coaxial Shells: A Study of Fluid-Structure Interaction

The study explores fluid-structure coupling in a complex system featuring a flexible shell connected to two rigid coaxial shells through circular step discontinuities. Utilizing the Donnell-Mushtari formulation for mathematical modeling and employing the mode-matching technique for solving the resulting boundary value problem, the analysis considers clamped and pin-jointed conditions. The investigation evaluates scattering powers and transmission loss, unveiling an inverse relationship in power propagation between the annular and inner shells. The study emphasizes the impact of parameters such as frequency, chamber length, and shell radii on system performance. Notably, adjustments to chamber dimensions and edge conditions offer avenues for achieving desired levels of attenuation.

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CP25

A Computational Comparison of Single Ventricle Patients Downstream Hemodynamics

Hypoplastic left heart syndrome (HLHS) is a congenital heart disease that accounts for 25–40% of all neonatal cardiac deaths. HLHS patients are born with an underdeveloped aorta and left heart, receiving a series of tsurgeries to create a univentricular circulatory system. Patients typically survive into early adulthood but suffer from reduced cardiac output leading to insufficient cerebral and gut perfusion. Clinical imaging data of the neck and chest vasculature is used to assess patients, but does not provide information in downstream vasculature. We utilize a 1D arterial network model to assess hemodynamics outside of the imaged region for HLHS patients and a control group of double outlet right ventricle patients (DORV). Clinical indices include blood pressure and flow outside of the imaged region, blood perfusion to organs of interest, wave intensity analysis, and shear stress. A sensitivity analysis was performed for the model and optimization techniques were also used to calibrate the model to each patient based on 4D-MRI flow data. This study successfully calibrates a 1D arterial network model to patient data and predicts clinical indices outside of the imaged region for each patient. Model outputs do show that HLHS patients have abnormal blood flow and reduced perfusion to key organs as is consistent with literature.

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CP25

Mode-Matching Analysis of Eigenvalue Problems Arising in the Study of Two-Dimensional Acoustic Waveguide Structures

Structural acoustics has gained significant intention towards the development of many engineering and applied mathematics problems alike. The major part of these contributions includes designing structures with the aim to control noise emanated from multiple sources. These naturally involve the wave scattering features at a discontinuity both in material properties and structures as investigated in the literature while studying the dissipative devices that are modelled for computational purpose. We study a mode-matching analysis of a two-dimensional waveguide problem subject to wave bearing boundaries. The underlying mathematical model characterizes the system to be non Sturm-Liouville whose solution suggests that how a choice of structure involving wave bearing boundaries is handled computationally. We aim to discuss the performance of reflected and transmitted regions of trifurcated lined waveguide backed by a line walled cavity involving multiple step discontinuities. Precisely we analyze the viability of the mode-matching technique and support our results with apposite numerical experiments. While performing the power balance the expressions for energy fluxes in different regimes are also the key finding for this study.

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CP25

Existence and Stability of Equilibria of Free-Falling Plates

Passively-falling plate systems, such as fluttering cards or gliding paper, are archetypal problems in flow-structure interaction at intermediate Reynolds numbers. We investigate equilibrium solutions of a quasi-steady nonlinear model of thin rectangular plates subject to gravitational and fluidic forces. We first demonstrate geometrically the existence and uniqueness of such equilibria for a set of fixed dimensionless parameters. We then examine a broad range of these equilibria through linear stability analysis, and present phase diagrams revealing a highly complex structure of stable and unstable regions including multiple Hopf bifurcation boundaries. We verify these findings via the full nonlinear model, and highlight some connections to unsteady flight modes. We propose a necessary condition for glider stability based on the derivative of the aerodynamic center of pressure, alongside other contributing factors for stability. We also identify a necessary condition for the stability of divers. Notably, we uncover a new distinct flight mode, emerging from a limit cycle, that supplements those previously documented. These results offer broad generalization to flat plates with arbitrary geometry and density, as well as to fluids of varying densities. We conclude by highlighting some connections to real examples of steady flight observed in nature.

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CP25

Thermo-Mechanical Stress Distribution in a Functionally Graded Microstretch Elastic Solid Half-Space Immersed in a Liquid under Fractional Order Derivative.

Abstract: This scientific article focuses on the analysis of distribution of mechanical stress and thermal stress in a functionally-graded material immersed in a liquid. Specifically, the study examines the formation of basic equations governing functionally-graded microstretch material and strain in the displacement is also examined. The Normal Mode Analysis method is applied to find the distribution expression. Coupling coefficients at the boundary are defined. Velocity of different plane waves are also calculated. The numerical results are illustrated and the of non-homogeneity parameters effects are also shown graphically. Keywords: Mechanical stress distribution Thermo-microstretch elasticity; functionally graded material; non-homogeneity.

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CP26

Numerical Modeling and Convergence Analysis of the Cahn-Hilliard-Navier-Stokes System Using a Combined Scalar Auxiliary Variable and Finite Difference Scheme

We present an overview and a numerical scheme for the Cahn-Hilliard-Navier-Stokes system by using both the Scalar Auxiliary Variable method along with a Finite Element Scheme. Our initial focus involves the development and analysis of a first-order numerical scheme, establishing its convergence for the model. Through extensive numerical simulations, we demonstrate the effectiveness of the proposed scheme in accurately simulating the Cahn-Hilliard-Navier-Stokes system. This study contributes to a deeper understanding of the system dynamics and provides a robust numerical framework for its simulation.

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CP26

Hele-Shaw Flow of Shear-Thinning Fluids

The Hele-Shaw flow describes the dynamics of an interface between two fluids of different viscosities trapped between two parallel plates separated by a very small gap, and the flow attracts attention because of its wide applications in engineering. Traditionally, the fluids involved in Hele-Shaw flow are Newtonian, when the interface displays a complicated fingering pattern called the Saffman-Taylor instability. If shear-thinning fluids are used, the interface morphology is different in that there is less fingering developed along the interface, among other differences. This project aims to understand why this difference occurs by employing numerical simulations. Computational results will be presented.

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CP26

Enstrophy Variation Via Self-Similar Collapse of Point Vortices on Inviscid Flows

We investigate enstrophy dissipation characterizing 2D turbulence in inviscid flows through point-vortex solutions of the 2D filtered Euler equations, which are a regularized 2D Euler equations. The preceding studies have shown that there exist three point-vortex solutions of the filtered equations and they converge to self-similar collapsing orbits and dissipate the enstrophy in the zero limit of a filter scale. In this study, we numerically show that the enstrophy dissipation could occur for four and five point-vortex solutions of the 2D filtered Euler equations.

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CP26

Dynamics of Elliptical Vortices with Continuous Profiles

The dynamics of elliptical vortices in 2D ideal fluid are computed using an adaptively refined and remeshed vortex method. Four examples with continuous profiles are considered comprising the compact MMZ and POLY vortices, and noncompact Gaussian and smooth Kirchhoff vortices. The phase portraits in a corotating frame all have two hyperbolic points and two sets of heteroclinic orbits. As the vortices start to rotate, two spiral filaments emerge and form a halo of low-amplitude vorticity around the core; this filamentation is attributed to vorticity advection along the unstable manifolds of the hyperbolic points. In the case of the Gaussian vortex the core rapidly axisymmetrizes, but later on it starts to oscillate and two small lobes enclosing weak vortical fluid form within the halo; this is attributed to a resonance stemming from the core oscillation. In the case of the MMZ, POLY, and smooth Kirchhoff vortices, the core remains elliptical for longer time, and the filaments entrain weak vortical fluid into two large crescent-shaped lobes which together with the core form a non-axisymmetric tripole; afterwards however the lobes repeatedly detrain fluid into the halo; this is attributed to a heteroclinic tangle near the hyperbolic points. While prior work suggested that elliptical vortices could evolve to become either an axisymmetric monopole or a non-axisymmetric tripole, the current results suggest they may oscillate between these states.

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CP26

Collective Dynamics of Self-Avoidant, Secreting Particles

Motivated by autophoretic droplet swimmers that move in response to a self-produced chemical gradient, here we examine the collective dynamics of individual motile agents using a simple reaction-diffusion system. The agents have an unlimited supply of a chemical, secrete it at a given rate, but are anti-chemotactic so move at a given speed in the direction of maximal decrease of this chemical. In both one- and two-dimensional periodic domains, we find intriguing long-time behavior of the system. Depending upon a non-dimensional parameter that involves secretion rate, agent velocity, domain size and diffusion, we find that the position of the agents either relax to regularly spaced arrays, approach these regular arrays with damped oscillation, or exhibit undamped, periodic trajectories. We examine the progression of particles that are initially seeded randomly, and we also examine the stability of the steady and periodic states.

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MS1

Scientific Machine Learning on Neuromorphic Hardware

The design of neuromorphic systems is motivated in part by the computational model theorized to underpin computation in the brain. The resulting system promises lower power requirements, while providing for highly parallel computations. This is achieved by sacrificing global memory access and reducing the complexity of operations. This has important ramifications on scientific machine learning (SciML) algorithms designed to run on these platforms. For instance, a physics-informed neural network (PINN) approximation the solution to a partial differential equation (PDE) must be adapted to a spiking neural network (SNN) compatible with the neuromorphic architecture. We describe our conversion approach, and modification of the SNN for execution on Intels Loihi-2 platform. Results will be presented showing the performance of our approach measured in terms of the accuracy, energy usage, and throughput characteristics of the implementation.

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MS1

Spiking Neural Networks for SciML

Machine learning in general, Scientific Machine Learning (SciML) specifically, has been accelerating in the past decade. An issue that has recently been surfaced relates to the sharp advances in software, that cannot seem to be matched highly performing hardware. This led researchers to explore alternative computation resources that are more energetically efficient, drawing inspiration from the human brain, that is still the most efficient learning machine in nature. The field of neuromorphic computing consists of chips designed to mimic neuronal activity and utilize it for machine learning. In this talk we explore the usage of such chips and focus on the mathematical challenges we faced when solving problems like regressing functions, operator learning, physics informed machine learning, numerical schemes, etc., on the neuromorphic chips. We show results of running those simulations in a spiking neural network framework, as well as running large scale physics simulations on the worlds' largest neuromorphic chip.

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MS1

Probabilistic Computing? Bet on Dice!

Operations in biological brains are probabilistic, and hence stochasticity has become intertwined with neuromorphic hardware, algorithms, and devices. Within this sea of stochasticity, we find a growing trend of new probabilistic computing devices for generating true random numbers. The ability to quickly and efficiently generate true random numbers at a device level suggests a future where stochastic elements are ubiquitous in computing. Current computing devices are largely focused on binary or two-state devices (i.e., coin flips), however, there may be inherent benefits to multi-state random draws (i.e., dice rolls) as well. We use mathematical analysis to establish a theoretical probabilistic framework for multi-state random draws and test our findings via device simulation and measured physical device data.

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MS1

Numerical Discrepancies Introduced by Neuromorphic Conversion of Physics-informed Neural Networks

Scientific Machine Learning (SciML) is a mathematical technique to provide numerical solutions to problems arising in the natural sciences, often in the form of partial differential equations. Since these models are tasked with modeling physical situations, they demand special attention be paid to the numerical behavior of their solutions. Physics-informed neural networks (PINNs) are a SciML tool that incorporates structure from the physics of a problem into the architecture of the neural network, relieving the network from having to simultaneously fit the data and the physical constraints during training. Recently, spiking PINNs were introduced to allow PINNs to be implemented on neuromorphic hardware, leading to potential gains in energy efficiency necessary for deploying PINN models in resource constrained environments. Due to the nonconventional, spike-based communication in neuromorphic hardware, along with the additional constraint of fixed-point representations of numerical quantities, conversion of PINN models to neuromorphic hardware introduces numerical discrepancies with their traditional implementations. This talk will cover the details of these discrepancies, how they manifest in the numerical behavior of the model, and include examples from real neuromorphic hardware, in this case Intels Loihi 2. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

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MS2

Blow-up Finite Elements

We develop a new family of finite elements which allow discontinuity at vertices while maintaining full continuity across edges. We can use these spaces to construct intrinsic discretizations of tangent vector fields on triangulated surfaces that are continuous across edges, avoiding an obstruction caused by the angle defect. Numerical evidence suggests that our method works well for the Bochner/connection Laplacian. Moreover, these spaces fit into a complex of differential forms previously studied in the 90s by Brasselet, Goresky, and MacPherson, who called them shadow forms. We instead call them blow-up Whitney forms, in light of our discovery that, if we blow up a simplex in the sense of Melrose's work on manifolds with corners, then blow-up Whitney forms correspond to the faces of the blow-up simplex, analogous to the way in which classical Whitney forms correspond to the faces of the original simplex. Finally, we discover a surprising probabilistic interpretation of the blow-up Whitney forms in terms of Poisson processes, which yields intuition and simpler computations and proofs. Work on generalizing blow-up Whitney forms to higher order is in progress.

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MS2

Extended Regge Complex for Linearized Riemann-Cartan Geometry and Cohomology

Regge calculus, a discrete scheme for general relativity and Riemannian geometry, was interpreted as a finite element fitting in a differential complex. In this talk, we show that the cohomology of the Regge complex in three dimensions is isomorphic to the infinitesimal-rigid-body-motion-valued de Rham cohomology. Based on an observation that the twisted de Rham complex extends the elasticity (Riemannian deformation) complex to the linearized version of coframes, connection 1-forms, curvature and Cartan's torsion, we construct a discrete version of linearized Riemann-Cartan geometry on any triangulation and determine its cohomology.

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MS2

Computable Reliable Bounds for PoincarFriedrichs Constants Via Cechde-Rham Complexes

We derive computable and reliable upper bounds for PoincaréFriedrichs constants of classical Sobolev spaces and, more generally, L^2 de-Rham complexes. The upper bounds are in terms of local PoincaréFriedrichs constants over subdomains and the smallest singular value of a finite-dimensional operator that is easily assembled from the geometric setting. Thus we reduce the computational effort when computing the PoincaréFriedrichs constant of finite element de-Rham complexes, and we provide computable reliable bounds even for the original L^2 de-Rham complex. The reduction to a finite-dimensional system uses diagram chasing within a Čechde-Rham complex.

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MS2

Finite Element Exterior Calculus for Hamiltonian PDEs

We consider the application of finite element exterior calculus (FEEC) methods to a class of canonical Hamiltonian PDE systems involving differential forms. Solutions to these systems satisfy a local *multisymplectic conservation law*, which generalizes the more familiar symplectic conservation law for Hamiltonian systems of ODEs, and which is connected with physically-important reciprocity phenomena, such as Lorentz reciprocity in electromagnetics. We characterize hybrid FEEC methods whose numerical traces satisfy a version of the multisymplectic conservation law, and we apply this characterization to several specific classes of FEEC methods, including conforming ArnoldFalkWinther-type methods and various hybridizable discontinuous Galerkin (HDG) methods. Interestingly, the HDG-type and other nonconforming methods are shown, in general, to be multisymplectic in a stronger sense than the conforming FEEC methods. This substantially generalizes previous work of McLachlan and Stern [Found. Comput. Math., 20 (2020), pp. 3569] on the more restricted class of canonical Hamiltonian PDEs in the de DonderWeyl grad-div form.

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MS3

Deep Neural Operators for Multiphysics Coastal Hydrodynamics

High-fidelity numerical models are commonly used to simulate physical phenomena in coastal and near-shore regions that involve nonlinear interactions between wave hydrodynamics, meteorological, and hydrological phenomena. Despite the tremendous progress in computational resources and methodologies, these high-fidelity models are still computationally expensive and require a significant amount of domain expertise. Moreover, in addition to the high computational cost, the challenges of capturing nonlinear spatial features using unstructured meshes across coupled models and the adoption of various empirical approximations render most of the existing high-fidelity, coupled wave-circulation models ineffective for use in ensemble-based forecasting systems and coastal hazard assessment studies. In this talk, we will present a deep neural operator framework inspired by the *deep operator network (DeepONet)* philosophy that can generate fast and accurate real-time predictions of various parametrized scenarios arising in coastal flows. We will explore different model formulations and demonstrate their merits and drawbacks using both a benchmark analytical problem as well as a realistic example of 2D tide-driven flow in Shinnecock Inlet Bay, New York. Moreover, a typical design and development pipeline for a model problem will be presented to highlight how such a framework might fit as a general approach for reduced order modeling in multi-physics engineering applications.

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MS3

More of a Good Thing: Stacking Deep Operator Networks

Physics-informed neural networks and operator networks have shown promise for effectively solving equations modeling physical systems. However, these networks can be difficult or impossible to train accurately for some systems of equations. Our novel multifidelity framework for stacking physics-informed neural networks and operator networks facilitates training by progressively reducing the errors in our predictions. We successively build a chain of networks, where the output at one step can act as a low-fidelity input for training the next step, gradually increasing the expressivity of the learned model.

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MS3

Self-Consistent Neural Operator for Extrapolation to Higher Reynolds Numbers

While data-driven approaches have become increasingly prevalent in solving partial differential equations (PDEs), the requirement of high-quality datasets is still a major challenge. To overcome this obstacle, data-free methods that rely on symmetry constraints and equation loss have been investigated. A key observation is that PDEs are inherently dimensionless, allowing domains of various sizes to be rescaled to a unit size with corresponding coefficients, such as the Reynolds number in the Navier-Stokes equation. Leveraging this scale-consistency, we propose sampling sub-domains of PDEs to create varied resolution sub-domain problems and enforce consistency among them. Given a dataset of a fixed domain size, we sample sub-domain instances to learns smaller scales and evaluate on larger virtual domain to extrapolate for larger scales. Further we design a full-scale neural operator to work across various domain sizes and boundary conditions. Characterized by the discretization-convergent property, neural operators maintain accuracy across arbitrary resolutions, converging as the resolution refine, which makes it a perfect candidate of full-scale modeling. Our experiments on the 2D stationary Darcy equation with varying coefficients and the dynamic Navier-Stokes equation at different Reynolds numbers demonstrate that scale-consistency reduces generalization error and improve model performance.

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MS3

Learning Diffusion for Stabilizing Linearized Chaotic Systems

Stochastic processes are used often in mathematical modeling of phenomena that appear to vary chaotically or randomly. We aim to incorporate stochastic modeling and explore the potential stabilizing effect on linearized chaotic systems. We introduce a stochastic diffusive term to obtain the Euler-Maruyama integration step as $\tilde{\mathbf{x}}_{n+1} = \tilde{\mathbf{x}}_n + \mathbf{J}(\mathbf{x}_n)\tilde{\mathbf{x}}_n \Delta t + \mathbf{\Sigma}(\mathbf{x}_n, \tilde{\mathbf{x}}_n)\Delta W_n$, where $\mathbf{J}$ is the Jacobian (drift), $\mathbf{\Sigma}$ is the diffusion matrix, and ΔW_n is the Wiener increment. Dietrich et al. (2023) use a neural network with a probabilistic loss function inspired by the structure of stochastic integrators to approximate the true drift and true diffusion used to generate the training data [Dietrich et al., Chaos 33, 023121, 2023]. Our work trains the network using data from a nonlinear dynamical system subject to perturbations. The resulting diffusion matrix $\mathbf{\Sigma}$ of the stochastic equation learned by the network is shown to be stabilizing. The motivation in using a neural network stabilization function is to enable controllable diffusion. The performance is assessed by comparing sample trajectories generated by the neural network to a scalar stabilization model derived through theory.

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MS4

Benchmarking Quantum Annealers for Combinatorial Optimization

Over the past decade, the usefulness of quantum computers for combinatorial optimization has been the subject of much debate. Thus far, experimental benchmarking studies have indicated that quantum computing hardware does not provide an irrefutable performance gain over state-of-the-art optimization methods. However, as this hardware continues to evolve, each new iteration brings improved performance and warrants further benchmarking. To that end, this work conducts an optimization performance assessment of D-Wave Systems most recent "Advantage Performance Update" computer, which can natively solve sparse unconstrained quadratic optimization problems with over 5,000 binary decision variables and 40,000 quadratic terms. This work demonstrates that classes of contrived optimization problems exist where this quantum annealer can provide run time benefits over a collection of established classical solution methods that represent the current state-of-the-art for benchmarking quantum annealing hardware. Although this work does not present strong evidence of an irrefutable performance benefit for this emerging optimization technology, it does exhibit encouraging progress, signaling the potential impacts on practical optimization tasks in the future.

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MS4

New Developments on Quantum Interior Point Methods

Interior Point Methods (IPMs) are the most efficient methods to solve linear optimization problems. However, the cost per iteration can be considerably high for large-scale problems. We highlight how quantum linear system solvers can reduce the cost per iteration in Quantum IPMs. However, QIPMs are not efficient for finding precise solutions. Another significant challenge is that the efficiency of these methods depends on the condition number of the coefficient matrix of the Newton systems. It is known that the condition number of the linear systems arising in IPMs may grow to infinity as optimality is approached. To address these challenges, we use three tools: iterative refinement methods, preconditioning, and regularization. We also compare the performance of these methods from both the theoretical and practical aspects.

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MS4

Quantum Computing and Quantum Communications in the Financial Industry

Finance has been identified as the first industry sector to benefit from quantum computing, due to the abundance of use cases with high complexity and the fact that, in finance, time is of the essence, which makes the case for solutions to be computed with high accuracy in real time. Typical use cases in finance that lend themselves to quantum computing are portfolio optimization, derivative pricing, risk analysis, and several problems in the realm of machine learning, such as fraud detection and extractive text summarization. This talk describes the state of the art of quantum computing for finance, focusing on the research work conducted by the quantum computing team at JPMorgan Chase in the area of quantum algorithms and applications for financial use cases. This presentation will also touch upon JPMorgan Chases research effort in the area of Quantum Key Distribution (QKD), the only key-exchange mechanism mathematically proven to be unconditionally secure and, therefore, resistant to quantum or classical computing attacks.

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MS4

Quantum Algorithms and Software for Nonconvex Continuous Optimization

Identifying efficient quantum algorithms for nonconvex optimization would be appealing for both theoretical and practical applications. A conventional approach to achieving quantum speedups in optimization relies on the quantum acceleration of intermediate steps in classical algorithms while maintaining the overall algorithmic trajectory and solution quality unchanged. We propose Quantum Hamiltonian Descent (QHD), which is derived from the path integral of dynamical systems corresponding to certain classical optimization algorithms, as a genuine quantum approach to nonconvex optimization. Specifically, we prove that QHD can efficiently solve a family of nonconvex continuous optimization instances, each characterized by exponentially many local minima. Meanwhile, a comprehensive empirical study suggests that representative state-of-the-art classical optimization algorithms/solvers, including Gurobi, would require super-polynomial time to solve such instances. We also propose several implementation techniques that enable us to run QHD on today's analog quantum computers for solving large-scale non-convex quadratic programming (QP) problems. Based on the QHD algorithm and its real-machine implementation, we have developed a user-friendly software package named QHDOPT, specifically designed for nonconvex optimization.

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MS5

Plasmid Loss in Spatially Constrained Microbial Populations

Plasmid DNA is commonly found in bacterial cells, and is used by synthetic biologists to program cells to have abilities necessary for experiments. Each time a cell divides, there is a chance that all plasmids are passed to one daughter cell, leaving the second daughter cell with no plasmids. In a finite population of dividing cells, plasmid loss eventually impacts the behavior of the whole population, as plasmid free cells have different DNA and grow exponentially after the first loss event. Because biologists frequently observe cell populations in very small microfluidic traps, we introduce a spatial model of a cell population undergoing plasmid loss, where dividing cells push out cells that are on the edge of the microfluidic trap. We explore how properties of single cells, such as division age, impact the behavior of the whole population in this model.

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MS5

Time-Dependent Antibody Kinetics for Previously Infected and Vaccinated Individuals via Graph-Theoretic Modeling

Modeling the deterioration of antibody levels is paramount to understanding the time-dependent viral response to infections, vaccinations, or a combination of the two. These events have been studied experimentally, but also benefit from a rigorous mathematical underpinning. Disease/vaccination prevalence in the population and time-dependence on a personal timeline simultaneously affect antibody levels, interact non-trivially, and pose considerable modeling challenges. We propose a time-inhomogeneous Markov chain model for event-to-event transitions coupled with a probabilistic framework for post-infection or post-vaccination antibody kinetics. This approach is ideal to model sequences of infections and vaccinations, or personal trajectories in a population. Here, we use synthetic data to demonstrate the modeling process as well as estimation of transition probabilities. This work is an important step towards a comprehensive understanding of antibody kinetics that will allow us to simulate and predict real-world disease response scenarios

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MS5

Effective Statistics of Molecular Motors with Nonlinear Springs

In this talk, we consider averaged systems which track the position two molecular motors attached to a cargo. Positions of motors and cargos are modeled as continuous time stochastic differential equations with switching terms to account for the attachment and detachment of motors from the microtubule. We show that the procession behavior can differ greatly depending on the choice of spring for modeling the motor tether. In particular, a nonlinear spring allows for temporarily unengaged motors. This requires an augmented state space when using a Markov chain analysis to account for both taut and relaxed motor configurations. We obtain effective statistics for velocity and diffusivity over a variety of ensembles, and test them against extensive numerical simulations.

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MS5

Modeling Mosquito Lifecycle Dynamics: A Comparative Study of Two Species in Lita, Ecuador

Aedes albopictus and Ae. aegypti are the primary vectors for arboviruses like dengue, Zika, and chikungunya in America. The presence of Ae. albopictus was first reported in Ecuador in 2017, and its gradual spread across the country raises concerns regarding disease dynamics, particularly given the existing dengue burden. Understanding the invasion patterns and interactions between this new vector and the established Aedes aegypti population is crucial for enhancing disease control strategies. To address this, we propose a model incorporating both species, accounting for seasonal variations, and estimating parameters using mosquito abundance data from Lita, Ecuador. Through numerical simulations, we explore population fluctuations driven by environmental heterogeneity and assess the impact of Aedes albopictus invasion in areas previously inhabited solely by Aedes aegypti.

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MS6

Quantum Algorithms for Computational Fluid Dynamics and Nonlinear Radiation Diffusion

In this talk we give an overview of recent developments of a quantum algorithm for solving systems of nonlinear partial differential equations (PDE) that provides a quadratic quantum speedup [1,2]. First, we briefly summarize the algorithm's construction and the regime where it provides a quadratic speedup. We then describe how the quantum oracles used in the algorithm can be implemented as quantum circuits so that the quantum PDE algorithm is now fully specified as a quantum circuit. We describe how the spatial discretization used in the quantum PDE algorithm can be implemented using finite-volume methods, replacing the finite-difference methods previously used, and show how WENO high-resolution schemes can be incorporated. Finally, we present a new application of the quantum PDE algorithm to nonlinear radiation diffusion as occurs in the optically thick plasmas produced in inertial confinement fusion. 1. F. Gaitan, Finding flows of a Navier-Stokes fluid through quantum computing, npj Quantum Inf. 6, 61 (2020). 2. F. Gaitan, Finding solutions of the Navier-Stokes equations through quantum computing recent progress, a generalization, and next steps forward, Adv. Quantum Technol. 4, 2100055 (2021).

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MS6

Quantum Computing of Fluid Dynamics Via Hamiltonian Simulation

Simulating fluid dynamics on a quantum computer is intrinsically difficult due to the nonlinear and dissipative nature of the Navier-Stokes equation (NSE) and scalar transport equation. We propose a framework for quantum computing of fluid dynamics via Hamiltonian simulation. For compressible or incompressible flows with finite vorticity and dissipation, we derive the hydrodynamic Schrdinger equation (HSE) by extending the Madelung transform. The HSE, a unitary operator on a two-component wave function, is more tractable to quantum computing than the NSE. The HSE flow can resemble a turbulent flow of entangled vortex tubes with the five-thirds energy spectrum scaling. Moreover, we transform the dissipative problem for scalar transport to a Hermitian one in a higher-dimensional space. We develop quantum algorithms for these Hamiltonian systems, which are validated on quantum computing simulators.

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MS6

Computational Fluid Dynamics on Quantum Computers

QubitSolve is developing a quantum-based solution for computational fluid dynamics (CFD). We have developed a variational quantum CFD (VQCFD) algorithm and implemented it in a software prototype as part of a project funded by the National Science Foundation. Currently, the quantum circuits in the software prototype are being tested on various quantum computing platforms, such as superconducting circuits, trapped ions, and neutral atoms. This presentation aims to discuss the performance data collected from these tests.

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MS6

Noisy Intermediate-Scale Quantum Algorithms for Differential Equations

Current quantum computers are sometimes referred to as noisy intermediate-scale quantum (NISQ) devices. They have relatively small qubit counts and lack quantum error correction. Nevertheless these devices provide us with interesting, non-classical computing capabilites. In this talk, I give an overview of our work at Quantinuum on exploring the capabilities of NISQ computers in the context of solving linear and nonlinear differential equations.

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MS7

A Mathematical and Data-Driven Approach for Enhancing Access to Local Produce in the Mid-Ohio Valley

The Community Food Initiative (CFI) non-profit organization tasked us with finding an efficient way to source produce at the Chesterhill Produce Auction (CPA). Using data analysis, computer science, and mathematics, we organized data given from various programs to model auction prices. We used these results to present the CFI with a prediction model of sustainable produce prices. Our goal was to maximize food distribution while minimizing cost.

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MS7

Crash Analysis for Lake Saint Louis Police Department

”Lake Saint Louis is a small city of just under 17,000 people in the same county as Lindenwood University. Originally a planned community, it is easily accessible by Interstate 64 and Interstate 70. It also contains two large lakes and shopping centers that attracts visitors to the area. As a result, there have been a number of traffic crashes in the area. The Lake Saint Louis Police Department (represented by Lieutenant Josh Gilliam) along with George Ertle, the City Administrator, has requested that Lindenwoods PIC Math group review data from 2019-2023 to identify patterns. We have reviewed the crash data at several locations and under multiple conditions and have uncovered some noticeable trends. We also have insights that may result in changing driver behavior or provide an engineering solution that may reduce collisions.”

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MS7

Statistical Analysis of Genome Sequences

”Many important pieces of biological information are stored in the DNA of every species. Part of the data stored in DNA is what is known as genome data. This data is made up of sequences of nucleotide bases, which biologists denote with the letters A, C, T, and G. Finding patterns, similarities, and differences between the genome data of different genera allows us to have a deeper understanding of the biological structure of living species. One angle that biologists have taken to understand genome data is through a method known as k-mer analysis. In this context, k-mers are strings of length k of the nucleotide bases. Our work aimed to explore different methods of k-mer analysis to assess their strengths and weaknesses, as well as to search for any interesting patterns regarding the genome data of different genera. ”

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MS7

Using Data Analysis to Help Fight Human Trafficking in Florida

Human trafficking is the illegal trade of people against their will who are exploited for commercial gain, labor services, or sexual acts. Rates of human trafficking victims have escalated in Florida, increasing the severity of this issue. In Tampa Bay, FL, the Strategic Alliance to Fight Exploitation (SAFE) was created to help mitigate human trafficking. In an effort to improve collaboration among SAFE organizations, the Trafficking in Persons (TIP) Lab of the University of South Florida conducted a survey. Using the data collected through that survey, this project aimed to identify services provided to human trafficking victims, the types of individuals being served, the largest gaps in resources, and areas for collaboration among the organizations in the SAFE coalition. After constructing a visualization of the survey with LATEX software, data cleaning and analysis were performed using R Statistical Software. Additionally, mathematical techniques from linear algebra and graph theory were used to showcase connections and gaps in the services provided by the SAFE coalition.

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MS7

Assessing the Impact of Climate Change and Water Quality on Crustacean Populations in Norwalk Harbor: A Statistical Analysis

Working with data provided by Harbor Watch, we compared the catch total of various crustaceans over time to multiple chemical variables. When factoring in the influence of temperature, salinity, and dissolved oxygen, our results include the usage of regression alongside data transformation to determine if each chemical change influenced population size. To achieve this, the data we were provided with had to be cleaned, organized, and have missing values filled to make the analysis as easy as possible. Using these results, we inform Harbor Watch on the potential trends in changing populations and relate these changes to environmental factors. It was noted that with rising temperatures, the populations of blue and horseshoe crabs’ increase. Similarly, as salinity rises, so does the population of horseshoe crabs. Lastly, as dissolved oxygen levels in saltwater decrease, the populations of sand shrimp, long-clawed hermit crabs, and horseshoe crabs also decline. These findings suggest that monitoring temperature and dissolved oxygen levels could be important for understanding crustacean populations.

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MS8

Generalizing Riemann Curvature to Regge Metrics in Any Dimension

The intrinsic curvature of an N-dimensional Riemannian manifold (M, g) with metric tensor g is given by the fourth-order Riemann curvature tensor. Regge calculus was originally developed for solving Einstein field equations in general relativity by discretizing the metric tensor by piece-wise constant metrics and approximating the curvature using angle deficits. Regge finite elements consist of piece-wise symmetric matrix-valued polynomials with single-valued tangential-tangential components. Due to their weak continuity, taking derivatives leads to distributions. Recently, a concept of approximating and analyzing curvature quantities like the Gauss curvature, scalar curvature, and Einstein tensor has been successfully developed. In this talk, we discuss the definition of the distributional Riemann curvature tensor in any dimension [Gopalakrishnan J., Neunteufel M., Schberl J. and Wardetzky M., Analysis of distributional Riemann curvature tensor in any dimension, arXiv:2311.01603, 2023]. We prove that in the H^{-2}-norm we obtain convergence towards the smooth curvature of rate $k+1$ if the discrete metrics interpolate the smooth metric tensor g into Regge finite elements of polynomial order k. In dimension $N=2$, the rate holds for all $k \geq 0$, whereas for $N \geq 3$, one requires $k \geq 1$. We confirm with numerical examples, implemented in the open-source finite element software NGSolve (www.ngsolve.org), that the theoretical rates are sharp.

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MS8

Bianchi Identity for Discrete Vector Bundles

In the smooth theory of vector bundles with connection the de Rham complex may be replaced by a sequence in which the spaces are vector bundle valued k-forms and the arrows are exterior covariant derivatives $d_\triangledown$. Then the curvature $F := d_\triangledown^2$ is an endomorphism valued 2-form and the Bianchi identity is $d_\triangledown F = 0$. For discrete vector bundles with connection on a simplicial complex X we show that discrete curvature emerges as a homomorphism valued 2-form from a combinatorial definition of $d_\triangledown$. This curvature satisfies a discrete Bianchi identity. We will hint at how these objects and operators can be constructed for a subdivision of X which allows the curvature to be defined on the 2-dimensional duals of co-dimension 2 primal simplices. Some of our constructions can then be shown to reproduce those introduced in [S. H. Christiansen and K. Hu, Finite Element Systems for vector bundles : elasticity and curvature, Found. Comp. Math., Vol. 23, 2023].

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MS8

Distributional Differential Operators on Riemannian Manifolds with Smooth and Regge Metrics

Several finite element discretization methods rely on elements that are not globally continuous. Using appropriate duality pairings, differential operators in the sense of distributions are well-defined. They can be used to construct and analyze mixed formulations such as the Hellan-Herrmann-Johnson (HHJ), tangential-displacement normal-normal stress (TDNNS), and mass conserving mixed stress (MCS) method. To compute curvatures of Riemannian manifolds, where the metric tensor is approximated by Regge finite elements, suitable (nonlinear) distributions are considered; see, e.g. [Gopalakrishnan J., Neunteufel M., Schberl J. and Wardetzky M., Analysis of distributional Riemann curvature tensor in any dimension, arXiv:2311.01603]. During the numerical analysis, differential operators arise, which seem to generalize distributional differential operators from the Euclidean to the covariant setting with smooth and Regge metrics. However, a systemic and rigorous derivation of these operators in the sense of distributions and analysis is lacking. In this talk, we discuss the necessary tools for defining distributional covariant differential operators on Riemannian manifolds, where the metric is smooth or a Regge finite element. We focus on the covariant incompatibility operator in arbitrary dimensions. We derive several other distributional differential operators from it. Convergence rates are tested by the open-source finite element software NGSolve (www.ngsolve.org).

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MS8

Shape Optimization with Unfitted Finite Element

Methods

We present a formulation of a PDE-constrained shape optimization problem that uses an unfitted finite element method (FEM). The geometry is represented (and optimized) using a level set approach and we consider objective functionals that are defined over bulk domains. For a discrete objective functional (i.e. one defined in the unfitted FEM framework), we derive the exact Frechet, shape derivative in terms of perturbing the level set function directly. In other words, no domain velocity is needed. We also show that the derivative is (essentially) the same as the shape derivative at the continuous level, so is rather easy to compute. In other words, one gains the benefits of both the optimize-then-discretize and discretize-then-optimize approaches. We illustrate the method on a simple model (geometric) problem with known exact solution, as well as shape optimization of structural designs. We also give some discussion on future work.

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MS9

Randomization-based Methods for Probabilistic Inference with Physics-informed Machine Learning Models

We propose a randomized approximate inference method for uncertainty quantification in physics-informed machine learning (PIML) models, with application to forward modeling and Bayesian inverse modeling. This approach targets the challenges in sampling the posterior distribution of PIML model parameters due to the ill-posedness introduced by physics-informed likelihoods. In our method, we generate samples approximating the posterior distribution of PIML model parameters by adding zero-mean Gaussian perturbations to the components of the PIML objective function. The covariances of these perturbations are chosen to ensure that the resulting randomization scheme exactly samples from the true posterior in the case of linear models. We apply the proposed method to Bayesian physics-informed neural network and conditional Karhunen-Loève expansions (B-PINN and B-PICKLE, respective) models for both forward and inverse modeling. For these problems, we characterize the ill-posedness of the inference problem in terms of the eigenspectrum of the Laplace approximation of the posterior and compare our method against Hybrid Monte Carlo sampling. We find that careful randomization can lead to accurate predictive posterior performance at reduced computational cost compared to Hybrid Monte Carlo. Finally, we discuss possible strategies for reducing the bias introduced by the randomization scheme.

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MS9

Feature-Adjacent Multi-Fidelity Physics-Informed Machine Learning of Nonlinear Operators for Partial Differential Equations

Recent developments in physics-informed operator learning, a method for learning nonlinear function mappings, have shown promise but face challenges in complex problems where high-fidelity data is required for accuracy and convergence. The production of high-fidelity data, however, is often prohibitively expensive. Our work addresses this by utilizing low-fidelity data to reduce reliance on high-fidelity data, considering the varying fidelity across different operator-related parameters. We extend the feature-adjacent multi-fidelity approach to operator learning, particularly in scenarios abundant in low-fidelity data, emphasizing the diverse range of fidelity levels present within these datasets. In our approach, the similarity between low- and high-fidelity solutions is enforced in a specially constructed feature space, which is created using an encoder. This feature space represents each low-fidelity data set and measures its proximity to the high-fidelity counterpart through a feature vector. The transformation from this feature space back to the original space is achieved with a decoder. The proposed approach markedly enhances prediction accuracy, as demonstrated in the challenging context of learning partial differential equation (PDE) solution operators.

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MS9

Extended Galerkin Neural Networks for Approximating Singular Variational Problems with Error Control

We present extended Galerkin neural networks, a variational framework for approximating general boundary value problems (BVPs) with error control. In particular, we introduce a new weighted least squares variational formulation and analyze its theoretical and numerical advantages for neural network approximation of general and singular BVPs. We demonstrate that extended Galerkin neural networks are capable of learning singular solution structures and incorporating them into a so-called enriched neural network architecture. Numerical results are presented for several problems including steady Stokes flow around re-entrant corners and in convex corners with Moffatt eddies. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-859727-DRAFT.

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MS9

Deep-Learning Reduced-Order Surrogate Modeling and Approximate Bayesian Inference

We propose a reduced-order deep-learning surrogate model for dynamic systems. The method uses space-time-dependent Karhunen-Loeve expansions (KLEs) of the state variables and space-dependent parameters to identify their reduced (latent) dimensions. Then, a DNN is employed to map the parameter latent space to the state variable latent space. Next, we present an approximate Bayesian framework for uncertainty quantification in inverse solutions obtained with the said surrogate model that accounts for both the data and model uncertainty.

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MS10

Sampling Balanced Forests of Grids in Polynomial Time

We prove a polynomial fraction of k-component forests in the $m \times n$ grid graph have equal numbers of vertices in each component, for any constant k. This resolves a conjecture of Charikar, Liu, Liu, and Vuong, and establishes the first provably polynomial-time algorithm for (exactly or approximately) sampling balanced grid graph partitions according to the spanning tree distribution, which weights each k-partition according to the product, across its k pieces, of the number of spanning trees of each piece. Our result follows from a careful analysis of the probability a uniformly random spanning tree of the grid can be cut into balanced pieces. Beyond grids, we show for a broad family of lattice-like graphs, we achieve balance up to any multiplicative $(1 \pm \varepsilon)$ constant with constant probability, and up to an additive constant with polynomial probability. More generally, we show - with constant probability - components derived from uniform spanning trees can approximate any partition of a planar region given by Jordan curves. This implies polynomial time algorithms for sampling approximately balanced tree-weighted partitions for lattice-like graphs. Our results have applications to understanding political districtings, where there is an underlying graph of indivisible geographic units that must be partitioned into k population-balanced connected subgraphs. This work appeared at STOC 2024.

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MS10

Evaluating Redistricting Justifications with Local Tree Walks

Tools from discrete sampling and optimization have become increasingly important for analyzing graph-based formulations of political redistricting, requiring both operationalizing legislative text and exploring complex Pareto frontiers. In this talk I will discuss recent applications and extensions of these techniques, including for court cases and line-drawing support, evaluating nonpartisan justifications for proposed plans, and balancing multiple population constraints to address within-cycle vote dilution. Along the way I will present related open problems and some proposals based on the cycle basis walk.

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MS10

Preventing Gerrymandering by Sampling Redistricting Plans

Redistricting is the task of redrawing district boundaries, i.e. partitioning a set of geographical units into a fixed number of parts (districts), subject to certain constraints on the balance, contiguity and compactness of the partitioning. Sampling redistricting plans is crucial for evaluating and detecting gerrymandering in redistricting plans: the idea is to compare a given plan with an ensemble of plans drawn from a certain distribution. We show that ReCom [DeFordDuchin-Solomon21]-a popular Markov chain to sample redistricting plans-is exponentially slow mixing on a natural and simple graph that is representative of real geographical maps. We show an alternative way to sample balanced, compact and contiguous redistricting plans using a variant of ReCom combined with rejection sampling.

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MS11

Better Software Practices How to Write Code You're Not Afraid to Share

Are you interested in a career in science or mathematics? If yes, the chances are very good that you will interact in some way with software. Software has become a foundation of discovery in computational science and engineering and faces increasing complexity in computational models and computer architectures. This session will introduce attendees to modern software design, tools, and practices that will be applicable to students across many different disciplines.

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MS11

Automatic Differentiation as a Tool for Computational Science

Automatic Differentiation (AutoDiff) is a powerful tool for the computation of derivatives of functions defined by computer programs. AutoDiff lies at the heart of frameworks for machine learning, modeling languages for mathematical optimization, and derivative-based uncertainty quantification techniques. In this minitutorial, we aim to introduce the basic concepts of automatic differentiation and demonstrate its use for gradient based optimization. Resources will be available at: https://github.com/sriharikrishna/siaman24.

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MS12

An Efficient Quantum-walk Inspired State Preparation Circuit

Continuous-time quantum walks (CTQWs) on dynamic graphs are a recently introduced universal model of computation that offers a new paradigm that describes quantum algorithms. While it is not straightforward to implement CTQWs on dynamic graphs, it is easy to construct a dynamic CTQW equivalent of a universal gate set in the circuit model. In this talk, we present an efficient dynamic CTQW inspired state preparation circuit.

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MS12

Quantum Circuit Simulation as a Graph Ordering Problem

One of the key problems in tensor network based quantum circuit simulation is the construction of a contraction tree which minimizes the cost of the simulation, where the cost can be expressed in the number of operations as a proxy for the simulation running time. This same problem arises in a variety of application areas, such as combinatorial scientific computing, marginalization in probabilistic graphical models, and solving constraint satisfaction problems. In this talk, we'll discuss how the computationally hard portion of this problem can be reduced to one of graph ordering, and show how an optimal contraction tree can be constructed relative to a given order in polynomial time. What's more, we will discuss how existing methods in graph ordering may be utilized to acquire quality contraction trees.

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MS12

How it Goes: Building an Empirical Performance Model for QA Computations

Empirical performance studies of annealing QPUs have exposed some unusual patterns that run contrary to expectations based on theoretical models. For example, in nearly all application scenarios, best-practice dictates that the QPU be used as a constant-time sampler, in the sense that anneal time is set to a fixed value that is selected reasons other than input size N. The talk will present an emerging empirical model of QA performance that identifies the main drivers of QA performance, explains these observations, and supports (limited) generalizations about performance in practical scenarios.

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MS12

A Dual Quantum Logarithmic Barrier Method for Linear Optimization

Quantum computing has the potential to speed up some optimization methods. One can use quantum computers to solve a linear system of equations via the Quantum Linear System Algorithm (QLSA). Quantum Linear System Algorithms (QLSAs) can be used as an oracle for algorithms that require solving a linear system of equations at each iteration. The dual logarithmic barrier method is used to solve linear optimization problems. This method, at each iteration, requires the solution of a linear system to compute Newton directions. In this paper, we use QLSA to solve the linear system at each iteration of the dual logarithmic barrier method. Due to the noise in contemporary quantum computers, the output of QLSA is noisy. Hence, we need to work with the inexact variant of the dual logarithmic barrier method. Thus, this paper proposes an inexact feasible dual quantum logarithmic barrier method for linear optimization. Convergence properties of the method are studied and we show that this method has $\mathcal{O}(\sqrt{n}L)$

iteration complexity, where L is the bit length of the input data.

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MS13

Multi-Attribute Decision-Making for Location Optimization

A difficult aspect of expanding a business is determining the best place to open up a new location. Working Fields is a staffing and peer support agency based in South Burlington, VT that works with individuals recovering from substance abuse or prior incarceration. We have partnered with Working Fields to find an ideal location for their new office in the greater Springfield, MA area. We have used web-scraping, data analysis and explored mathematical models such as TOPSIS (Technique of Order Preference by Similarity to the Ideal Solution) to assess the quality of potential locations which would be best for a new office. In this presentation we will share our primary conclusions and methods.

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MS13

Detecting Infrastructure Vulnerabilities via ODE Perturbations

According to the Department of Homeland Security, cybersecurity threats to critical infrastructure are one of the most significant strategic risks for the United States. Cyber-physical systems can be modeled using dynamical systems, giving hackers a means to model their attacks. In collaboration with our partners at Oak Ridge National Laboratory, we explore methods that could be used to tamper with critical infrastructure. We model various critical cyber-physical infrastructures as linearized ODE and find minimal perturbations that destabilize these systems. We also prove some more general results about minimal destabilizing perturbations.

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MS13

Analyzing College Competencies

”College competencies are areas of expertise that form the foundation of a students higher education experience and skillset. To ensure each student is achieving the desired level of these skills regardless of the subject area of their program, Champlain College implemented a system to rank each competencys relevance to each course. We partnered with the Provosts Office to analyze the competency mapping for each majors curriculum in order to evaluate the general education at Champlain College. We will discuss our use of various data analysis techniques to determine a metric by which we can establish a baseline that represents an adequate grasp of each competency and then share our conclusions.”

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MS13

An Investigation of Rural Autonomous Driving with Big Data

DriveOhio serves as the state’s hub for smart mobility technology on the ground and in the air. DriveOhio’s Automated Driving Systems project explored how connected and automated semi trucks and passenger vehicles could improve safety for drivers, passengers, and other travelers in rural settings. The YSU PIC Math team worked with DriveOhio to analyze the data generated by the passenger vehicle deployments and identify points where the technology may not perform as well as expected. This work informs additional research to further examine the specific characteristics that may challenge automated driving technologies in a rural area.

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MS13

Modeling Water Consumption in Springdale: Scenario Analysis

Text to come.

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MS13

Addressing Understaffing in Non-Profit Meal Services

”For nearly 40 years, Project Open Hand (POH), a nonprofit founded by Ruth Brinker in 1985, has been serving older adults and people with disabilities in the San Francisco Bay Area. First established as a reaction to the AIDS outbreak, POH expanded significantly to encompass a wide range of health problems, and it now serves hundreds of meals per day. This project aims to increase POH’s operational performance, by addressing the problem of how many new employees POH should hire in order to guarantee service continuity and employees welfare. Utilizing the data provided by POH on employee status, paid time off (PTO), including vacation pay and sick leave, and current staffing schedules, we created a calculator that determines the required number of additional full-time (FTE) and part-time (PTE) employees needed to meet the work demand on a day to day basis. Furthermore, we provided Project Open Hand with a thorough overview of using this calculator, including directions for adjusting computations and the required adjustments in the future. Finally, we created numerous staffing routines to include the new hired employees. Such schedules are based on potential operational scenarios, readjusting FTE appropriations based on the days with the most affordable staffing levels. This project is part of the PIC Math program of the Mathematical Association of America (MAA) and the Society for Industrial and Applied Mathematics (SIAM). Support is provided by the National Science Foundation (NSF grant DMS-1722275)."

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MS14

An Immuno-Epidemiological Model of Foot-and-Mouth Disease in African Buffalo

We present a novel immuno-epidemiological model of Foot-and-Mouth Disease (FMD) in the African buffalo population. Upon infection, the hosts can undergo two phases, namely the acute and the carrier stages. In our model, we divide the infectious population based upon these two stages so that we can dynamically capture the immunological characteristics of both phases of the disease and to better understand the carriers role in transmission. We first define the within-host immune kinetics dependent basic disease reproduction number and show that it is a threshold condition for the local stability of the disease-free equilibrium and existence of endemic equilibrium. By using a sensitivity analysis (SA) approach developed for multiscale models, we assess the impact of the acute infection and carrier phase immunological parameters on the basic reproduction number. Interestingly, our numerical results show that the within-carrier infected host immune kinetics parameters and the susceptible individual recruitment rates play significant roles in disease persistence, which are consistent with experimental and field studies.

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MS14

Combining Data-Driven and Model-Driven Approaches to Understand West Nile Virus Dynamics Under Climate Change

Climate change will change the risk of mosquito borne illnesses because mosquito populations are directly impacted by changes in temperature and hydrology in their environment. This is a complex system of interconnected environmental, ecological, and epidemiological processes that are typically modeled separately due to incompatible scales and disparate and incomplete data. We built a modular modeling framework that links earth systems models, mosquito population models, and epidemiological disease models at a common scale in order to facilitate calibration to historical data as well as developing predictions of future risk. This approach allows us to exploit our mechanistic understanding of the *Culex* mosquito life cycle and West Nile Virus disease dynamics in conjunction with sparsely collected trap and infection data to expand our modeling capability from data rich regions to the whole of the continental US.

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MS14

Foot and Mouth Disease and the Immune System: a Quest for Mechanisms for the Persistence of Fmdv in African Buffalo

The rise of interactions between wildlife and humans increases the need to understand the relationship between different ecological and epidemiological processes within and among different interacting populations. Foot-and-mouth disease viruses (FMDV) are among the most infectious pathogens known to man, and African buffalo (*Syncerus caffer*) act as a reservoir host for FMDV in the sub-Saharan region of the African continent. Because of the impact on international livestock trade that Foot-and-mouth disease can cause, and its ubiquitous characteristic of persisting in wild populations of African buffalo while remaining highly contagious, raises the question of how this pathogen persists in the wild. In this talk, we will present current modeling work concerning the propagation of FMDVs in their reservoir host, the dynamics for the loss of acquired immunity, its role in the facilitation and stabilization of the persistence of this fast-spreading pathogen in wildlife populations, and how some of this pathogen's evolutionary mechanisms affect the pathogen's dynamics in the wild.

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MS14

Adaptive Management of Infectious Disease: Stochastic Programming for Genetic Biocontrol

Mosquitoes are responsible for a significant percentage of the global infectious disease burden. Biocontrol is critical to mitigating this problem, but its efficacy and cost varies according to geographic region, intervention technology, and vector species. Current state-of-the-art methods for intervention planning omit the mathematical optimization methods that could accommodate local-level operational objectives and limitations. This generates potential efficiency and equity gaps that stand to be exacerbated as the climate warms, a phenomenon that is shifting the range of thermo-sensitive arthropods and the diseases they carry. Here, we develop a stochastic programming approach to produce optimal biocontrol intervention strategies using genetic-based technologies given uncertain daily weather variability. We discuss the application of this work to the ecologically appropriate design of public health trials.

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MS15

Beyond Pair-Based STDP Learning Rules for Mixed-Signal Neuromorphic Chips

Spike-timing-dependent plasticity $STDP$ is a prevalent learning mechanism in the brain. Several STDP learning models have been proposed based on neurophysiological data from various brain regions. While the pair-based STDP model has been widely implemented in neuromorphic chips and Spiking Neural Networks $SNNs$, it is recognized that multi-spike models of synaptic plasticity, such as the triplet and suppression STDP models, better align with neurophysiological data in the brain compared to the pair-based STDP model. Moreover, implementing any ideal STDP-based learning model in CMOS-based neuromorphic chips requires synapses with multi-bit resolution. High-resolution synapses offer better performance but come at a cost in terms of silicon area and power consumption. In this talk, I will present two simplified and hardware-friendly STDP learning models developed for implementation in mixed-signal neuromorphic chips. In these models, the resolution of synaptic efficacy is restricted to under 4 bits, and the update in efficacy at any point in time is limited to a single bit. The potential deterioration in performance due to low-resolution synapses is compensated by including additional biologically plausible variables, such as the effect of spike triplets and the influence of neurotransmitters on STDP learning, in the model. The talk will also cover circuits designed to implement these learning models in neuromorphic chips.

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MS15

Codesign of Magnetic Tunnel Junction Devices using Reinforcement Learning and Evolutionary Optimization

Novel devices and novel computing paradigms are key for energy-efficient, performant future computing systems. However, designing devices for new applications is often time-consuming and tedious. Here, we investigate the optimization of spin-orbit torque and spin transfer torque magnetic tunnel junction models as the probabilistic devices for true random number generation. We leverage reinforcement learning and evolutionary optimization to vary key device and material properties of the various device models for stochastic operation. Our optimization methods generated different candidate devices capable of generating stochastic samples for a desired probability distribution, while also minimizing energy usage for the devices.

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MS15

Machine Learning for Tower Classification and Jet

Prediction in a Heavy Ion Colliding Application

Jet-finding is a widely pursued task for heavy-ion collision experiments, whose aim is to identify and characterize the jets present after a collision event. In this application, we use exploratory data analysis and correlation analysis to gain insights about experimental setup and characteristics of the data of which there were two types: experimental data from proton-proton collisions and synthetic data generated using PYTHIA software. There have been many approaches for producing jet-finding models. These approaches vary greatly by type of model and cost function used, amount of theoretical knowledge used to structure the model, volume of data required, type of classification or prediction produced, and level of accuracy achieved. Two machine learning problems are explored in this application: a binary classification task where we aim to identify towers belonging to the leading jet, and a multiclass prediction task where we aim to identify which jet, of many possible, each tower belongs to. Accuracy, correlation, and error analyses are conducted for both machine learning tasks to gain insights on differences in model performance across both types of data, and across events with different characteristics of interest. *SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525*

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MS16

Inf-Sup Stability of Trace Fem for Parabolic Surface PDEs

The Trace Finite Element Method (TraceFEM) solves surface PDE problems by using an unfitted mesh in the bulk surrounding a surface and using basis functions in the bulk. This talk considers parabolic problems on a fixed surface. We propose a TraceFEM semidiscrete scheme of the surface heat equation. The key feature of our method is in addition to stabilizing the solution with the normal derivative volume stabilization, we also stabilize the time derivative with a different stabilization scaling. We prove that this scheme satisfies a parabolic inf-sup stability property in the spirit of Tantardini and Veeser (2016). Consequences of inf-sup stability include symmetric error estimates, optimal rates of convergence under minimal regularity, and additional compactness of discrete solutions, which will be useful for extending to nonlinear problems. This work is joint with R.H. Nochetto (UMD), M. Shakipov (UMD), and V. Yushutin (Clemson).

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MS16

Nodal FEM for the Surface Stokes Equation

The Stokes and Navier-Stokes problems formulated on surfaces present a number of challenges distinct from those encountered for the corresponding Euclidean equations. In the context of numerical methods, these include the inability to formulate standard surface finite element velocity fields which are simultaneously continuous (H1-conforming) and tangential to the surface. In this talk we present a surface counterpart to the Euclidean MINI element which is the first FEM for the surface Stokes problem which does not require any penalization. We will also briefly discuss extension to other nodal Stokes FEM such as Taylor-Hood elements. This is joint work with Michael Neilan.

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MS16

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

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

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MS16

Meshfree Surface Parametrization with Partial Differential Equations

We discuss meshfree methods for surface partial differential equations and how they may be used to generate parametrizations of surfaces with desired properties. In particular, we look at generating conformal parametrizations and parametrizations with geodesic parameter curves. This is done by solving the Cauchy-Riemann and eikonal equations, respectively. For the eikonal equation, we also discuss high-order methods for solutions with a single point of non-differentiability, which may be used for parametrizations partially based on the distance from a single point. Numerical examples on scattered point clouds defining surfaces will be shown.

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MS17

Limiting and Efficient Implementation of the Active Flux Method

Many of the most popular solvers in Computational Fluid Dynamics (CFD) rely on the projection of the states into one dimension depending on the mesh orientation, and the application of a Riemann solver to the discontinuous data to find the upwind flux. The result is unsatisfactory representation of the physics and loss of accuracy. The Active Flux method was introduced as an alternative approach to this. The foundation of it is the distinction between the advection disturbances that are carried by the flow and the acoustics disturbances that propagate through the flow. This allows the treatment of each with the correct data. The separation of advection and acoustics offers us the opportunity to apply limiters to each of them separately. The acoustics equations are not simultaneously diagonalizable and no maximum principles can be found, therefore no existing limiters based on the ”maximum principles” can be applied. In this talk, we address the challenging task of developing a limiter for the acoustics equations in the Active Flux method. Results of a converging-diverging shock with notable symmetry will be demonstrated.

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MS17

Non-Intrusive Parametric Model Reduction via Data-Driven Operator Inference

Numerical simulation of dynamical systems is a primary means of understanding their behavior. However, simulations of large-scale systems impose significant computational expenses for outer-loop applications, such as uncertainty quantification, optimization, and inverse problems. Model reduction seeks to alleviate this burden by constructing reduced-order models (ROMs) that accurately approximate the dynamics of the underlying system but are significantly cheaper to evaluate. Such ROMs are key enablers for outer-loop applications on large-scale dynamical systems. One major challenge in developing ROMs is the limited training data for large-scale systems. This issue is aggravated in situations where, in addition to having a high-dimensional state space, the governing equations are parameterized. In this presentation, the authors present a framework for model reduction of parameterized time-dependent partial differential equations (PDEs) with affine parametric dependence, which combines the rigor of projection-based model reduction with the convenience of machine-learning methods. The parametric structure of the ROM is directly embedded into the ROM. The operators of the ROM are learned using the Operator Inference (OpInf) method. OpInf is a scientific machine learning method that combines data-driven learning and physics-based modeling. The resulting ROM can map parameter values to approximate PDE solutions efficiently.

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MS17

Developments in Meshless Model Reduction

The present work addresses limitations of traditional dimensionality reduction applied to meshless nonlocal methods in multiphysics modeling and simulations. Meshless nonlocal methods (MNMs) are versatile computational frameworks that enable effective modeling and simulation of complex multiphysics phenomena, from magnetohydrodynamics in astrophysics to multiphase flows in additive manufacturing. However, MNM methods are significantly less sparse in their numerical infrastructure relative to more traditional local/mesh-based methods such as finite element, finite volume, or finite difference methods. As a result, MNM methods can be more computationally expensive than traditional approaches. Model reduction would be a prime candidate to reduce the expense of these frameworks. However, traditional model reduction is not fit for the unstructured nature of meshless methods since it relies on structured data and fixed numerical topology to extract low-dimensionality. This work presents an approach to enable meshless model reduction through reference spaces where unstructured meshless integration points can evolve in a structured low-dimensional space. The proposed approach will be showcased on a series of fluid dynamic simulations via the smoothed-particle hydrodynamic framework.

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MS17

The Quest for High-Quality, High-Order Meshes: The Good, The Bad, and The Ugly

The efficiency of high-order methods in achieving high accuracy at a low cost rapidly deteriorates when the computational mesh is not optimal. High-order methods are also not yet robust enough to perform well on coarse meshes, but perhaps this is a natural consequence of failing to generate high-quality, high-order (curved) meshes. One wonders, ”Without improving the mathematics behind current high-order methods, would tackling challenges in creating high-quality, curved meshes bring out the superior performance of high-order methods we have been looking for?” This talk focuses on goal-oriented, node movement strategies to create optimal high-order, finite-element meshes for computational fluid dynamics. These node movement strategies exploit the synergistic relationship between vertex and high-order geometry node movements to size, stretch, and warp/curve mesh elements, which essentially adapts the basis functions used in the geometry approximation. To distinguish these node movement strategies from the traditional r-adaptation, we refer to the proposed node movement strategies as qr-adaptation, where q refers to the redistribution of high-order geometry nodes and r refers to the redistribution of vertex nodes.

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MS17

Numerical Dissipation Control in High Order Methods for Compressible Turbulence: Recent Development

This talk presents recent advances in high order finite difference method development for optimal numerical dissipation control in long time integration of direct numerical simulation, large eddy simulation and implicit LES computations of compressible turbulence for gas dynamics and MHD. The focus is on shock/turbulence interactions using adaptive blending of high order structure-preserving non-dissipative methods (classical central, Padé and dispersion relation preserving) with high order shock-capturing methods in such a way that high order shock-capturing methods are active only in the vicinity of shock/shear waves, and high gradient and spurious high frequency oscillation regions guided by flow sensors. The adaptive blending of more than one method falls under two camps: Hybrid methods and nonlinear filter methods. They are applicable for unstructured finite volume, finite element, discontinuous Galerkin and spectral element methods. The work represents the culmination of over 20 years of high order method developments and hands-on experience by the authors and collaborators in adaptive numerical dissipation control by the high order nonlinear filter approach. By examining the construction of these two approaches the nonlinear filter approach is more efficient and less CPU intensive while obtaining similar accuracy. A representative variety of test cases of comparing the various blending of high order methods with standalone standard methods will be illustrated.

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MS18

Mac-Inspired Social Network Modeling with Application to Social Insect Colonies

In 2003, I was first introduced to the concept of social network modeling by Mac during my initial year as a graduate student at UA. Subsequently, my interactions with Mac profoundly influenced my academic journey, shaping my master’s thesis on Ramanujan Graphs at UA, guiding my doctoral studies, and informing my current research at ASU. Mac’s unwavering dedication, mentorship, and leadership have been instrumental in my academic development and continue to positively impact my career trajectory. Inspired by Mac’s work and guidance, we have leveraged social network modeling tools to explore the implications of spatial heterogeneity on information and pathogen dissemination within social insect colonies. Many of our collaborative endeavors in this field involve Asma Azizi, a former Ph.D. student of Mac and former postdoc at ASU. This trajectory underscores the profound influence of Mac’s mentorship and leadership, which have not only shaped my academic pursuits but also fostered impactful collaborations and advancements in our understanding of complex systems.

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MS19

3:1 Nesting Rules in Redistricting

In legislative redistricting, most states draw their House and Senate maps separately. Ohio and Wisconsin require that their Senate districts be made with a 3:1 nesting rule, i.e., out of triplets of adjacent House districts. We seek to study the impact of this requirement on redistricting, specifically on the number of seats won by a particular political party. We compare two ensembles generated using Markov Chain Monte Carlo methods; one which uses the ReCom chain to generate Senate maps without a nesting requirement, and the other which uses a chain that generates Senate maps with a 3:1 nesting requirement. We find that requiring a 3:1 nesting rule has minimal impact on the distribution of seats won. Moreover, we study the impact the chosen House map has on the distribution of nested Senate maps, and find that an extreme seat bias at the House level does not significantly impact the distribution of seats won at the Senate level.

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MS19

Aggregating Community Maps Using Hierarchical Clustering

During the 2021 redistricting cycle, our team worked to quantify communities of interest by collecting and synthesizing thousands of community maps in partnership with grassroots organizations and/or government offices. In most cases, the spatialized testimony collected included both geographic and semantic dataa spatial representation of a community as a polygon, as well as a written narrative description of that community. In this talk, we outline our aggregation pipeline that started with spatialized testimony as input, and output processed community clusters for a given state with geographic and semantic cohesion.

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MS19

Graph Neural Networks for Modeling Census Dual Graphs for Redistricting

Graph Neural Networks (GNNs) have emerged as a powerful tool in recent years for analyzing complex graph structures, particularly those with meaningful annotations. In the context of political redistricting, geographical connections are represented by planar graphs, with districts represented by connected subgraphs. Our study applies GNNs to comprehend the underlying structure of the graphs used for redistricting in the USA, including those generated by data from the Census and relevant state agencies. This allows us to generate large collections of similar graphs for evaluating the performance of redistricting algorithms. This GNN approach also reveals connections between local graph topology and demographic attributes, highlighting the relationship between node features and demographic information such as population density, income level, and educational attainment. We also explore motifs within these graphs and their correlation with rural and urban categorization by the Census. Lastly, we assess the GNNs capacity to predict changes over time in partisanship estimates, population density, and other metrics using the learned graph representations.

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MS19

Visualizing Ensembles of Redistricting with Optimal Transport

Methods for visualizing ensembles of redistricting plans allow us to uncover the redistricting baseline for a state, compare the effect of policy choices, identify outliers, and more. Ideally, these methods should take into account the geography of the maps in the ensemble, not just vote shares. In this talk, I'll discuss some ways in which ideas from optimal transport can help us develop visualization methods. I'll describe some natural metrics on the space of redistricting plans, and briefly present a method for finding barycenters using one of these metrics. Finally, I'll spend some time talking about some recent joint work on embedding ensembles of redistricting plans into simpler spaces using semi-relaxed Gromov-Wasserstein divergence.

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MS20

Waveform Relaxation Methods for Cardiac Simulations

Waveform relaxation (WR) is a promising approach to speeding up simulations of cardiac electrophysiology. WR is a method of dividing up a problem domain, such as the spatial domain in a PDE problem, so that the subproblems may be solved independently over the time domain. The solutions are then iteratively refined by using the results from adjacent subdomains as a boundary condition. An advantage of WR compared to traditional methods of spatial parallelization is that much more parallel computation can be performed without requiring communication. However, WR-based algorithms must achieve fast convergence if they are to provide any practical benefit. While some WR algorithms have been demonstrated to converge quickly for simple problems such as the heat equation or wave equation, these methods remain mostly untested on more complex models such as those used in cardiac simulations. In this presentation, I explore the accuracy of several WR algorithms as well as the practical speedup compared to serial simulation and traditional parallelization.

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MS20

Simplifying Biophysical Models of Cardiac Dynamics to Maintain Traveling Wave Properties

Detailed biophysically realistic ion-channel models have been used to provide insight to the dynamic behavior of cardiac cells and how cells respond to a variety of inputs and treatment options. Detailed models can have dozens or hundreds of dynamic variables, making them computationally expensive. Therefore, properties of traveling waves are commonly studied in qualitative systems such as the Fitzhugh-Nagumo or Barkley models. While the qualitative models are well understood mathematically, they lack they specificity necessary to make direct connections with biology. In single cell studies, is common to simplify the biophysical models by retaining the important processes and ensuring that simplifications maintain similar firing behaviors. However, we find that many of the simplified models that have been developed for single cells do not retain key properties when applied to spatially extended tissue. We present simplifications to well-known ion-channel models that reduce the number of dynamic variables and show that these modifications retain critical properties of traveling waves and specificity needed for detailed studies.

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MS20

A General-Purpose WebGL Implementation of Cardiac Cell Models in Multi-Dimensional Tissue

Numerical simulations are widely used in various fields of medical science to provide insight into the basic understanding of diseases and for diagnostic and treatment planning purposes. The simulations are especially useful in the study of cardiac arrhythmia, which remains one of the leading causes of death in the United States and globally. Due to the complexity and the high computational demand of the cardiac cell models used for modeling arrhythmias in the tissue, scientists often use supercomputers to carry out such simulations. GPU computing has been introduced as an alternative to offering high-performance computing on personal computers in recent years. Specifically, WebGL has been proposed as a cross-platform GPU implementation that is portable and freely available on all modern browsers. In this work, we present a WebGL implementation platform that is developed independently of the cardiac-cell model of choice. As a result, this platform can be used with a wide variety of computational cell models. The users can either use a library of the models we have implemented, or design, implement, and import their own cell model of choice as a file into the program to utilize a wide variety of program features designed to facilitate the study of arrhythmias in 2D and 3D tissue.

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MS20

Excitation Waves in Unconventional Experimental Systems

The propagation of action potentials and chemical waves are well known examples for excitable behavior in spatially distributed systems. These traveling waves as well as related vortex structures have attracted interest in the context of the human heart, slime mold colonies, and the Belousov-Zhabotinsky reaction. These systems demonstrate the effectiveness of excitation waves for the relay of information over macroscopic distances, a feature often utilized by living organisms. This talk will introduce a few lesser-known systems that could expand the impact of our communities' work to applications in materials and corrosion engineering. One of these systems is the formation of inorganic structures such as heart-shaped leaves, helices, and funnels that self-organize in solutions of barium and silicate ions under the influx of CO2. The intriguing life-like shapes of these inorganic biomorphs are at least partly controlled by travelling excitation fronts and related nonlinear reaction-diffusion processes raising intriguing new questions regarding pinned rotors and subexcitable dynamics. The second example is the progression of corrosion on and within certain metal alloys of commercial relevance. We will introduce reaction-diffusion models of these solids considering activating microscale heterogeneities as well as (cell-like) grain structures. Lastly, we will discuss possible mitigation strategies that are based on a morphogenetic interpretation of the corrosion process.

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MS22

Body Composition: Insights Through Regression and Machine Learning

In this talk we discuss mathematical alternatives to dual energy x-ray absorptiometry (DXA) scans. DXA scans are a costly method of measuring body composition variables such as appendicular lean mass, bone density, and body fat percentage. These variables are fundamental benchmarks in researching osteoporosis, obesity, nutrition, and healthy aging. We employ various regression, supervised learning, and semi-supervised learning techniques, comparing and contrasting their performance on a data set encompassing information on 846 patients. The information is obtained through cheap 3D visual scans of each patient.

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MS22

Spectral and Fictitious Doman Methods for Efficient Simulation of DNA Origami

Development of new sensors to improve measurement of nucleic acids, proteins and small molecules is an active area of research with applications to viral diagnostics, cancer mutant screening and bio-surveillance. At the sensor surface on these devices there are background electrolytes together with DNA that have been folded into a desired shape through a process known as DNA origami. Measurements are taken by detecting capacitive changes at the surface in response to an applied potential. A useful mathematical model describing this process takes the form a set of Nernst-Planck equations that describe evolution of the electrolyte concentrations, which are coupled to a Poisson's equation that describes evolution of the potential. Spectral methods are well-loved for their excellent convergence properties, despite traditional limitations to simple geometries. It will be shown that for this application situating spectral methods within a fictitious domain formulation accommodates complex geometries, and offer an accurate and efficient way of solving this nonlinear system of partial differential equations.

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MS22

Robust Data-Driven Recovery of Conservation Laws with Limited Data

Conservation laws are an inherent feature in many systems modeling real world phenomenon, in particular, those modeling biological and chemical systems. If the form of the underlying dynamical system is known, one can use methods in linear algebra and algebraic geometry to identify the conservation laws. Our work focuses on using data-driven methods to identify the conservation law(s) and the limitations therein. Building upon previous work, we expand the idea of using a Singular Value Decomposition (SVD) to identify conservation law(s) within a system while keeping the amount of required data to a minimum. We will discuss features we look for in the recovery process as well as what makes our approach more suitable for low data situations compared to existing methodology. Finally, we will mention how identifying conservation laws can be used in other data-driven dynamics recovery algorithms, such as SINDy.

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MS22

Predicting Fixational Eye Movements using PDEs

The human visual system is extremely complicated, but certain phenomena exhibited by it may be modeled in a relatively simple fashion. I describe ongoing work on a model for automatic eye movements, which occur over distinct length and time scales, as a response to a variety of neuro-physiological causes. Particular attention will be given to fixational eye movements (FEMs), which constitute the tiniest movements when our eyes are fixed on a target.

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MS23

Teaching Exponentials and Logarithms through Video Games

This talk presents an innovative educational tool designed to enhance college algebra students' understanding of exponential and logarithmic functions through a video game. Set in a fictional lab in Nevada, the game offers interactive lessons that cover key concepts in exponential growth, exponential decay, and logarithms through real-world scenarios. Students will explore: water treatment processes to learn about exponential growth, radioactive decay to understand exponential decay, and sound waves to grasp logarithmic functions. This engaging approach aims to deepen conceptual understanding and promote active learning. The game is intended for integration into courses in colleges in Nevada, allowing instructors to decide how to implement the game into their courses.

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MS23

Competition, Resource Dependency and Social Organization among Queen Ants Pogonomyremex californicus

For our study, we choose to model the behavior among a species of queen ants, Pogonomyremex californicus. This particular species of ants has been found to have two subspecies that vary in behavior. The most common and ancestral sub-species are queens that found colonies alone. The other subspecies have been found to form a cooperative group of queen ants that found a single colony together (as a result of an evolutionary process). We refer to these queen types as solitary queens and cooperative queens respectively. In lab experiments, these queen types have been found to exhibit different behaviors i.e. personalities. In previous work, we created an ODE model based on these two queen types. We used a Lotka-Volterra model to model competition between the two queen types. The model yielded four outcomes: coexistence, bistability, solitary queens outcompeting cooperative queens, and cooperative queens outcompeting solitary queens. We expand upon this work by extending the model to include the impact of resource availability as well as social organization of adult ants affected by brood care and foraging for broods. We aim to address the following questions with our modeling framework: 1. How does dependency on resource availability impact the survival of either queen type? 2. How does social organization along with resource dependency change the impacts of survival of either queen type? 3. What new conditions must be met for queen survival?

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MS23

Study of Hyphal Growth in Fusing and Non-fusing Mycelia Using a Multiscale Model of fungal growth

Bacterial-fungal interactions play a fundamental role in many processes including crop biofuel development and biosystem design. In this work, we focus on the interactions between the fungus, Laccaria bicolor, and the bacterium, Psuedomonas fluorescens, and their integral role in the fitness of the roots of Populus species. Laccria bicolor synthesizes malate which stimulates growth and chemotaxis of P. flourescens. Furthermore, P. flourescens provides L. bicolor with thiamine thereby increasing fungal mass. We developed a multiscale computational model to investigate these interdependent interactions.The growth and branching of the fungal mycelia are modeled using an off-lattice spatial discrete submodel which is dependent on both diffusive and active translocation of internal nutrients and uptake of external nutrients. Malate secretion acts as a source of diffusive chemoattractant for P. fluorescens. The bacteria colony are represented by point sources of diffusing thiamine.

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MS25

Geometric Understanding of Deep Learning

This work introduces an optimal transportation (OT) view of generative adversarial networks (GANs). Natural datasets have intrinsic patterns, which can be summarized as the manifold distribution principle: the distribution of a class of data is close to a low-dimensional manifold. GANs mainly accomplish two tasks: manifold learning and probability distribution transformation. The latter can be carried out using the classical OT method. From the OT perspective, the generator computes the OT map, while the discriminator computes the Wasserstein distance between the generated data distribution and the real data distribution; both can be reduced to a convex geometric optimization process. Furthermore, OT theory discovers the intrinsic collaborative-instead of competitive-relation between the generator and the discriminator, and the fundamental reason for mode collapse. We also propose a novel generative model, which uses an autoencoder (AE) for manifold learning and OT map for probability distribution transformation. This AE-OT model improves the theoretical rigor and transparency, as well as the computational stability and efficiency; in particular, it eliminates the mode collapse. The experimental results validate our hypothesis, and demonstrate the advantages of our proposed model.

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MS25

Shape-Prior Image Segmentation Using Harmonic Beltrami Signature

This talk presents a novel approach for addressing the image segmentation problem with shape prior by introducing the Harmonic Beltrami Signature (HBS). Segmentation of degraded images is challenging, often resulting in missegmentation. The incorporation of shape information through a shape signature becomes crucial to enhance accuracy. The proposed method utilizes the HBS, a Beltrami coefficient represented as a complex-valued function, to describe the shape prior. By effectively incorporating the HBS into the quasiconformal segmentation model, shape-prior topology-preserving image segmentation can be achieved. Extensive experimental results demonstrate the efficacy of the proposed method.

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MS26

A Two-moment Radiation Transport Method for Relativistic Fluid Velocities

When modeling radiation transport through a moving fluid, the use of momentum space coordinates associated with a frame of reference comoving with the fluid greatly simplifies the inclusion of radiation-matter interactions. However, this choice of momentum space coordinates complicates the discretization of the phase-space advection operator by the appearance of velocity-dependent terms. In this context, we consider a multidimensional, spectral two-moment model which includes special relativistic effects to order all orders of v/c, where v is the fluid velocity and c is the speed of light, and we present a numerical method for evolving this model. The method uses the discontinuous Galerkin method for phase-space discretization and implicit-explicit time-stepping. The method is designed to maintain physical radiation moments during evolution. Numerical results that demonstrate the properties of the proposed method will be presented.

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MS26

A Symplectic Deep Autoencoder for Hamiltonian Systems

In this talk, we introduce a novel symplectic deep autoencoder for model order reduction (MOR) of simulating parametric Hamiltonian systems with high dimensional state variables. The existing MOR techniques for parametric Hamiltonian systems suffer two limitations. First, the inherent symplectic structure of Hamiltonian systems is not necessarily inherited by the reduced order model. This may lead to instability and blowup of the system energy. Second, due to non-dissipative nature of Hamiltonian systems, the popular global linear subspace solution representation becomes less effective, and it is related to the slow decay of the Kolmogorov n-width of the solution manifold. To overcome the difficulties, we propose a deep autoencoder using HenonNets that can preserve the symplectic structure. HenonNets are constructed by composing a sequence of Henon maps which are parametrized by neural networks. Since a Henon map is symplectic, a HenonNet preserves symplectic structures when used to learn a nonlinear embedding of the solution manifold. Hence, the reduced system is still Hamiltonian, and the system energy and long-term stability is preserved. A collection of numerical tests is presented to verify the effectiveness of the proposed MOR technique.

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MS26

Conservation Properties of the Augmented Basis Update Galerkin Integrator for Kinetic Problems

Numerical simulations of kinetic problems can become prohibitively expensive due to their large memory footprint and computational costs. A method that has proven to successfully reduce these costs is the dynamical low-rank approximation (DLRA). One key question when using DLRA methods is the construction of robust time integrators that preserve the invariances and associated conservation laws of the original problem. In this work, we demonstrate that the augmented basis update & Galerkin integrator (BUG) preserves solution invariances and the associated conservation laws when using a conservative truncation step and an appropriate time and space discretization. We present numerical comparisons to existing conservative integrators and discuss advantages and disadvantages.

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MS26

A Conservative Relaxation Crank-Nicolson Fnite Element Method for the Schrödinger-Poisson Equation

We propose a novel mass and energy conservative relaxation Crank-Nicolson finite element method for the Schrödinger-Poisson equation. Utilizing only a single auxiliary variable, we simultaneously reformulate the distinct nonlinear terms present in both the Schrödinger equation and the Poisson equation into their equivalent expressions, constructing an equivalent system to the original Schrödinger-Poisson equation. Our proposed scheme, derived from this new system, operates linearly and bypasses the need to solve the nonlinear coupled equation, thus eliminating the requirement for iterative techniques. We in turn rigorously derive error estimates for the proposed scheme, demonstrating second-order accuracy in time and $(k+1)$th order accuracy in space when employing polynomials of degree up to k. Numerical experiments validate the accuracy and effectiveness of our method and emphasize its conservation properties over long-time simulations.

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MS27

Free Elections in the Free State

In this talk I will present an ensemble analysis investigating the State Senate and Executive Council Districts in New Hampshire, which have not been previously subjected to a quantitative analysis. Using Recombination, a method of generating random samples from the space of plausible electoral maps, large ensembles are analyzed using the vote data from multiple elections. We observe that for both the number of seats won and the vote margins, the ensembles are highly sensitive to which election is used to obtain the vote data. However, across elections, partisan symmetry measures tell a more consistent story of unbalanced districts. Additionally, I will discuss local configurations and the impact of non-partisan traditional criteria on these maps.

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MS27

Comparison of Enumeration and Sampling Methods in Creating Montanas 2nd Congressional District

The 2020 decennial census data resulted in an increase from one to two congressional representatives in the state of Montana. The state underwent its redistricting process in 2021 in time for the November 2022 congressional elections, carving the state into two districts. This paper analyzes the redistricting process and compares the adopted congressional map to the space of all other possible maps. In particular, we look at the population deviation, compactness and political outcomes of these maps. Since the space is small enough to enumerate we also analyze how well the algorithms in the R package 'Redist' and the Python package 'Gerrychain' sample from the space of possible maps.

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MS27

Case Studies of Short Burst Optimization for Multiple Redistricting Criteria

In complex and non-convex energy landscapes like those that occur in the discrete context of partition sampling for redistricting, optimal states can be difficult to discover. In 2023 Cannon et al. demonstrated that ?¿'short bursts', biased random walks performed in a small number of steps and repeated, led to significantly better performance than simple biased walks in finding global optima in this redistricting context. In this talk we will present case studies applying short bursts to a variety of traditional redistricting criteria. Applying this method on real-world redistricting data allows us to explore tradeoffs between metrics and the corresponding Pareto frontiers. We also investigate applications of short bursts to continuous sampling and optimization problems and present some results about short bursts on simple random walks on labeled graphs.

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MS27

Quantifying the Non-responsiveness and Dilution of Minority Voting Power of the 2021 Georgia Districting Plan via Parallel Tempering

To audit political district maps, one may determine a baseline for the expected distribution of partisan outcomes by sampling an ensemble of maps. One approach to sampling is to precisely codify redistricting policy preferences between maps. Such preferences give rise to a probability distribution on the space of redistricting plans, and Metropolis-Hastings methods allow one to sample maps from the specified distribution. Although these approaches have nice theoretical properties and have successfully detected gerrymandering in legal settings, sampling from policy-driven distributions is often computationally difficult. Yet, there is no algorithm that can be used off-the-shelf for checking maps under generic redistricting criteria. In our recent work, we mitigate the computational challenges through a parallel tempering method and, for the first time, validate that such technique is effective at the scale of statewide precinct graphs. We develop these improvements through the first case study of Georgia district plans. Our analysis projects that recent elections in Georgia will be largely fixed even as public opinion shifts toward either party and the partisan outcome of the 2021 enacted plan does not respond to the will of the people. Only 0.12% of the 160K plans in our ensemble were similarly non-responsive. Our analysis also shows that the 2021 plan overly packs African Americans into four districts and thereby diminishes their voting power in critical swing districts.

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MS28

From Correlations to Betti Curves: The ABCs of Topological Data Analysis for Matrix Analysis

Topological data analysis (TDA) is an emerging subfield of applied mathematics that can bring new insights to data. Persistent homology, a popular TDA algorithm, is traditionally applied to point cloud data. Yet persistent homology can also be a powerful technique for analyzing matrix structure. We will start from the basics, building up to the definition of homology and Betti curves. Importantly, different null models produce distinctive sets of Betti curves. This lets us use Betti curves to compare data to null models. As an application, we will analyze neural correlation matrices from calcium imaging data of spontaneous activity in zebrafish larvae optic tectum. We will also provide a demo using open source software for TDA algorithms.

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MS28

Phase-Amplitude Methods for Reduced Order Representation of Oscillatory Dynamical Systems

Phase-amplitude-based methods have a rich history in the physical, chemical, and biological sciences for reduced order representation of limit cycle oscillators. These techniques provide a universal representation for the dynamics of both coupled and externally forced oscillators that enable rigorous mathematical analysis in applications that would otherwise be intractable. This tutorial session provides a high-level overview of phase-based reduction methods originally developed by Winfree and Kuramoto that have been fruitfully applied to understand emergent behaviors (e.g., synchronization, entrainment, chimeras) in populations of weakly coupled oscillators, for instance, with applications to neurological rhythms and circadian oscillations. We will also discuss more recent extensions to this theory that simultaneously consider amplitude coordinates which ultimately enable the careful study of strongly coupled oscillations in regimes beyond where the weak coupling assumptions are valid. As part of this tutorial session participants will have the opportunity to obtain hands-on experience with a recently developed Python toolbox that can be used to compute the necessary terms of the phase-amplitude reduced order equations for general systems of ordinary differential equations that display limit cycle oscillations. The tutorial will be run on Google Collab.

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MS29

Detecting Changes in Dispersion in COVID-19 Incidence Time Series Using a Negative Binomial Model

Metrics of variability are often overlooked and useful ways to understand epidemic dynamics. For instance, superspreading of SARS-CoV-2 can be elucidated by utilizing such metrics. Our method identifies shifts in population-level incidence dispersion, allowing a more complete and predictive understanding at both the individual and population level, and allowing practitioners to prepare surge capacity in certain months. Although classical theory predicts that there will be less dispersion when incidence is higher, we consider a more general negative binomial regression framework to account for processes that may also affect the spread of cases. We investigate changes in dispersion and find that there are increases in dispersion around holiday periods in many US counties, concurrent with incidence increases. In addition, highly overdispersed patterns occur more frequently later in time series, consistent with more heterogeneity in transmission, susceptibility, and reporting. Our method is robust to changes in incidence and to population size, allowing for quantification of dispersionindicative of superspreading dynamicswithout artifactual contributions from these features.

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MS29

Co-Infection in Pinnipeds: Musings on Biological Problems That Need Mathematical Solutions As Presented by a Biologist

As a disease ecologist, I am often confronted with problems that require mathematical solutions. California and Stellar Sea Lions are commonly infected with a urogenital carcinoma. We have found that male sea lions with this carcinoma have altered immune function - with elevated levels of an immunosuppressive cytokine (IL10) - which may make them important in the transmission of other infectious pathogens like leptospirosis. We are interested in understanding how altered susceptibility, in animals with cancer, may lead to super-spreading of other common pathogens and which types of pathogens are likely to be affected. We have data on cancer status, immune status, over 50 sea lions, but an immuno-epidemiological mathematical model would improve our ability to make conclusions. Pacific Walrus live in the arctic and are exposed to rapid changes in diet and habitat. We are interested in understanding how exposure to parasites and diseases may be affected by global climate change, particularly in whether parasites that are of risk to human health may be disproportionately affected. Recent work has found toxoplasma in walrus samples, and we have found an increase in a zoonotic tapeworm in walrus consuming higher trophic level prey. We are interested in using mathematical models to understand parasite and disease transmission in a changing climate in the arctic. For this we have data on approximately 35-40 walrus that would allow us to test predictions.

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MS29

Modeling Many Parasites and Pathogens in Desert Bighorn Sheep

Desert bighorn sheep live in fragmented interacting populations, which have been studied as networks built from genetic and movement data. My colleagues have recently used large-scale molecular techniques to identify many parasites and pathogens in sheep in these populations. In this talk, I will show how this data is being used to study how the network structure of the sheep populations impacts the dynamics of parasite and pathogen transmission and, in turn, the evolution of immunity within the sheep populations.

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MS29

High and Dry: Environmental Conditions Drive Opportunities of Disease Transmission in Desert Bighorn Sheep

Heterogeneity in host contact patterns, influenced by individual and group traits, can affect pathogen invasion and persistence. However, the role of climate and landscape in shaping animal contact ecology and disease dynamics remains unclear. We examine this by integrating long-term GPS and environmental data into network analyses and disease dynamic models, focusing on eight Desert Bighorn Sheep (DBS) populations in the Mojave Desert characterised by extreme environmental fluctuations. We investigate (i) whether environmental variation drives contact synchrony, (ii) the importance of individual traits versus population-level conditions in structuring contacts, and (iii) the consequences for disease outbreak size and persistence. Our analyses reveal that rainfall, temperature, and sex-reproductive season interactions significantly affect social contacts, with demographic variables showing varied effects across temporal scales. By scaling up and refining contact networks based on different infectious periods, we capture mating patterns and quantify the impact of spatiotemporal environmental and demographic factors on DBS contacts, offering insights into wildlife ecology and disease transmission.

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MS30

Pose Graph Optimization

In researching graph theory, the goal was to create code in Python and optimize a pose graph using the minimum cycle basis (MCB) and all pairs shortest path (APSP). Starting with all pairs shortest path, it was constructed using the lexicographical Dijkstra algorithm, ensuring a consistent APSP. The true shortest paths for any undirected graph were found using only positive weighted graphs (a parameter of Dijkstra's algorithm). With an accurate APSP checked with results from Networkx, the MCB was constructed by use of the Horton set and Gaussian Elimination. In doing so, MCB for any given graph (the biggest one tested had 808 nodes and 827 edges) was computed, with its results also checked by Networkx. Now, while there wasn't enough time to learn the techniques necessary to implement code to optimize a pose graph using the MCB, we learned about its process and its influence in robotics because of its ability to minimize the error between predicted and observed data.

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MS30

Comparative Analysis of Iterative Methods for Solving Separable Nonlinear Least Square Problems

In this talk, we will present a comparative analysis of the Gauss-Newton, alternating least squares, and variable projection methods for solving separable nonlinear least square problems. Furthermore, we will show these methods' accuracy and running time in the context of fitting nonlinear functions to both simulated and real data.

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MS30

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To Come

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MS30

Mathematical Modeling, Analysis and Simulation of Patient Journey in Drug Addiction

This work develops a mathematical model to study the dynamics of addiction as individuals go through their detox journey. Addiction is treated as an infectious disease in this work and is modeled via compartmental models described by differential equations that help to understand the non-linear dynamics of various sub-populations among the drug users. A detailed mathematical analysis along with the derivation of the basic reproduction number for the proposed model is also presented. We also introduce a Physics Informed Neural Network approach that helps to estimate the parameters in the model efficiently.

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MS30

Cost-Benefit Analysis of Yearly Mammograms: A Social Justice Approach to Individualized Medicine

”Breast cancer is the second most common cancer and the leading cause of death among women worldwide. To combat this, the United States Preventative Service Task Force (USPSTF) has suggested that women get biennial mammograms starting at age 40 and continue to do so until the age of 74. Despite this however, mortality rates, particularly in women of color, remain high and the taxing cost of the procedures makes continuous access to them difficult for lower income communities. Our research concluded that women of color, especially those with low income, are less likely to seek medical attention because they do not have insurance or have lower-quality health care. When they do get medical attention for mammograms, they are diagnosed with higher stages of breast cancer. We utilized machine learning algorithms to determine how often a woman should receive a mammogram based on risk factors such as race/ethnicity, age, body mass index, and breast density, among others. Next, we created a point system to determine each individual patient’s risk of getting breast cancer based on said risk factors and then used unsupervised clustering algorithms to place the patients in different categories based on their accumulated points. It is our hope that placing patients in proper protocols will help decrease their spending on mammographic procedures and reduce false positives.”

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MS31

Quantifying Fairness in Electoral Redistricting

An emergent trend of research in recent years is rooted in ‘quantitative justice’– that is the mathematical, computational, and statistical analysis of problems that are often sourced in the real world where the topic under investigation or the rationale for the analysis are rooted in addressing societal inequity. In this context, mathematical tools are used to quantify notions of “fairness” in a given domain, and the analysis often has the potential to impact both the mathematical research community as well as society at large. A particular societal problem that has received a significant amount of interest in recent years is studying fairness in electoral redistricting. In this talk, we will emphasize how tools from applied algebraic topology and metric geometry can be utilized in electoral redistricting, and more generally how techniques related to shape comparison and object matching can be applied to problems in real world contexts.

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MS31

Quantifying Hierarchy and Documenting Inequity in PhD-Granting Mathematical Sciences Departments in the United States

In this paper we provide an example of the application of quantitative techniques, tools, and topics from mathematics and data science to analyze the mathematics community itself in order to quantify inequity and document elitism. This work is a contribution to the new and growing field recently termed “mathematics of Mathematics,’ or “MetaMath.’ Our goal is to rebut, rebuke, and refute the idea that the mathematical sciences in the United States is a meritocracy by using data science and quantitative analysis. Using research and data about PhD-granting institutions in the United States, we quantify, document, and highlight inequities in departments at U.S. institutions of higher education that produce PhDs in the mathematical sciences. Specifically, we determine that a small fraction of mathematical sciences departments receive a large majority of federal funding awarded to support mathematics in the United States and that women are dramatically underrepresented in these departments. Additionally, we quantify the extent to which women are underrepresented in almost all mathematical sciences PhD-granting institutions in the United States.

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MS31

Data Science Tools for Community-Driven Police Accountability

Recent years have highlighted the urgent need for transparency and accountability within police departments across the United States. Though data is legally mandated to be publicly accessible, in practice, there are persistent barriers in obtaining and analyzing such data. Consequently, the public are generally unable to take data-informed action toward social justice. This talk will detail open-source tools for collecting, organizing, and understanding police data. Tools such as optical character recognition, language and topic modeling, and spatial inference are employed, with future opportunities to address challenges of anonymized and missing data. The mission of this ongoing work is to work alongside communities to increase easy access and understanding of public data by addressing these technological and analytical challenges.

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MS31

Dynamics of Female Gender Representation in Academic Mathematics

Women remain underrepresented in academic mathematics. In this project, we study the dynamics of female gender representation among the faculty of doctorate-granting mathematics departments. We abstract academic genealogies as a multitype branching process in which advisors generate graduated PhD students, and estimate the parameters of this process by fitting a mechanistic model of academic careers to a data set derived from the Mathematics Genealogy Project. Upon fitting our model, we find that male academics enjoy an advantage in production of new PhD students relative to their female colleagues, and that this influences the next generation due to homophily effects. Our formalism suggests that, without substantial structural shifts, gender representation in most subfields of mathematics will increase slightly before leveling out well short of parity. We close with some reflections on our models limitations and what it suggests about interventions to the representation of women in academic mathematics. Joint work with Phil Chodrow, Harlin Lee, Anna Haensch, Juan G. Restrepo, and Mason A. Porter.

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MS32

Stochastic Modeling for Periodic Time Series Data

Stochastic modeling for epidemiological time series involves the use of various statistical techniques to analyze and interpret data collected over time in the field of epidemiology. These time series data typically include information about the occurrence of diseases or health-related events over a specific period. Seasonal variation is present in many environmental and biological systems from growth and maturation of plant and animal populations to infectious disease outbreaks. Periodic mean-reverting stochastic differential equations (SDEs) realistically capture seasonal variability. We discuss some periodic mean-reverting SDE models and fit them to seasonally varying influenza and temperature data with $dX(t) = r(\beta(t) - X(t))\,dt + d\beta(t) + \sigma X^p(t)\,dW(t)$, $r, \sigma > 0$ for $p = 0, 1/2, 1$ with periodic mean $\beta(t)$. It is shown that the SDE with $p = 0$ is related to the well-known Ornstein-Uhlenbeck diffusion process with an asymptotic normal distribution. The diffusion terms in the SDE model with $p = 1/2$ and $p = 1$ are related to the Cox-Ingersoll-Ross (CIR) process and to geometric Brownian motion (GBM), respectively. It is shown that the higher-order moments of the CIR and GBM processes are periodic, provided they exist. A problem involving missing influenza data is handled with a modified MissForest algorithm. Model parameters in the SDE models are fitted to data in two steps. First, the mean of the data is fit to a proposed periodic function $\beta(t)$, and parameters are estimated with a least squares method. Second, the parameters r and σ are fit to the SDE model with a maximum likelihood method. In conclusion, leveraging advanced statistical modeling techniques such as stochastic time series models and machine learning algorithms can provide valuable insights into epidemiological time series data, enabling more accurate predictions and a better understanding of environmentally driven disease dynamics.

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MS32

Simplex Slicing: An Asymptotically-Sharp Lower Bound

We show that for the regular n-simplex, the 1-codimensional central slice that's parallel to a facet will achieve the minimum area (up to a 1-o(1) factor) among all 1-codimensional central slices, thus improving the previous best known lower bound (Brzezinski 2013) by a factor of $\frac{2\sqrt{3}}{e} \approx 1.27$. In addition to the standard technique of interpreting geometric problems as problems about probability distributions and standard Fourier-analytic techniques, we rely on a new idea, mainly *changing the contour of integration* of a meromorphic function.

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MS32

Polyglot Entrainment for Higher Dimensional Neuronal Dynamic Models

The entrainment of biological oscillators is a classic problem in the field of dynamical systems and synchronization. We explore a novel type of entrainment mechanism referred to as polyglot entrainment (multiple disconnected 1:1 regions) for higher dimensional nonlinear systems. Polyglot entrainment has been recently explored only in two-dimensional slow-fast models in the vicinity of Hopf bifurcations. Heading towards generality, in this study, we investigate the phenomenon of polyglot entrainment in higher-dimensional conductance-based models including the four-dimensional Hodgkin-Huxley model and its reduced three-dimensional version. We utilize dynamical systems tools to uncover the mechanism of entrainment and geometric structure of the null surfaces to explore the conditions for the existence of polyglot entrainment in these models. In light of our findings, in the vicinity of HB, when an unforced system acts as a damped oscillator and the fixed point is located near a cubic-like manifold, polyglot entrainment is observed.

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MS33

Mathematical Insights into the Quantification of Endosomal Escape

The endocytosis process is the main uptake mechanism to transport peptides, proteins, and other biological agents into the cell. When therapeutic drugs enter the cell, they are encapsulated in endosomes. During the intracellular delivery process, these drugs must escape the endosome to reach the cytosol and their desired cancer-infested target. While many membrane-permeating instruments and processes have been developed to ensure that drugs can enter the cell, the efficiency and efficacy of endosomal escape has not been well-studied. We developed a mathematical model to quantify the endosomal escape of siRNA over a series of drug delivery experiments. Fusogenic peptides were developed that electrostatically bind with siRNAs to aid with cell uptake and promote endosomal escape. Peptides are known to enhance cellular uptake of biological agents but not endosomal escape. Our work is very important in that it specifically quantifies endosomal escape and proves this to be true. With a combination of stochastic simulation models, dynamical systems, parameter estimation, and statistical validation methods, our novel quantification approach answers many questions about measuring endosomal escape. Additionally, our work can be used to develop agents that specifically increase endosomal escape in drug delivery in cancer therapy.

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MS33

Rigidity and Resilience in Network-like Biomaterials

We examine rigidity and resilience in network-like biomaterials, addressing key questions in the rational design of biomimetic soft materials. I will begin by discussing the potential structural mechanisms responsible for the robust and resilient mechanical properties in cytoskeletal and extracellular matrix networks. Using rigidity percolation theory, we investigate the impact of their composite and heterogeneous structures on cell and tissue mechanics, with a focus on tunability and resistance to damage. Following this, I will discuss our work in developing colloidal networks using functionalized clock proteinskey components in biological timekeepingto engineer materials with self-assembly dynamics and material properties that can be regulated on a timed schedule. By harnessing protein-based reaction networks, we aim to infuse synthetic materials with robust life-like characteristics. Our findings demonstrate how understanding the emergent structure-function relationships in biological and bio-hybrid network systems can guide the creation of biomimetic materials.

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MS33

Multi-Timescale Plasticity in Working Memory

Our brains retain relevant information about our environment on short timescales of a few seconds through a process termed working memory. However, identifying what features of our environment are important depends on our beliefs about the environmental statistics. Our beliefs are updated based on experiences over long timescales (minutes or hours) and by our most recent experiences, creating serial biases. Here, we develop a neural field model of working memory that incorporates both long-term experience and recent observations and compare a low dimensional approximation to human behavior. Our neural network model describes the non-linear dynamics of neural activity, in which a stimulus activates neurons with preferences for those stimulus features. Connectivity between active neurons is strengthened and decays with time since a preferred stimulus, representing updating beliefs about the environmental statistics. The plasticity rules that govern connectivity changes occur on both short and long timescales independently. Our neural network can be approximated by a low-dimensional model that describes neural activity as a particle moving through an energy landscape. The shape of the energy landscape, which mimics the connectivity of the network model, is updated based on experience with multi-timescale decay terms. This reduced model is then used to fit the strength and decay rates of long- and short-term biases in human behavior.

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MS33

A Deep Learning Approach for the Electrical Impedance Tomography Problem

Electrical Impedance Tomography (EIT) can map electrical property distributions within the body using a surface electrode array. EIT systems using a circumferential array applied to the abdomen can be used to monitor acute intra-abdominal hemorrhages in trauma patients. A half array ('hemiarray') applied only to the anterior abdomen may be more practical. However, severe reconstruction artifacts result in posterior regions using standard EIT reconstruction methods. In this talk, we introduce novel machine learning-based approaches for standard full and hemiarray EIT reconstructions, demonstrating superior reconstruction characteristics compared to conventional methods.

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MS34

Oblique Projection for Solving High-Dimensional Partial Differential Equations on Low-Rank Matrix and Tensor Manifolds

Time-dependent basis reduced-order models (TDB ROMs) have successfully been used for approximating the solution to nonlinear stochastic partial differential equations (PDEs). For many practical problems of interest, discretizing these PDEs results in massive matrix differential equations (MDEs) that are too expensive to solve using conventional methods. While TDB ROMs have the potential to significantly reduce this computational burden, they still suffer from the following challenges: (i) inefficient for general nonlinearities, (ii) intrusive implementation, (iii) ill-conditioned in the presence of small singular values and (iv) error accumulation due to fixed rank. To this end, we present a scalable method for solving TDB ROMs that is computationally efficient, minimally intrusive, robust in the presence of small singular values, rank-adaptive and highly parallelizable. These favorable properties are achieved via oblique projections that require evaluating the MDE at a small number of rows and columns. The columns and rows are selected using the discrete empirical interpolation method (DEIM), which yields near-optimal matrix low-rank approximations. We 2 show that the proposed algorithm is equivalent to a CUR matrix decomposition. Numerical results demonstrate the accuracy, efficiency, and robustness of the new method for a diverse set of problems.

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MS34

Sequential-in-Time Training of Nonlinear Parametrizations for Model Reduction

It is well understood that the performance of linear model reduction methods is limited for the large class transport-dominated problems. We discuss methods based on nonlinear parametrizations to overcome the limitations of linear methods in terms of error decay. One question that immediately arises is how the dynamics can be described after the non-linear parametrization has been applied: Even if the governing equations are linear in the solution fields, the dynamics of the non-linear parameters are not. We will build on the Dirac-Frenkel variational principle to formulate the dynamics in the non-linear parametrization and demonstrate the approach on numerical experiments.

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MS34

Space-Time Model Reduction Using Spod Modes

Most reduced-order modeling (ROM) strategies operate by first finding a compressed representation of the state of the full-order system and then evolving this representation according to ODEs derived from either the full-order model or from data. Examples of this approach include all Petrov-Galerkin methods and ROMs based on nonlinear encodings, such as autoencoder manifolds and spectral submanifolds. In this talk, we explore a different paradigm: we find a compressed representation of the entire space-time trajectory of the system, then solve a set of algebraic equations for the coefficients that encode the trajectory in the space-time representation. The promise of this approach is that many fewer degrees of freedom are required to represent a trajectory to some accuracy when the reduction is done in space and time in tandem as compared to when it is done only in space. We use spectral POD (SPOD) modes as the space-time encoding. These offer a substantial compression of space-time trajectories relative to space-only reductions and possess desirable properties such as analytic time dependence and space-time separability. We derive a method to solve for the SPOD coefficients and demonstrate the performance on two forced linear problems. At the same CPU time, the SPOD methods error is two orders of magnitude lower than the POD-Galerkin and balanced truncation errors.

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MS34

Data-driven Modeling of Transitions in Fluid Flows Using Spectral Submanifolds

We present a rigorous method of model-order reduction for a class of canonical shear flows, particularly plane Couette flow and pipe flow. In these flows, an extended turbulent state can coexist with the stable laminar. In this case, the boundary between the coexisting basins of attraction, often called the edge of chaos, is the stable manifold of an edge state. We show that a low-dimensional submanifold of the edge of chaos can be constructed from velocity data using the recently developed theory of spectral submanifolds (SSMs). These manifolds are the unique smoothest nonlinear continuations of nonresonant spectral subspaces of the linearized system at stationary states. We use very low dimensional SSM-based reduced-order models to predict transitions to turbulence or laminarization for velocity fields near the edge of chaos.

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MS35

Data Assimilation in Medical Models and Digital Twins

One of the growing areas of interest in the context of biological and medical models is the question of how to personalize a model to a target organism or patient in order to improve model predictions. This question is inherently tied to data assimilation (DA): the process of calculating the "optimal' combination of observational and model data which determines the next model state while taking into account the errors present in both sources. Most existing DA methods have evolved from the context of numerical weather prediction and are tailored toward ordinary or partial differential equations models. However, little work has been done to extend the application of this methodology into the context of more complex models, including stochastic and multiscale models. In our work, we consider how to extend a well-known DA method, the ensemble Kalman filter, so that it may be applied to three stochastic models of increasing complexity. We explore the benefits and limitations of this method in doing so and discuss the open questions that still exist within this area of research.

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MS35

Stochastic Modeling of Asian Long-Horned Beetle Invasion

The Asian long-horned beetle (*Anoplophora glabripennis*) in an invasive wood-boring pest in the eastern United States. It destructively feeds on maples and other hardwood trees, often killing its host and disrupting native ecologies. A multi-institutional effort has been made to mark the presence and distribution of the beetle in the US states. Currently, metapopulation models are used to calculate infestation rates based on tree species, type of land usage, and patch size. Utilizing raw field data, we have constructed several models to evaluate factors influencing beetle spatial distribution, identify high-risk areas, and anticipate its spread. Spatial stochastic models were used to understand the dynamics between regions based on infestation level, host availability, and proximity to other infestations, as well as predict long-term spread patterns of the beetle. We also used patch models to understand infestation spread based on the presence/absence of an infested neighbor or region.

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MS35

Extinction Probability in Population Models Before Reaching a Quasi-Stationary State

A fundamental question in population ecology concerns the likelihood of persistence of two or more interacting species and, conversely, the risk of extinction of one or more of these species. The importance of quantifying this extinction risk can be observed in models of cancer immunotherapy, where treatment success is described by an extinction event. While it is well understood that the mean-field description fails to capture species extinction, stochastic simulation reveals trajectories resulting in extinction events before entering a metastable state. Our analysis shows that these trajectories occur with high probability and, unlike previous studies, require only small fluctuations from the mean-field trajectory. We derive a modified boundary condition to the Fokker-Planck approximation describing the probability of extinction prior to entering the metastable state. Our analysis of this model allows us to quantify extinction risk, and reveals the important role of initial population size.

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MS35

Modeling the Dynamics of Legionnaires' Disease

Legionnaires' disease (LD) is an atypical pneumonia caused by the inhalation of the bacteria of the genus Legionella suspended in aerosolized water. In 2018, there were nearly 10,000 LD cases reported by health departments in the United States. True incidence should be higher as LD is likely underdiagnosed. We develop and analyze an ODE-based model to examine the factors that may have contributed to the increase in LD outbreaks.

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MS36

High Order Unconditionally Strong Stability Preserving (SSP) Implicit Two-derivative RungeKutta Schemes and their Extensions

We construct a novel family of fully-implicit, high-order, unconditionally strong stability-preserving (SSP) second-derivative RungeKutta schemes designed for equations containing stiff terms. This approach has been validated to possess the asymptotic-preserving property, which preserves the asymptotic limit of the equation, and the scheme automatically reduces to a high order time discretization for the limiting system. Additionally, the inherent contractivity of the SSP method ensures the uniqueness of solutions in the stage equations of the implicit Runge-Kutta method. David I. Ketcheson has demonstrated the existence of a second-order unconditionally SSP RungeKutta method that incorporates downwind conditions. Our research, however, reveals that employing this method directly, even when integrating the backward derivative condition, fails to work. Instead, by leveraging this idea with the downwind conditions and integrating it with additive RungeKutta methods, we have developed a new family of second-order SSP methods that eliminate time-step limitations for various problems, including the Broadwell model, the radiative transport equation, and the Bhatnagar-Gross-Krook (BGK) kinetic equation. In this talk, we provide a summary of the key theorems and present the corresponding numerical results associated with the models. This is a joint work with Andrew Christlieb, Sigal Gottlieb and Zachary J. Grant.

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MS36

Energy-Preserving Explicit Runge-Kutta Methods

Using a recent characterization of energy-preserving B-series, we derive the explicit conditions on the coefficients of a Runge-Kutta method that ensure energy preservation up to a given order in the step size. Such pseudo-energy-preserving methods can be expected to behave like energy-preserving methods over moderate time intervals. We provide examples of pseudo-energy-preserving methods up to order six, and apply them to Hamiltonian ODE and PDE systems. We find that these methods exhibit significantly smaller errors, relative to other Runge-Kutta methods of the same order, for long-time simulations.

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MS36

Invariant Conservation Law-Preserving Wave Equation Discretizations with Applications to Fiber-Reinforced Materials

Symmetry- and conservation law-preserving finite difference discretizations are obtained for linear and nonlinear one-dimensional wave equations on five- and nine-point stencils, using the theory of Lie point symmetries of difference equations, and the discrete direct multiplier method of conservation law construction. In particular, for the linear wave equation, an explicit five-point scheme is presented that preserves the discrete analogs of its basic geometric point symmetries, and six of the corresponding conservation laws. For a class of nonlinear wave equations arising in hyperelasticity, a nine-point implicit scheme is constructed, preserving four point symmetries and three local conservation laws. Other discretization of the nonlinear wave equations preserving different subsets of conservation laws are discussed.

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MS37

Mac's Career and the Mathematical Modeling & Analysis Group at Lanl

Mac Hyman obtained his PhD in 1979 at the Courant Institute, NYU, and subsequently joined Los Alamos National Lab as a member of the Mathematical Modeling and Analysis group in Theoretical Division. His PhD research with Peter Lax was on novel numerical methods and computer software for solving a wide range of PDEs. We will explore his career and impact at the center of computational physics and supercomputing in the largest US national laboratory. As co-founder of the Center for Nonlinear Studies (CNLS), he became closely involved in the discovery of new solitons and their applications, as well as the subtle numerical methods required for describing a wide range of other nonlinear phenomena. His early work on mathematical models to study the AIDS epidemic also started a lifelong fascination with mathematical epidemiology.

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MS38

Computational Harmonic Analysis Research at Michigan - Dearborn (charm'd)

To come

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MS39

Recent Advances in Weak Form-Based Data-Driven Modeling

Data-driven discovery of governing equations in the weak form has proven to be highly computationally efficient as well as robust in the presence of substantial measurement noise. In this talk, we will provide a brief overview of the developed numeical methods including batch and online equation learning and parameter estimation. Our main focus of the talk will cover recent results in applying the weak form to discover accurate reduced order models, learned from noisy data. Time permitting, we will also discuss recent results which provide a theoretical justification for the robustness of the method in comparison to strong form- and smoothing-based methods.

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MS39

Discovering Sparse Dynamics of Nonlinear Oscillatory and Chaotic Systems from Noisy Partial Observations Using Sensitivity Analysis.

Complex multi-component physical, biological, and chemical systems are often only partially observable despite rapid advancements in experimental measurement techniques. A key challenge is, therefore, discovering predictive nonlinear dynamical models and their parameters directly from incomplete, noisy experimental observations. We develop an automated differential equation inference framework to find sparse, predictive, nonlinear models from a few noisy partial observations of a system's state. By combining differential equation sensitivity analysis and ranked-choice model selection with sparse library-based learning methods, we can account for model symmetries introduced by the unobserved variables and incorporate robustness to noise. After validating our method using the FitzHigh-Nagumo oscillator and the chaotic Lorenz attractor, we demonstrate the framework's broad applicability to various experimental datasets from squid neuron activity, Belousov-Zhabotinsky reactions, and bacterial swarming experiments.

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MS39

Learning Differential Equations from Single Trajectories Based on Feature Selection with Explicit Sparsity Control

Learning differential equations (ODEs or PDEs) from single trajectory data is a rising research field with important applications in various fields. It can automatically find the differential equations satisfied by the observational data, and the identified models can be used to validate theory or to discover new dynamics. Different frameworks have been proposed in the literature, e.g., SINDy , weak-SINDy, weak-IDENT, and many network-based. In this talk, we will focus on a stream of works based on optimizations with l0-sparsity restriction. We shall demonstrate the benefit of the framework that allows explicit control of the complexity of the candidate models, thus avoiding redundancy in the validation process. Under this paradigm, we will talk about Robust-IDENT, a robust method for identifying constant coefficient PDEs based on successively smooth differentiation and a multi-shooting error accumulation scheme. We will also discuss GP-IDENT, an effective method for finding PDEs with varying coefficients. Various examples will be presented.

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MS39

Sparse-Optimization for Discovering Differential Algebraic Systems from Data

Differential Algebraic Systems (DAEs) form a broad category of differential equations wherein ordinary differential equations (ODEs) are combined with algebraic equations, resulting in a highly coupled system. DAEs typically arise due to the separation of time scales, conservation laws, or algebraic constraints in the dynamical systems. Sparse optimization represents a recently expanding set of techniques used to discover the model of a dynamical system from a model library and data. Despite the extensive study of numerical solvers for DAEs in the literature and their wide range of applications, model discovery algorithms for such systems remain a less explored area of research. Previous approaches focused on using quasi-steady state approximations to reduce the system of DAEs into an implicit system of ODEs, and then trying to discover the reduced system. However, the reduction often introduces numerical instability, and existing algorithms based on Sparse Inference of Nonlinear Dynamics (SINDy) have highly correlated library terms due to algebraic relationships between candidate features in the library. We propose a novel method called Sparse Optimization for Differential Algebraic systems (SODAs), that can identify the full system of DAEs without any reduction. Additionally, we demonstrate that this method can handle higher levels of noise in the data and work with simpler candidate library functions compared to the existing methods to discover implicit ODE systems.

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MS42

Topology Optimization of Spin-Photon Interfaces Using Computationally Optimized Compact Models

We present a topology-optimization framework for a dipole model simulation of a spin-photon interface to a color center in a diamond microdisk. We propose a gradient-based optimization method that relies on the gradient of the position of the scattering holes in a silicone-nitride grating layer. The proposed topology includes constraints which allows for a manufacturable design while maintaining a high collection efficiency into the ZPL. The proposed topology demonstrates high quantum efficiencies into low numerical apertures. The use of an optimized digital twin potentially allows for the integration into existing quantum network simulations.

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MS42

Machine Learning Applications on Gamma Emission Tomography for the Verification of Spent Nuclear Fuel

Radioactive waste from nuclear-energy facilities poses challenges for the world both for both safe, long-term disposal of material and ensuring nonproliferation of weapons of mass destruction. Spent nuclear fuel assemblies contain plutonium, an element that can be used to make nuclear weapons, and a mission of the International Atomic Energy Agency (IAEA) is safeguarding against its illicit use. Confirming that the nuclear material contained in spent fuel is not being diverted for non-peaceful activities and determining whether countries are abiding by their nonproliferation responsibilities is an essential component of providing assurance to the international community. Verifying the declaration of the geometry of a spent-fuel assembly can be accomplished by determining the distribution of radioactive material. Ideally, one would measure the distribution of plutonium, but the distribution of any fission product can be used for this metric of integrity. The IAEA uses the Passive Gamma Emission Tomography (PGET) device to perform a measurement and reconstruction of cross-sectional activity from gamma emitters in spent-fuel assemblies. Reconstructed images are analyzed to determine the number of pins present in the assembly. Unfortunately, image artifacts and variations in pin-to-pin burnup complicate unambiguous counting of pins. Figures of merit have been developed where individual pin intensities of the assemblies are compared to a neighborhood of average pin intensities to determine missing rods based on a statistical deviation. Due to the complex relationship in the pin-pin burnups, this method was unable to effectively identify missing pins. Machine learning can recognize complex patterns in radiographic images through large amounts of data and automated optimization methods. This study describes a machine-learning approach for discriminating missing pins for verification of nuclear material.

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MS42

Intrinsic Projection (ip) of Irk Methods for Differential Algebraic Equations

We present the new technique of Intrinsic Projection (IP) for Implicit Runge-Kutta (IRK) Methods applied to differential-algebraic equations (DAEs). IP does not require the accurate evaluation of any additional Jacobian like for standard Projected Implicit Runge-Kutta Methods and is therefore simpler to implement. (IP) for IRK methods is analyzed for index 2 DAEs, in particular, we give results about existence and uniqueness, and some error estimates. For index 2 DAEs IP for IRK methods is shown to lead to the same order of error estimates as standard Projected Implicit Runge-Kutta Methods, but at a lower computational cost. Some preliminary results for index 3 DAEs will also be given.

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MS43

An Efficient Flux-variable Approximation Scheme for Darcy's Flow

We present an efficient numerical method to approximate the flux variable for the Darcy flow model. An important feature of our new method is that the approximate solution for the flux variable is obtained without approximating the pressure at all. To accomplish this, we introduce a user-defined parameter $\delta > 0$, which is typically chosen to be small so that it minimizes the negative effect resulting from the absence of the pressure, such as inaccuracy in both the flux approximation and the mass conservation. The resulting algebraic system is of significantly smaller degrees of freedom, compared to the one from the mixed finite element methods or least-squares methods. We also interpret the proposed method as a single step iterate of the augmented Lagrangian Uzawa applied to solve the mixed finite element in a special setting. Lastly, the pressure recovery from the flux variable is discussed and an optimal–order error estimate for the method is obtained. Number of examples are provided to verify the proposed theory and algorithm, some of which are from more realistic models such as SPE10.

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MS43

A C^0 Finite Element Method for the Triharmonic Problem

Consider the 6th-order triharmonic problem in a polygonal domain with the simply supported boundary condition. The finite element approximation to such high-order problems often involves sophisticated construction of the bilinear form and of the finite element space. We propose a new C^0 finite element algorithm to solve these problems. Our methods are intuitive, easy to implement, and applicable to both convex and nonconvex domains. We give finite element error analysis and report numerical results to validate the algorithms.

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MS43

Pressure Robust Schemes for Incompressible Flow

The incompressible fluid model is widely used in various fields in engineering and science and their numerical solutions are of prominent importance in understanding complex, natural, engineered, and societal systems. There has been considerable interest in mathematical modeling and algorithm development. One of the critical challenges is the development of the pressure robust scheme and achieve the desired mass conservation with low cost. Our effort aims at designing the low-cost divergence preserving finite element method and in turn, achieve viscosity independent velocity error estimates. Translating this result to the incompressible fluid equations, our algorithm is robust with varying viscosity permeability values and large pressure gradients. The crucial component is to integrate the h(div) velocity reconstruction operator to the discretization in the proper form. In this talk, we shall present our algorithm development, and then demonstrate the stability and convergence analysis theoretically and numerically. The profiles of benchmark tests indicate that our algorithm outperforms other non-divergence preserving numerical schemes.

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MS43

H^1-Conforming FEM on Curvilinear Meshes: Theory and Practical Realization

Several classes of finite element methods can be naturally posed on non-standard meshes. Among the H^1-conforming methods, the most well-known is the Virtual Element Method (VEM). Boundary element based finite element methods (BEM-FEM), developed around the same time, are quite similar to VEM in the way that the local finite element spaces are defined–in terms of Poisson problems with polynomial source and boundary data. The most significant difference between BEM-FEM and VEM is how they discretize the underlying PDE, with BEM-FEM working more directly with implicitly-defined bases, and VEM using projections and stabilization schemes to work with polynomials. Our work in this direction may be considered an evolution of the BEM-FEM approach, with the BEM aspect replaced by a Nyström solver. Such modifications have made it more natural to allow for mesh cells that may have curved edges and may not even be simply connected. A challenge for such methods is to develop appropriate quadratures for computing the types of integrals needed to form associated element stiffness matrices. Most approaches resort to ”brute force” techniques that involve subdividing the given (polyhedral) mesh cell in simpler cells and applying known quadratures at that level. We take a different approach, in which the relevant volumetric integrals are reduced to integrals along the boundary, and all computations that are needed to compute these integrals take place on the boundary of the mesh cell.

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MS44

Anomaly Detection Using Wintap (a Flexible, Ex-

tensible Endpoint Data Sensor for Research and Cyber Defense) and PySparkPlug (a Python Package for Distributed Heterogeneous Density Estimation)

Sensors can collect a wide array of metrics on Windows process behavior. Monitoring these metrics can provide valuable information about when a process misbehaves, either from an operation or a security standpoint. We introduce the Wintap endpoint sensor–an agent that records, summarizes, and aggregates information about Windows processes from a variety of sources and presents it in an easily accessible format. We also demonstrate how Wintap-reported values can be used to effectively characterize process behavior and alert analysts to events of interest. We model these values using PySparkPlug, a density estimation tool that can be used to model complex and heterogeneous distributions. We use this tool to identify anomalies in features such as image loads, file activity, and network activity. We then demonstrate how these anomalies can be aggregated to allow us to identify benignware that has been introduced into a sample dataset.

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MS44

Introduction to Math and AI for Cybersecurity

The speed, scale, complexity, and ubiquity of cyber-attacks has never been more evident and their far-reaching impacts on society demonstrate the critical need for robust security solutions to reduce the success of cyber-attackers when (not if) they compromise critical networks. The rapid evolution of malicious cyber actors activities makes todays static and rules-based cyber-defense capabilities, which require a priori knowledge of precise attacker tactics, unsustainable. As such, artificial intelligence (AI) is rapidly becoming an essential component of modern cybersecurity systems and mathematics, as the bedrock of AI, plays a critical role in ensuring the resiliency of these security solutions. The evidence of a cyber-attack lies in telemetry captured by sensors on the network and requires transformation into certain mathematical objects such as arrays, vectors, graphs, and hypergraphs before applying a rigorous mathematical theory (to include AI) and deriving critical insights for the defense of cyber systems. For example, there is a growing body of work applying combinatorial and topological techniques to these transformations of cyber data, demonstrating promise as part of a battery of techniques. This talk will provide the necessary background to help mathematicians become more familiar with the cyber domain, while using language and concepts familiar to a general mathematical audience. Well also preview concepts that will be covered in subsequent talks.

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MS44

Mathematics to Secure Elections: Cyber-Focused Risk Assessments for Socio-Technical Critical Infrastructure

Mathematics tools and techniques can be broadly applied to election systems, which are socio-technical U.S. critical infrastructure. In this presentation, we discuss attack trees, a cybersecurity framework that enables the systematic exploration of potential cyber, physical, and insider threats to electoral systems. By leveraging principles of operations research and probability theory, we assess vulnerabilities and propose resilient defenses against actors seeking to compromise democratic processes. We also explore other examples of applied mathematics in election systems, including information theory to examine potential weaknesses in poll worker security behaviors and identify poll worker security practices to improve to ensure election integrity. By examining diverse mathematical disciplines, this presentation aims to bridge the gap between mathematical theory and applications to the broader area of U.S critical infrastructure, with the goal of stemming a discussion regarding potential new research areas and applications.

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MS44

Deep Reinforcement Learning for Adversarial Network Packet Generation

Recent advancements in artificial intelligence (AI) and machine learning (ML) algorithms, coupled with the availability of faster computing infrastructure, have enhanced the security posture of cybersecurity operations centers (defenders) through the development of ML-aided network intrusion detection systems (NIDS). Concurrently, the abilities of adversaries to evade security have also increased with the support of AI/ML models. Therefore, defenders need to proactively prepare for evasion attacks that exploit the detection mechanisms of NIDS. In this talk, we introduce a novel deep reinforcement learning (DRL) framework for conducting red team evaluations of the defender's NIDS. This adversarial DRL framework is trained to generate functional malicious network packets. By systematically perturbing raw malicious packets, our framework disguises them as benign while retaining functionality. Experiments with publicly available data showcase the superior performance of our approach, achieving an average adversarial success rate of 66.4% across various ML models and attack types. Our investigation reveals that over 45% of successful adversarial samples were out-of-distribution packets, evading classifiers' decision boundaries. Insights from this study can aid defenders in improving their NIDS against evolving adversarial attacks.

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MS45

Deep Learning-Based Prediction of Electrical Ar-

rhythmia Circuits from Cardiac Motion

The heart's contraction is driven by electrical excitation propagating through the muscle. Identifying the electrical triggers or drivers of heart rhythm disorders remains a key goal in cardiac electrophysiology. In our previous work we demonstrated in simulations the feasibility of predicting 3D electrical wave dynamics from ventricular deformation mechanics using deep learning. However, validating this approach experimentally presents significant challenges. In this talk, I will address these challenges and present our latest findings on implementing a deep learning-based approach for the prediction of electrical activity from the heart's motion experimentally. We have developed a novel electro-mechanical imaging system, including a 12-camera panoramic optical mapping system, capable of capturing synchronized electrical and mechanical dynamics of beating hearts. With this system we generate an ex vivo training dataset consisting of corresponding electrical and mechanical data. I will discuss the dataset generation process, the development of our deep learning model, its accuracy in predicting electrical dynamics, and future directions aiming to improve diagnosis and treatment options for heart rhythm disorders.

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MS45

Atrial Fibrillation Initiation and Organization in a Mechanistic Model of Atrial Remodeling and Calcium Homeostatic Regulation

Atrial fibrillation (AF) is the most common cardiac arrhythmia characterized by chaotic electrical activity that inhibits normal atrial contraction. Rapid activation of cardiac cells elevates intracellular calcium (Ca_i), which drives electrical remodeling of ion channels. These changes ultimately lead to a decrease in Ca_i, suggesting that electrical remodeling is a homeostatic feedback process. While this adaptation succeeds in maintaining Ca_i within a physiological range, the associated remodeling leads to a significant reduction in action potential duration (APD) and refractory period, and thus to an increased risk of arrhythmia. Here, we develop a model that couples ion channel feedback expression to the Courtemanche model of atrial electrophysiology describing ionic current conductances dynamics regulated by feedback system with a set Ca_i as its target. The model provides a mechanistic explanation for AF initiation and progression. We show that at fast pacing rates, or in the presence of spiral waves, feedback drives remodeling, maintaining calcium homeostasis. Simulations predict remodeling in atrial tissue over long periods of time, illustrating spiral wave stabilization, maintenance and breakup, consistent with the time progression of AF. Using a minimal description of calcium homeostatic mechanisms in atrial tissue, we are able for the first time to track the long term progression of pro-arrhythmic AF remodeling.

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MS45

Enhanced Ca2+-Driven Arrhythmias in Female Patients with Atrial Fibrillation: Insights from Computational Modeling

Accumulating evidence demonstrates substantial sex-related differences in atrial fibrillation (AF), which is the most common arrhythmia, with female patients faring worse with the condition. In this study, we aim to gain a mechanistic understanding of the Ca2+-handling disturbances and Ca2+-driven arrhythmogenic events in males vs. females and establish their responses to Ca2+-targeted interventions. By integrating known sex-differential components into our computational spatiotemporal atrial cardiomyocyte model, we found that female vs male atrial cardiomyocytes in AF exhibit greater propensity to developing arrhythmia-promoting spontaneous Ca2+ release events and elevated beat-to-beat variability in action potential-elicited Ca2+ transients. Computational analyses provided novel mechanistic insights into these sex differences. Furthermore, simulations of tentative Ca2+-targeted interventions identified potential treatment strategies that attenuated Ca2+-driven arrhythmogenic events in female atria (e.g., tubule restoration, and inhibition of ryanodine receptor and sarcoplasmic/endoplasmic reticulum Ca2+ ATPase), which reveal additive efficacy when applied in combination. Our study uncovers and validate sex-specific AF mechanisms and establishes that AF treatment may benefit from sex-dependent strategies informed by sex-specific mechanisms.

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MS45

Bistability of Early Afterdepolarizations Promotes Cardiac Arrhythmias

Early afterdepolarizations (EADs) are oscillations of the action potential (AP) plateau which are known to induce cardiac arrhythmias. At the single cell levels these oscillations are highly irregular and vary from beat-to-beat. This is because voltage repolarization is highly sensitive to stochastic processes at the subcellular level such as calcium cycling. Because of this randomness it is not understood how EADs behave in cardiac tissue composed of millions of cells. In this study we show that electrical coupling forces EADs to exhibit bistability in cardiac tissue. We show that once this bistability transition occurs paced cardiac tissue becomes unstable to electrical wave break and reentry. These results suggest that bistability of EADs in cardiac tissue promotes cardiac arrhythmias.

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MS47

Utilizing Mathematical Modeling and Computation to Gain Insight into Epidemics

Studying epidemics with mathematics gives insight to various questions such as vaccination analysis with COVID-19 and behavioral considerations for Ebola. We will discuss the use of mathematical models to capture different dynamics during an epidemiological outbreak and the associated questions these models address. Further, we will explore the computational tools used to analyze the models such as incorporating data through parameter estimation, management from control theory, and sensitivity analysis.

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MS47

Mathematical Modelling of Covid-19 Dynamics

The COVID-19 pandemic has ravaged global health and national economies worldwide. Testing and isolation are effective control strategies to mitigate the transmission of COVID-19, especially in the early stage of the disease outbreak. In this paper, we develop a deterministic model to investigate the impact of testing and compliance with isolation on the transmission of COVID-19. We derive the control reproduction number $\mathcal{R}_C$, which gives the threshold for disease elimination or prevalence. Using data from New York State in the early stage of the disease outbreak, we estimate $\mathcal{R}_C = 7.989$. Both elasticity and sensitivity analyses show that testing and compliance with isolation are significant in reducing $\mathcal{R}_C$ and disease prevalence. Simulation reveals that only high testing volume combined with a large proportion of individuals complying with isolation have great impact on mitigating the transmission. The testing starting date is also crucial: the earlier testing is implemented, the more impact it has on reducing the infection. The results obtained here would also be helpful in developing guidelines of early control strategies for pandemics similar to COVID-19.

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MS47

Assessing the Impact of the Wolbachia-Based Control of Malaria in An Endemic Setting

Malaria is one of the deadliest infectious diseases globally, causing hundreds of thousands of deaths each year. Efforts to control malaria involve disease surveillance, traditional mosquito controls, and the deployment of malaria vaccines. Wolbachia is a natural bacterium that can infect mosquitoes and reduce their ability to transmit diseases, and it has been used as an alternative strategy to combat dengue epidemics in the field. Extensive laboratory work has been done to introduce Wolbachia in Anopheles mosquitoes for malaria control with promising results. We develop and analyze a new mathematical model to assess the potential use of Wolbachia-based strategies for malaria control in the endemic regions. The model describes the complex Wolbachia transmission dynamics among mosquitoes, which is then coupled with malaria-specific disease features among humans with dynamical immunity feedback. We derive the basic reproduction number of the malaria disease transmission, which is a function of Wolbachia prevalence in mosquitoes. The resulting system presents bifurcations in both Wolbachia transmission in mosquitoes and malaria transmission in humans, which leads to potential malaria elimination.

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MS47

Unconditionally Energy Conservative and Positivity Preserving Methods for Wasserstein Gradient Flows

This talk introduces three innovative first-order dissipative numerical schemes tailored for a broad spectrum of Wasserstein gradient flows. These schemes are designed to preserve positivity and ensure energy dissipation across computations. Notably, the third scheme presents a groundbreaking approach that involves splitting the energy functional and incorporating a scalar auxiliary variable, which satifies the conservation of positivity and energy dissipation. Furthermore, we develop fully discrete schemes that adhere to these fundamental properties, cementing the robustness of our methodologies. The performance of our schemes is thoroughly evaluated through numerical experiments, which substantiate their theoretical accuracy and computational effectiveness. Our contributions significantly enhance the understanding of Wasserstein gradient flows and provide viable computational methods to navigate the intricacies of complex dissipative systems.

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MS48

Implicit Quantum Algorithm for Linear Differential Equatins

Many dynamical systems around us are governed by linear ordinary differential equations (ODEs). Typically, such systems feature dynamics at slow timescales which we are ultimately interested in as well as dynamics at much faster timescales, making them stiff. Solving such systems numerically explicitly requires a timestep that is much smaller than that dictated by the desired precision, rendering the algorithm inefficient. This is a limitation that quantum ODE solvers also suffer from, as they incorporate explicit timestepping techniques. In this work, we develop a quantum algorithm that solves ODEs via implicit timestepping, therefore circumventing the timestep limitation of existing explicit quantum ODE and increasing the efficiency of simulating stiff dynamics. Through a comparative analysis with existing ”one-shot” quantum algorithms those that output the solution at the final simulation time only we show that our algorithm has a better scaling with simulation time if one is interested in a time-integrated observable. We also show that our algorithm is flexible enough to become one-shot, if desired.

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MS48

Tensor Networking for Solving the LES-FDF Transport.

Large eddy simulation (LES) via the filtered density function (FDF) methodology has proven very effective for reliable and affordable computation of chemically reactive turbulent flows. Due to their inherent capabilities, the equations governing the transport of FDF are high dimensional. It is shown that tensor networks (TN) can deal with such a large dimensional transport in a very effective manner. These networks are employed here to tackle the Fokker-Planck form of the FDF instead of the Langevin form as is typically done via Monte Carlo methodologies. Demonstrative simulations are conducted of a chemically reactive flow, governed by a time-dependent five-dimensional modelled Fokker-Planck equation.

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MS48

Quantum-Inspired Simulations of Turbulent Combustion

The matrix product state (MPS) representation, developed for approximating the state of quantum many-body systems, exploits their correlation structure to accurately capture the underlying physics in a low-rank form (i.e., in a massively reduced state space). Here, this quantum-inspired methodology is employed for simulating chemically reacting turbulent flows. In doing so, the governing differential operators representing compressible, reacting turbulent flows are recast in the context of MPS, and their dynamics is simulated with various degrees of truncation. Simulations are performed to assess the effects of the Reynolds number, the Mach number and chemical heat release ratios on the compositional structure of the flow. The results via MPS-reduced order solutions are appraised against those generated via direct numerical simulation of the same flows. Advances on the simulation of reacting turbulent flows on quantum computing devices are also discussed.

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MS49

The Interplay Between Genomic Surveillance and Public Health Interventions

Pandemics pose a complex challenge in which epidemiological surveillance is essential but not sufficient to achieve containment. Waning immunity and the emergence of new variants that modify the population’s immunity profile and cause breakthrough infections, are main obstacles in controlling viral spread. Therefore, understanding the genomic composition of ongoing outbreaks is critical to characterize the expected disease dynamics, elucidate epidemiological outputs, and to inform potential intervention strategies. In this talk, I will introduce a modeling framework that integrates genomic surveillance, multi-variants dynamics and intervention strategies. I will discuss the effects of competing dynamics among variants, determined by the novel variant’s importation/emergence time, relative infectiousness and cross-infection, on both the variants detection time and the effectiveness of different intervention scenarios during a pandemic progression. We found that (i) the novel variants detection conditions are determined by the competitive dominance, modulated by the populations susceptibility; (ii) different intervention scenarios result in better outcomes depending on the target metric; (iii) the transmission process' characteristics inherently limit detection and the impact of intervention strategies.

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MS49

Mathematical Modeling of Microemulsions

Microemulsions can be mathematically modeled by a 4th order Cahn-Hilliard initial boundary value problem involving a sixth order nonlinear time dependent equation. This talk focuses on presenting a novel numerical splitting method/scheme simulating the microemulsion process and will show that this numerical method is uniquely and unconditionally solvable. Here, the C^0 Interior Penalty finite element method is used for the spatial discretization while the time discretizations are based on a modified convex splitting of the energy of the systems.

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MS49

Imex Methods for Thin Film Equations and Cahn Hilliard Equations with Variable Mobility

We consider a class of splitting schemes using implicit-explicit (IMEX) time stepping to obtain accurate and energy-stable solutions to thin-film equations and Cahn-Hilliard models with variable mobility. The splitting method gives a linear constant coefficient implicit step allowing for efficient computational implementation. The influence of the stabilizing splitting parameters over the numerical solution is studied computationally with choices of initial conditions. In addition, we compute energy-stability plots for the proposed methods for different choices of splitting parameter values and different sizes of the timestep. The methods improve the accuracy of the original bi-harmonic- modified (BHM) approach and retain the energy-decreasing property while reaching second order accuracy. Numerical experiments are presented to demonstrate the performance of the proposed methods.

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MS49

Improved Rational Approximation of Near-to-far Propagation Kernels for the Wave Equation

The 3-space, 1-time dimensional scalar wave equation, or 3 + 1 wave equation, describes how scalar or acoustic waves move through space and time. A special set of solutions to this equation, called multipole solutions can be used to understand how waves spread out from a central point. This work looks at how to predict the behavior of these waves as they move from one distance to a much larger distance from the center. Starting with a time series of wave data recorded at a smaller radius r1, the goal is to predict the wave data at a much larger radius r2. This prediction accounts for the time it takes the wave to travel from r1 to r2 and any changes in the waves shape. The process is described using a mathematical tool called a Laplace convolution, which involves the original time series and a kernel made up of exponential functions. Each multipole solution is identified by an integer l, which corresponds to its angular momentum. The kernel for the near-to-far prediction is a sum of l exponential functions, and its Laplace transform is a sum of l simple poles. However, as l increases, the calculation of these kernels becomes inaccurate with standard double-precision storage due to exponentially growing residues. This work explores the use of the Alpert-Greengard-Hagstrom algorithm to approximate these kernels more accurately. The algorithm is applied to a case with $l = 64$, a moderately large value, and also to the scaled Bessel function J1(t)/t, by approximating its Laplace transform as a rational function.

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MS52

A Mathematical Model to Investigate the Potency and Longevity of Phage Cocktails for Combating Antibiotic-Resistant Infections

With the global health threat of antibiotic resistant bacteria infections, a renewed interest has emerged in phage therapy the use of bacteriophages to treat pathogenic bacterial infections. However, the intricate dynamics between phages, target bacteria, and the emergence of phage resistance bacteria present challenges for achieving successful clinical outcomes. We developed a mathematical model of phage-bacteria interactions with data from *in vitro* experiments to explore outcomes for various combinations of treatment: single phage, double simultaneously (cocktail), or double sequentially. Our findings show that simultaneous administration of two highly potent and asymmetrical binding phage strains improved overall cocktail potency. This treatment strategy exhibits greater lysis potency, higher phage proliferation, most significantly reduced bacterial density, and longer delay in resistance evolution compared to other tested combinations. Nevertheless, all two-phage cocktail treatments showed an emergence of multi-phage resistance. Our study underscores the importance of a biologically-motivated modeling framework for assessing the impact of individual phage properties on treatment outcomes.

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MS52

Individual Motivations, Collective Behaviors: Increasing the Realism of Social Psychological Theory in Models of Emergent Collective Action

One of the foundational challenges in modeling emergent behaviors in human social systems is how to understand the coupled bidirectional influences between internal individual beliefs, perceptions, and decisions and the external influence of observations of others. In this talk, we will explore a model of collective action rooted in a well-supported explanatory theory from social psychology: the theory of planned behavior. We will further incorporate known biases in perception due to recency and primacy effects. We will show how a single, uniform explanatory model of individual action can lead to highly complex collective dynamics. We will end with a brief discussion about how such models can improve our understanding and prediction of, and ultimately our ability to influence, the behaviors of social groups.

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MS52

Most Probable Transition Path to An Ice-Free State in the Arctic

We consider a stochastic Arctic energy balance model with periodic forcing and a piecewise-smooth drift, where the periodic state may transition from a stable perennially ice-covered state to a stable perennially ice-free state as a rare event. We calculate the most probable transition path from the ice-covered to the ice-free state as the minimizer of the Friedlin-Wentzell rate functional, with a correction term necessary for the minimizer to cross the switches in the system. We compare this path to transition paths generated through Monte Carlo simulations. This provides an initial case study of the theoretical most probable transition path in a physically-informed piecewise-smooth model.

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MS52

Using Persistent Homology to Analyze Access to Resources with Heterogenous Quality

Ideally, all public resources (e.g. parks, grocery stores, hospitals, etc.) should be distributed in a way that is fair and equitable to everyone. However, this is not always the case. Quantifying how much (or little) access individuals have to certain resources is a complex problem. Previous work has shown that tools from topological data analysis (TDA) can be useful in determining ”holes” in the locations of resource locations based on geographic locations and travel times [Hickok et al., Persistent homology for resource coverage: a case study of access to polling sites, 2023]. Some resources may necessitate incorporation a notion of quality. As a case study, we look at public parks, which are heterogenous in many ways. Having access to a park that is hundreds of acres with basketball courts, baseball diamonds, and an aquarium is inherently different than having access to a small patch of grass with an overgrown tennis court. Here we present an exploration of the access to public parks in Chicago using persistent homology, a tool from TDA.

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MS53

Data Assimilation for a Porous Media Model

We propose the use of a continuous data assimilation algorithm for miscible flow models in a porous medium. In the absence of initial conditions for the model, observed sparse measurements are used to generate an approximation to the true solution. Under certain assumption of the sparse measurements and their incorporation into the algorithm it can be shown that the resulting approximate solution converges to the true solution at an exponential rate as time progresses. Various numerical examples are considered in order to validate the suitability of the algorithm.

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MS53

Nonlinear Algorithms InData Assimilation and Large-Time Behavior of Differential Equations

A continuous data assimilation method proposed by Azouani, Olson, and Titi in 2014 introduced a linear feedback control term to dissipative systems. In this talk, we will focus on the insights of nonlinear variations of the AOT algorithm and distinguish the clear connections to the large-time behavior of physical systems, analytical and otherwise.

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MS53

A proof of Onsager Conjecture for SQG

We construct weak solutions for the surface quasi-geostrophic (SQG) equation which do not conserve the Hamiltonian. The weak solutions are in C^0- space. Thus our result gives a proof of the Onsager type of conjecture for the SQG, since it is known that the Hamiltonian is conserved in space with higher regularity.

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MS53

Effect of the Noise on the Statistical Features of 3D Turbulent Flow

The stochastic equations are often used as a complementary model to the deterministic one to better understand the role of small perturbations and the randomness. In this talk, considering the stochastic 3D NavierStokes equations with both shear and periodic boundary conditions, we demonstrate how to quantify the effect of the randomness on the bulk and statistical features of the applied flow.

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MS54

Model Order Reduction Using Shape-Morphing Modes

We present recent advancements for fast and scalable computation of reduced-order nonlinear solutions (RONS). RONS is a framework for reduced-order modeling of time-dependent partial differential equations (PDEs), where the reduced solution has nonlinear dependence on time-varying parameters. RONS provides an explicit set of ordinary differential equations (ODEs) to optimally evolve the time-varying parameters. Additionally, RONS allows us to easily enforce conserved quantities of the governing PDE in the reduced solution. When the reduced-order solution contains many parameters, formation and integration of the RONS equation becomes computationally expensive. To overcome this computational bottleneck, we introduce symbolic RONS, collocation RONS, and regularized RONS. These new approaches allow applications of RONS to problems which require many parameters in the reduced solution. We demonstrate the ability of RONS to produce fast and accurate reduced-order models by applying these new methods to several examples, including the Kuramoto-Sivashinsky equation and an 8-dimensional Fokker-Planck equation. LLNL-ABS-859766

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MS54

Data Assimilation for Shape-Morphing Reduced-Order Models

Shape-morphing modes, which depend nonlinearly on time-varying parameters, have opened a new paradigm in reduced-order modeling and numerical solution of partial differential equations (PDEs). The parameters of the model evolve according to a set of ordinary differential equations (ODEs) known as RONS. In this talk, we introduce data assimilation into this framework. In particular, using a linearized version of RONS, we show that discrete observational data can be used to nudge the shape-morphing solution closer to the true solution of the PDE. We also introduce a method, based on QR factorization with column pivoting, to inform the optimal location of the sensors for gathering the observational data. We demonstrate, on several numerical examples, that the resulting data-assimilated shape-morphing solutions accurately approximate the true solution of the PDE.

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MS54

Temporally Aperiodic Spectral Submanifolds and Their Applications in Soft Robotics

In this talk we discuss the recent extension of the current theory for spectral submanifolds (SSMs) to general non-autonomous dynamical systems that are either weakly forced or slowly varying. Restricting the dynamics onto these SSMs provides one with a mathematically rigorous model reduction technique. We further validate this by computing low dimensional temporal SSMs and their reduced dynamics for aperiodically forced high-dimensional nonlinear systems from equations. We also discuss an application of these ideas for optimal control of soft robots purely from data. Specifically, we design a novel model predictive control scheme and test it on a high-dimensional nonlinear finite element model describing a soft trunk robot. We find our method outperforms the state-of-the-art techniques for trajectory tracking control tasks.

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MS56

Continuous Data Assimilation of a Discretized Barotropic Vorticity Model of Geophysical Flow

We consider continuous data assimilation applied to a finite element spatial discretization and backward difference temporal discretization of the barotropic vorticity model of geophysical flow. We prove that with sufficient measurement data and properly chosen nudging parameter (guided by our analysis), the proposed algorithm achieves optimal long-time accuracy for any initial condition. While our analysis requires nudging of both the streamfunction and vorticity, our numerical tests indicate that nudging only the streamfunction can be sufficient.

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MS56

A Block Factorization Based Preconditioner for Resistive MHD Simulations

We discuss a block preconditioner for the visco-resistive low Mach number compressible magnetohydrodynamics model. This model requires the solution of the governing partial differential equations (PDEs) describing conservation of mass, momentum, and thermal energy, along with various reduced forms of Maxwells equations for the electromagnetic fields. The resulting systems are characterized by strong nonlinear and nonsymmetric coupling of fluid and electromagnetic phenomena, as well as the significant range of time- and length-scales that these interactions produce. These characteristics make scalable and efficient iterative solution, of the resulting poorly-conditioned discrete systems, extremely difficult. The block preconditioner considered here is based on an approximate operator splitting approach which can isolate certain coupled systems, allowing them to be handled independently. Here we use the splitting to create two independent 2x2 block systems, a magnetics-flow system and a magnetics-constraint system. Targeting ARM architectures, the supercomputer Fugaku in particular, we investigate various preconditioner reuse options to reduce setup costs. We demonstrate this approach for various resistive MHD problems that are relevant to magnetic confinement fusion applications.

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MS56

A Second Order Numerical Scheme for a Sixth-Order Cahn-Hilliard Type Equation modeling Microemulsions

In this talk we present a second-order in time approximation for a sixth-order Cahn-Hilliard type equation which models the dynamics of phase transitions in ternary oil-water-surfactant systems. For its spatial discretization, we decompose this nonlinear sixth-order parabolic equation into a mixed formulation comprising a system of three second-order (in space) equations, one of which is parabolic while the other two equations are algebraic. We discuss the key properties of unconditional stability and unique solvability for our scheme and demonstrate its numerical performance through results of selected computational experiments.

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MS56

Filtered Subspace Iteration for Singularly Perturbed Self-adjoint Operators

Subspace iteration is one of the oldest algorithms for solving eigenvalue problems. In this presentation, we will use the filtered subspace iterations in the perturbed FEAST method to approximate a finite cluster of eigenvalues of an unbounded self-adjoint operator in a Hilbert space. A rational function of the operator is constructed such that the eigenspace of interest is its dominant eigenspace, and a subspace iteration procedure is used to approximate this eigenspace. The computed space is then used to obtain approximations of the eigenvalues of interest. A convergence analysis will be shown that how the error in eigenspaces decreases.

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MS57

Vector Space Embeddings and Data Maps for Cyber Defense

Vast amounts of information of interest to cyber defence organizations comes in the form of unstructured data; from host-based telemetry and malware binaries, to phishing emails and network packet-sequences. All of this data is extremely challenging to analyse. In recent years there have been huge advances in the methodology for converting more traditional unstructured media into vectors, however, leveraging such techniques for cyber defence data remains a challenge. Imposing structure on unstructured data allows us to leverage powerful data science and machine tools. Structure can be imposed in multiple ways, but vector space representations, with a meaningful distance measure, have proved to be one of the most fruitful. In this talk, we will demonstrate a number of techniques for embedding cyber defence data into vector spaces. We will then discuss how to leverage manifold learning techniques, clustering, and interactive data visualization to broaden our understanding of the data and enrich the data with expert feedback. At the Tutte Institute for Mathematics and Computing (TIMC) we believe in the importance of reproducibility and in making research techniques accessible to the broader cyber defense community. To that end this talk will leverage several open-source libraries and techniques that we have developed at TIMC: Vectorizers, UMAP, HDBSCAN, ThisNotThat and DataMapPlot.

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MS57

A Combinatorial Approach to System Testing

The National Institute of Standards and Technology (NIST) estimates that \$60 billion dollars are spent each year due to inadequate software testing, despite the fact that 50–80% of development budgets go to testing. Testing every possible configuration is unrealistic for all but the simplest systems, and so carefully designing a test strategy is essential for identifying and fixing errors. As systems become more complex and interconnected, errors become more difficult to detect. A system which has thirty parameters has over a billion different configurations which must be tested to be 100% confident that the system is error-free. To reach 90% confidence, however, we need as few as 10 tests—and a few assumptions. Combinatorial testing applies the theory of combinatorial designs to produce a testing plan which will ilicit erorrs—when they exist—efficiently and effectively. This area combines classical problems in pure math, including a centuries-old false conjecture by Euler, with real-world applications.

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MS57

Magnitude and Cybersecurity

The theory of magnitude connects the theory of enriched categories to geometry, information theory, and algebraic topology, among other areas. Meanwhile, it enables remarkable capabilities in areas such as outlier detection, optimization, and topological characterizations of discrete data. We give an overview of the theory, its connections, and emerging applications to cybersecurity, including a proof of concept software fuzzer.

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MS57

Do You Trust Me? Securing AI from the Ground Up Through Verification, Transparency, and Fairness

Artificial Intelligence (AI) and Machine Learning (ML) have shown incredible promise in a wide variety of domains. However, the majority of use cases considered such as movie recommendations or semantic characterization of product reviews - are relatively low-risk. We argue that to enable AI/ML in high-risk domains such as cybersecurity, autonomous actuation and control, or medical workflows, we must consider the security of AI/ML algorithms throughout the model development and deployment process. We will discuss metrics, tools, and techniques to quantify and increase AI/ML model robustness and trust, including verification, transparency, and fairness. We will also describe how these approaches can be leveraged throughout AI/ML model development and deployment pipelines to enable Secure AI.

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MS58

Predicting Bifurcations in Cardiac Systems with Machine Learning

Cardiac systems can undergo bifurcations - abrupt and significant changes in dynamics when a parameter crosses a threshold. These bifurcations can correspond to life threatening cardiac arrhythmia, so predicting them and understanding their origin is of great interest. In this talk, I will discuss our work on using machine learning to approach these problems. In particular, I will show how a machine learning classifier can be trained to predict a bifurcation to alternans in chick heart aggregates, and how reinforcement learning can be used to discover stimulus protocols that lead to reentry in different tissue geometries.

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MS58

Particle Swarm Optimization for Developing Populations of Models for Cardiac Simulations

Human cardiac cells exhibit high variability not only across patients but even within the same individual's heart. Capturing this variability in simulations of cardiac electrophysiology models is useful for obtaining a more complete and robust understanding of cardiac dynamics, particularly when studying the effects of specific interventions. One approach for representing such variability involves using virtual cadres of cardiac patients: large populations of models with different dynamics but whose overall variability for certain biomarkers matches that of real tissue. We introduce a modification of particle swarm optimization for rapidly generating populations of cardiac models fitting user-specified biomarker criteria. This approach avoids converging to a single global minimum while still exploiting the swarm intelligence to explore parameter space. Our browser-based WebGL implementation takes advantage of GPU hardware for increased speed and usability, while also yielding a greater proportion of acceptable parameter sets than using random initializations. We present initial results of using this tool to generate populations of cardiac models under various constraints.

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MS58

Machine Learning Reveals Physiological Differences in Atrial Fibrillation Patients Who Experience Long-Term Versus Acute Success from Ablation

Background: It is unclear why many patients with long-term freedom from atrial fibrillation (AF) after ablation did not exhibit acute termination, yet others with acute AF termination may not show long-term success. We hypothesized that different combinations of multimodal data in AF patients predict acute or long-term response to ablation, and that these distinct phenotypes may be revealed by machine learning (ML). Methods: We studied 561 patients from the Stanford AF ablation registry (66+/-10y, 28% women) in whom we extracted 71 data elements: electrogram (EGM) features, ECG features, structural features, lifestyle features and clinical variables. We used 30% of cohort as a hold-out test set. We compared 6 ML models to predict both outcomes, used Shapley explainability analysis to identify the phenotypes for each outcome. Results: The best model for termination was more predictive than for long-term outcome (AUROC 0.83, Random Forest vs 0.65, logistic regression, respectively; $p < 0.001$) and both had distinct predictive components. Phenotypes of long-term success were 100% explained by clinical and lifestyle features, while phenotypes for termination were 80% explained by electrical features. Conclusions: Long-term and acute responses to ablation in AF patients reflect distinct physiology. These findings may help improve identification of likely responders.

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MS58

Simulations of Low-Energy Defibrillation with a Rotating Field: Insights from a Computational Study

Heart disease is the leading cause of mortality in the US despite the existence of many treatment methods to aid cardiovascular problems. Cardiac arrhythmias, such as ventricular fibrillation (VF), ventricular tachycardia (VT) and atrial fibrillation (AF), are a major contributor to sudden cardiac death. While the traditional clinical treatment to VF, a high-energy fibrillation shock, is effective, side effects like severe pain and myocardial damage can lead to increased mortality and decreased quality of life. In this talk, we will be talking about simulation results from low-energy defibrillation with a rotating field, a more effective approach for the treatment of AF, VT and VF.

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MS59

Intrastep, Stage-Value Predictors for Diagonally-Implicit Runge–Kutta Methods

To better identify the necessary attributes of good stage-value predictors (SVPs), numerous SVPs are designed for an existing: ESDIRK4(3)7L[2]SA (Kennedy2019) and a new: ESDIRK4(3)8L[2]SA (eight stages) scheme. Both are stiffly-accurate, stage-order two, explicit, singly-diagonally implicit Runge–Kutta (ESDIRK) schemes. Tradeoffs are studied in the parameter spaces enforcing the constraints on accuracy, linear stability, nonlinear stability and coefficient size to determine which objectives correlate with effective predictors. The SVPs are tested in challenging external aerodynamics simulations (10^7 DoFs) using the compressible Navier-Stokes equations (CNSE). An entropy stable spectral collocation formulation is used for discretizing the spatial terms in the equations. Simulations are performed at a wide variety of temporal error tolerances. At lax temporal error tolerances, the most efficient SVPs are those designed with second-order accuracy and the stability properties: A-stability, L-stability, rather than high accuracy constraints. Simulations requiring tight error tolerances are better suited for SVPs designed using high accuracy constraints. Designing SVPs with enhanced stability properties is tedious but worthwhile. Simulation times are reduced with optimal SVPs by as much as 100% on some stages, with combined stepwise improvements of between $50 - 100\%$ for both methods.

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MS59

Modified Patankar Linear Multistep Methods for Production-Destruction Systems

A wide variety of mathematical models for real life problems are given in the form of positive and conservative Production-Destruction differential Systems (PDS) [U. an der Heiden, M.C. Mackey, The dynamics of production and destruction: Analytic insight into complex behavior, J. Math. Biol., 16 (1982)]. Patankar-type schemes are linearly implicit integrators for PDS, traditionally based on Runge-Kutta schemes and specifically designed to be unconditionally conservative and positive [J. Huang, W. Zhao, C.W. Shu, A Third-Order Unconditionally Positivity-Preserving Scheme for Production-Destruction Equations with Applications to Non-equilibrium Flows, J. Sci. Comput., 79 (2019); S. Kopecz, A. Meister, Unconditionally positive and conservative third order modified Patankar-Runge-Kutta discretizations of production-destruction systems, Bit Numer. Math., 58 (2018)]. Here we extend the Patankar approach to linear multistep methods and prove that the resulting schemes retain, with no conditions on the step size, the positivity of the solution and the linear invariant of the continuous-time system. Moreover, we provide results on arbitrarily high order of convergence achieved through an embedding technique for the Patankar weights denominators. Finally, we report numerical tests that confirm the theoretical results and show that Modified Patankar Linear Multistep Methods are competitive and can have higher accuracy and better performance than Modified Patankar Runge-Kutta methods.

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MS59

High Order Runge-Kutta Methods for Stiff, Semilinear Differential Equations

Runge-Kutta methods are one of the most popular families of integrators for solving ordinary differential equations, essential in simulating dynamical systems arising in physics, engineering, biology, and various other fields. Unfortunately, classical error analysis for Runge-Kutta methods relies on assumptions that rarely hold when solving stiff ordinary differential equations (ODEs): an asymptotically small timestep and a right-hand side function with a moderate Lipschitz constant. Without idyllic assumptions, Runge-Kutta methods can experience a problematic degradation in accuracy known as order reduction. While high stage order remedies order reduction, it is only viable for expensive, fully implicit Runge-Kutta methods. In this talk, I will discuss recent advancements in deriving computationally practical Runge-Kutta methods that truly attain high order for semilinear ODEs. Our new, stiff analysis leads to rich and interesting connections with the set of rooted trees.

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MS59

Step into the Complex World

Operator splitting methods of order greater than two require backward integration on every operator. This is known to cause instability issues in certain applications. One possible remedy is to consider operator splitting methods with complex-valued coefficients. Moreover, little is known about operator splitting methods for N-split problems other than the first-order Lie-Trotter method and the second-order Strang-Marchuk method. In this talk, we will present a pair of second-order complex-valued operator splitting methods that can be generalized to N-split problems. We will compare the accuracy and efficiency of these methods with the Strang–Marchuk method and propose extensions to high-order methods.

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MS60

Equity, Diversity, And, Inclusion (EDI) in the SIAM Community and Beyond: An Update

As SIAM's first Vice-President for Equity, Diversity, and Inclusion (EDI) I will use this opportunity to present an update on various initiatives that are happening at SIAM and other organizations that will enhance EDI in the mathematical and computational sciences communities that SIAM serves.

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MS60

Effective Student Programs for Improving EDI in STEM at Oak Ridge National Laboratory

It is important for students, in particular diverse students, to be well informed about career opportunities beyond academia and industry to increase their opportunities in STEM. This talk will introduce an interactive session and discussion for undergraduate and graduate students who are actively looking for diverse career path options including opportunities in terms of internships, research collaborations, and postdoctoral program opportunities at DOE national laboratories (particularly the case of Oak Ridge National Laboratory [ORNL]). I will discuss the fundamental importance of student internships and of integrating a broad set of internship experiences in shaping a better position for career paths. I will answer questions about STEM careers at National Laboratories and how this setting can provide exposure, training, experience, and fun to redirection your career priories with perhaps unexpected results. I will conclude the session by introducing the portfolio of student programs for diverse students at ORNL.

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MS60

EDI Panel Discussion

EDI panel discussion moderated by Ron Buckmire.

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MS61

Bounds on the Global Attractor of 2D Incompressible Turbulence

Analytic bounds on the projection of the global attractor of 2D incompressible turbulence in the palenstrophy–enstrophy plane [Dascaliuc, Foias, and Jolly 2005, 2010] are observed to vastly overestimate the values obtained from numerical simulations. This is due to the lack of a good estimate for the inner product of the solenoidal part of the advection $B(u,u)$ of the velocity u and the biLaplacian $\Delta^2 u$. Sobolev inequalities like Ladyzhenskaya and Agmon's inequalities yield an upper bound that is not sharp. For statistically isotropic turbulence, we show that the expected value of this term is in fact zero. The implications for estimates on the behaviour of the global attractor are discussed.

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MS61

Nonlinear and Linear Evolution Equations Via Transformations at the Level of Naturally Associated Stochastic Structures

Certain PDE have naturally associated stochastic structures that can be exploited to construct deterministic solutions to associated initial-boundary value problems and study their long-time behavior. We use the framework of YZX stochastic models to connect solutions of the the so-called α-Riccati equation (a non-linear model used to describe ageing, but which can also be viewed as a simplified analogy to the self-similar Navier-Stokes equations) to the solutions of the Pantograph equation (a non-local linear ODE which has applications ranging from combinatorics to cell division modeling, and which functionally represents a linearization of the α-Riccati equation about a steady state). The key observation is that this connection, somewhat reminiscent of the Cole-Hopf transform for Burgers equation, is established for the associated stochastic structures, rather for the equations themselves. As a result, we obtain non-uniqueness for the corresponding Cauchy Problem for the α-Riccati equations from a solution of the Pantograph equations, obtained via the stochastic cascades. Notably, the Pantograph equation solutions that we obtain are consistent with the algebraically decayed solutions mentioned by Kato and McLeod in 1971. Based on the ongoing joint work with Tuan Pham, Enrique Thomann, and Edward Waymire.

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MS61

The Batchelor-Howells-Townsend Spectrum, Large Velocity Case

We consider the behavior of a passive tracer θ governed by $\partial_t\theta + u \cdot \nabla\theta = \Delta\theta + g$ in two space dimensions with prescribed smooth random incompressible velocity $u(x,t)$ and source $g(x)$. In 1959, Batchelor, Howells and Townsend (J. Fluid Mech. 5:113) predicted that the tracer (power) spectrum should scale as $|\theta_k|^2 \propto |k|^{-4}|u_k|^2$ for $|k|$ above some $\bar{\kappa}(u)$, with different behaviour for $|k| \lesssim \bar{\kappa}(u)$ predicted earlier by Obukhov and Corrsin. In this paper, we prove that the BHT scaling does indeed hold probabilistically for sufficiently large $|k|$, asymptotically up to controlled remainders, using only bounds on the smaller $|k|$ component.

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MS61

On Well-Posedness of Mildly Regularized Active Scalar Equations in Borderline Sobolev Spaces

We consider the initial value problem for a family of 2D generalized surface quasi-geostrophic equations (gSQG) when perturbed by logarithmic Laplacian dissipation. These equations interpolate between the 2D incompressible Euler equation and the SQG equation, and extrapolate beyond SQG to a family with more singular velocities. Previous studies by Bourgain & Li, Elgindi & Masmoudi, Crdoba & Zoroa-Martinez, and Jeong & Kim have established the ill-posedness of this family at critical regularity levels. In this talk, we address the question of well-posedness (in the Hadamard sense) in a setting of borderline regularity. We establish that mild logarithmic dissipation recovers well-posedness in scenarios where the corresponding unperturbed equation exhibits ill-posedness. Additionally, this type of dissipation confers a mild smoothing effect instantaneously. A key aspect of our proof involves identifying a suitable linearized system that captures the inherent commutator structure associated with the gSQG equation.

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MS62

Modeling Single-Cell and Spatial Transcriptomic Data with Optimal Transport

The emerging single-cell and spatial genomics techniques allow us to elucidate the governing rules of multicellular systems with unprecedented resolution and depth. These datasets are often high-dimensional, complex, and heterogeneous. Mathematical tools are needed to extract biological insights from such data. In this talk, we will discuss several computational methods based on optimal transport for exploring the tissue structures, temporal signatures, and cell-cell communication processes on single-cell and spatial genomics data. We will also discuss supervised optimal transport motivated by these biological applica-tions where application-induced constraints are enforced in the optimal transport problem.

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MS62

Knot Data Analysis for Biomolecular Interactions Using Multiscale Gauss Link Integral

Over the past decade, topological data analysis (TDA) has become a powerful tool in data science, with its main technique being persistent homology. This method tracks topological properties as point cloud data evolves, using algebraic topology. Despite the significance of knot theory and related mathematical subjects, their practical applications have been limited due to localization and quantization challenges. To address these issues, we introduce knot data analysis (KDA), a new approach that incorporates curve segmentation and multiscale analysis into the Gauss link integral. This results in the multiscale Gauss link integral (mGLI), which not only reveals global topological features of knots and links at an appropriate scale but also provides multiscale feature vectors to capture local structures and connections within each curve segment at different scales. We demonstrate its representative ability on biomolecules and molecular interactions through protein flexibility analysis and protein-ligand binding affinity predictions. The pro-posed mGLI significantly outperforms other state-of-the-art methods including earlier persistent homology-based methods. Our approach enables the integration of artificial intelligence (AI) and KDA for general curve-like objects and data.

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MS62

Tree Distinguishing Polynomial and Its Applications in Biosciences

Polynomial invariants, such as the Tutte polynomial for graphs and the Jones polynomial for knots, are essential mathematical objects for studying discrete and topological structures. They encode structural in-formation and can be represented as vectors or matrices. These polynomials allow the analysis of exten-sive structures using modern data analytic tools. Discrete structures, especially trees, emerge in many are-as of biosciences and record important biological information. In this talk, we introduce an easy-to-compute and interpretable polynomial that is a complete invariant for trees. We apply this tree distinguishing polynomial to study pathogen evolution and nucleic acid structures. With this approach, we reveal dis-tinct evolutionary patterns of seasonal and tropical human influenza virus A H3N2 as well as a strong correlation between nascent RNA secondary structures and R-loop formation.

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MS63

Hodge Decomposition Method for the 3D Quad-Curl Problem

Using the Hodge decomposition for a divergence-free vector field, we develop a finite element method for the quad-curl equation in three dimensions. This approach allows the fourth-order problem to be reformulated as three second-order saddle point systems: two Maxwell systems and a Stokes system. Analysis and results are presented for a Nedelec-P1 discretization for Maxwells equations, and a P2-P1 Taylor-Hood method for Stokes equations.

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MS63

General Degree Divergence-free Finite Element Methods for the Stokes Problem on Smooth Domains

We construct a divergence-free, isoparametric method for the Stokes problem on smooth domains. This method builds on the Scott-Vogelius finite element pair with arbitrary polynomial degree greater than two, which is known to be a divergence-free method when implemented on affine elements. In order to preserve the divergence free property in the isoparametric framework, we use the Piola transform to modify the functions in the discrete velocity space. We also distribute the edge degrees of freedom at particular quadrature points. These choices ensure weak continuity across element edges that allow us to prove that the method converges with optimal order in the energy norm. We also prove that the discrete velocity error has optimal convergence in L^2.

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MS63

A Nonvirtual Virtual Element Method with Punctured Mesh Cells

Unconventional mesh geometries incorporating polygonal and curvilinear cells are the subject of increasing interest to those seeking numerical solutions of partial differential equations. This flexibility in mesh construction holds the promise of significantly reducing the degrees of freedom involved in obtaining a finite element solution when compared to conventional meshing techniques. In recent work, we extend the mesh geometry even further by allowing planar mesh cells to be multiply connected, i.e. have holes. We use the same function space as that used in virtual element methods (VEM), consisting of implicitly-defined solutions to Poisson problems with polynomial data. Unlike VEM, we construct and compute with basis functions directly, rather than taking projections and introducing stabilization terms. By leveraging notions from complex analysis, we efficiently obtain the H^1 semi-inner products and L^2 inner products of these basis functions by performing computations solely on cell boundaries. An additional benefit of this approach is that the values, gradient, and higher derivatives of the finite element solution can be cheaply obtained in the interior of mesh cells, and not just on the skeleton.

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MS63

A parameter-free and pressure-robust enriched

Galerkin method for Navier-Stokes equations

In this talk, we present and analyze a parameter-free and pressure-robust enriched Galerkin (EG) method for the steady incompressible NavierStokes equations. Unlike traditional EG methods which enrich the Continuous Galerkin (CG) space with Discontinous Galerkin (DG) functions defined on elements, we enrich the CG sapace with a DG space of piecewise constants along edges in 2D or on faces in 3D. The DG space acts as a correction to the normal component of the CG space to ensure stability. We utilize weak derivatives to achieve a parameter-free property and employ test function reconstruction to ensure pressure robustness. We establish error analysis demonstrating the existence, uniqueness, and convergence of the method. Numerical experiments validate our theoretical findings.

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MS64

Linear and Nonlinear Kalman Filter Designs for a Cardiac Ionic Model

Cardiac arrhythmias are sometimes preceded by alternans, which is a beat-to-beat (period-2) alternation in the electrical waves that govern contractions in the heart. Two possible causes of alternans are instabilities in either the cellular membrane potential dynamics or the intracellular calcium dynamics, respectively leading to either voltage-driven or calcium-driven alternans. There is increasing interest in developing data assimilation algorithms to reconstruct cardiac variables that are not directly measurable yet may be important to alternans and arrhythmia formation. At present, little is known about the impact of alternans mechanisms on data assimilation performance. In response, we applied computational methods from control theory to the Shiferaw-Sato-Karma (SSK) nonlinear ODE model of alternans. We designed a linear data assimilator (the Kalman Filter or KF) for the SSK model, and we showed that a control-theoretic model property called observability typically predicted which types of simulated measurements (e.g., membrane potential or intracellular calcium) yielded more favorable KF performance measures, such as steady-state estimation error. The types of measurements that yielded the best KF performance were found to depend on alternans mechanism. In addition, we applied a nonlinear assimilator called the Unscented Kalman Filter (UKF) to the SSK model, and we confirmed the ability of the UKF to reconstruct certain missing variables in simulation tests.

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MS64

A Modified Fitzhugh-Nagumo Model that Reproduces the Action Potential and Dynamics of the Ten Tusscher et al. Cardiac Model in Tissue

The Fitzhugh-Nagumo FHN) model is a two variable model that is used to simulate the electrical activation of cardiac and neural cells. Due to its simplicity the two variable FHN model lacks many dynamics observed in cardiac tissue. Meanwhile, complex ionic models such as the 19-variable Ten Tusscher et al. (TNNP) model are capable of reproducing these dynamics. To aid in bridging the gap between the two models, we have parameterized a modified version of the FHN model, which is better suited for reproducing cardiac dynamics which the original FHN model. These previously applied modifications mainly add a nullcline at zero voltage for the fast variable (eliminating hyper polarization) and modify the slow variable nullcline from linear to quadratic (allowing for alternan behavior and a better fit to experimental cardiac data). Using particle swam optimization (PSO) to fit the action potentials of several pacing period, we have parameterized the modified FHN model to match the action potential patterns and properties seen in two dimensional simulations of the TNNP model. This parameterized model allows for proof-of-concept investigation in cardiology that can help guide more time-consuming simulations with complex ionic models.

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MS64

Quantifying Changes in Experimental Fibrillation Patterns Induced by a New 3D Cardiac Defibrillation Method

We have been developing a new, 3D low-energy defibrillation method, which works by applying an electric field to the surface of the heart to modify the shape of the filaments around which scroll waves rotate so that they shrink and disappear. In this talk, we present the analysis of experimental optical mapping data related to our method, generated at Georgia Institute of Technology. Particularly, we will present evidence of dynamical changes in wave propagation patterns consistent with how we expect our method to work.

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MS65

Characterizing the Complexity of Fibrillation from Models and Experiments with Lyapunov Exponents

Lyapunov exponents can be used to quantify the degree of chaos in a nonlinear system. We calculate the Lyapunov exponent in time and as function of space to quantify different types of spiral wave breakup dynamics supporting ventricular fibrillation (VF). We use a Nonlinear Time Series Analysis (TISEAN) algorithm to analyze the input voltage signal from simulations of VF for various point in space in order to also quantify a Lyapunov exponent in space. We present results from simulations of several ionic cardiac models for various parameters and from optical mapping experiments in various mammalian species including rabbits, porcine and human.

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MS65

Dreaming of Electrical Waves: Generative Modeling of Cardiac Excitation Waves Using Diffusion Models

Electrical waves in the heart form rotating spiral or scroll waves during life-threatening arrhythmias such as atrial or ventricular fibrillation. The wave dynamics are typically modeled using coupled partial differential equations, which describe reaction-diffusion dynamics in excitable media. More recently, data-driven generative modeling has emerged as an alternative to generate spatio-temporal patterns in physical and biological systems. Here, we explore denoising diffusion probabilistic models for the generative modeling of electrical wave patterns in cardiac tissue. We trained diffusion models with simulated electrical wave patterns to be able to generate such wave patterns in unconditional and conditional generation tasks. For instance, we explored inpainting tasks, such as reconstructing three-dimensional wave dynamics from superficial two-dimensional measurements, and generating parameter-specific dynamics. We characterized and compared the diffusion-generated solutions to solutions obtained with biophysical models and found that diffusion models learn to replicate spiral and scroll waves dynamics so well that they could serve as an alternative data-driven approach for the modeling of excitation waves in cardiac tissue. For instance, we found that it is possible to initiate and evolve ventricular fibrillation (VF) dynamics. However, we also found that diffusion models 'hallucinate' wave patterns when given insufficient constraints.

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MS65

Bifurcation Structure of Traveling Wave Solutions in Electrophysiological Models of Cardiac Tissue

In the heart, repeated waves of electrochemical activity propagate through the tissue, triggering the coordinated contractions that allow the heart to pump blood. The propagated waves can be modeled as traveling wave solutions in spatially-distributed excitable medium in which local dynamics have been represented by highly idealized models (such as the two-variable FitzHugh-Nagumo equations) and high-dimensional biophysically-detailed models (such as the ten-variable ten Tusscher et al. model). In general, traveling waves in models of cardiac tissue cannot be computed analytically, and therefore suitable numerical methods are a necessity. It is common to solve for traveling wave profiles with root finding methods, and then continuation methods can capture the dependence of the existence of waves and their properties, such as wave speed, on cardiac model parameters and the frequency of the waves. Current numerical methods for computing traveling wave solutions are adequate for idealized models but are lacking for the more computationally demanding detailed-biophysical models. We develop robust and efficient numerical methods for computing traveling wave solutions, dispersion curves, and bifurcation scenarios for the high-dimensional models. We use these numerical methods to uncover potential fundamental differences between the bifurcation structure of travelling waves in the highly idealized and in biophysically-detailed cardiac models.

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MS65

Automated Computation of Strength-Interval Curves Using Actors

Strength-interval (SI) curves are used to quantify the relationship between the response of excitable tissue as a function of the strength and duration of an electrical stimulus. In the context of cardiac electrophysiology, SI curves characterize the refractoriness of cardiac tissue as a function of inter-stimulus interval length. Although usually collected experimentally, this type of information can now also be obtained computationally. However, the computational generation of SI curves can be labor intensive and time consuming due to its iterative nature, the number and size of computations required, and the amount of researcher intervention involved. In this presentation, we demonstrate how the actor model of concurrent programming can be used to automate the process of SI curve generation, relieving much of the burden on the researcher while maximizing use of the available computational resources. Computational resource utilization is optimized by the dynamic monitoring and assessment of the overall benefit of each actor's momentary resource usage. The automatically generated SI curves are produced in significantly less time compared to current practice and with virtually no manual intervention. A newly proposed concurrent actor-based look-ahead bisection method for the location of the activation thresholds is also described.

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MS67

Multiphysics Time-integration for Turbulent Combustion at the Exascale

Turbulent reacting flow systems are often modeled with coupled time-dependent partial differential equations (PDEs). Solving such equations can easily tax the worlds largest supercomputers. One pragmatic strategy for attacking such problems is to split the PDEs into components that can more easily be solved in isolation. This generic operator-splitting strategy leads to a set of ordinary differential equations (ODEs) that need to be solved as part of an outer-loop time-stepping approach. In many combustion applications, the ODEs to be solved can be very stiff, exhibiting timescales that span many orders of magnitude. The SUNDIALS library provides a plethora of robust time integration algorithms for solving these ODEs on exascale-capable computing hardware, yet for many complex applications (such multicomponent fuels or emissions predictions), the chemical models remain too complex to solve using reasonable resources. The Quasi-Steady State Approximation (QSSA) can be an effective tool for reducing the size and stiffness of the simulations. In this talk, I will discuss the use of the SUDIALS library of ODE solvers together with automatic code generation tools to solve complex turbulent reacting flow problems using QSSA models.

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MS67

A Generalization of Operator Splitting Methods for Multi-Physics Applications

Partitioned integrators have been of great interest in solving multi-physics time dependent PDEs. They are designed to treat the various sub-system dynamics individually to improve time to solution. Generally, they rely on defining how the sub-system should be integrated to maintain accuracy and stability requirements. To bypass this requirement operator splitting and co-simulation methods are used. However, these methods have known limitations on their stability and accuracy. In this presentation a new approach will be presented called the Generalized Operator Splitting (GOS) methods. The GOS methods allow for any integration scheme to be utilized on the sub-systems and only describes how systems should be coupled. Deriving higher order methods, the efficiency of the methods, potential for parallelism, and their numerical properties will be presented.

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MS67

Performance and Accuracy Implications for Time Integrators Used with Adaptive Mesh Refinement

Adaptive mesh refinement allows for dynamic allocation of resources to improve the accuracy and performance of PDE simulations. However, time integrators tend to use the method of lines as a building block, with lower-order methods dominating most codes. We show that there are benefits of a more holistic space-time discretization approach, where accuracy in space and time are considered together. At the same time, we try to address some of the typical parallel bottlenecks in these algorithms, which can be mitigated by flexibly considering work and communication in both space and time. Solutions range from completely new algorithms to relatively non-intrusive approaches, each with different parallel performance characteristics. We demonstrate these with a few examples: higher-order and parallel in time methods applied to ice sheet modeling with a global time step; a novel multi-rate Runge-Kutta method applied to local time stepping for vortex dynamics; and a very high-order space-time splitting method applied to advection-diffusion systems. In each case, well compare error, efficiency, and speedup for parallel scaling and discuss tradeoffs of each compared to traditional approaches.

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MS67

Low-Synchronization Arnoldi Methods with Application to Exponential Integrators

Higher order exponential integrators require computing linear combination of exponential likeφ(A)-functions of large matricesA. Recent advancements in computational linear algebra allows efficient approximation of theφ-functions by exploiting the equivalence with a linear ordinary differential equation. The resulting adaptive Krylov methods can be very efficient in serial when little or no prior knowledge of the spectrum ofA is available. However, in parallel communication is of paramount importance in the formulation of methods for distributed architectures. The Arnoldi iteration in Krylov subspace methods is a computational bottleneck due to the global communication for normalization and inner products needed at each Arnoldi-step. We aim to improve the scalability of exponential integrators by introducing low-synchronization Arnoldi methods. The resulting orthogonalization algorithm has an accuracy comparable to modified Gram-Schmidt yet better suited for distributed architecture, as there is only one global communication per iteration. We present geophysical based numerical experiments which validate that reducing global communication leads to better parallel scalability and improved performance of exponential integrators for large scale parallel simulations.

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MS68

Consistent Nonlinear Filtering Via Measure Transport

The Bayesian inference step at the core of filtering algorithms is challenging for high-dimensional and non-Gaussian state-space models. While ensemble Kalman filters (EnKF) can yield robust estimates of the state in many practical systems, these methods are limited by linear transformations and are generally inconsistent with the Bayesian solution in the large-sample limit. In this presentation, I will discuss how measure transport can be used to construct couplings that map a prior ensemble into a collection of posterior samples. This approach can be understood as a natural generalization of the EnKF to nonlinear updates, and can reduce the intrinsic bias of the EnKF with a marginal increase in computational cost. In small- sample settings, we show to robustly learn these maps under sparse and low-rank structural assumptions and we demonstrate their benefit for filtering applications in chaotic dynamical systems and turbulent flow estimation.

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MS68

Optimal Bounds on Enhanced Dissiaption for Flows Generated by Certain Random Dynamical Systems

In many situations, the combined effect of advection and diffusion causes enhances dissipation. There are several situations where this is studied and quantified. One situation of interest is when the underlying flows are exponentially mixing. In this case a heuristic argument indicates that enhanced dissipation should be observable on time scales of order $O(|\log\kappa|)$, where κ is the molecular diffusivity. However, in general, one can only prove enhanced dissipation occurs on time scales of order $O(|\log\kappa|^2)$. In this talk we will study a class of random flows for which one can prove enhanced dissipation occurs on time scales of order $O(|\log\kappa|)$. This is joint work with SJ Son and W. Cooperman.

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MS68

Controlling Long-Time Mass Transfer and Energy Dissipation to Obtain Global Solutions in a Micro-Scale Model of Superfluidity

We investigate a micro-scale model of superfluidity derived by Pitaevskii in 1959 to describe the interacting dynamics between the superfluid and normal fluid phases of Helium-4. This system consists of the nonlinear Schrödinger equation and the incompressible, inhomogeneous Navier-Stokes equations, coupled to each other via a bidirectional nonlinear relaxation mechanism. The coupling permits mass/momentum/energy transfer between the phases, and accounts for the conversion of superfluid into normal fluid. We prove the existence of solutions in $\mathbb{T}^d$ $(d = 2, 3)$ for a power-type nonlinearity, beginning from small initial data. Depending upon the strength of the nonlinear self-interactions, we obtain solutions that are global or almost-global in time. The main challenge is to control the inter-phase mass transfer in order to ensure the strict positivity of the normal fluid density, while obtaining time-independent a priori estimates. We compare two different approaches: purely energy based, versus a combination of energy estimates and maximal regularity. The results in this presentation are from recent collaborations with Juhi Jang and Igor Kukavica.

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MS68

Controland Analysis of Long-Time Statistics and Behavior of Fluids Equations

Large-time behavior of Newtonian fluids has been a topic of interest for centuries, relying on the analysis and simulation of the Navier-Stokes equations and their extensions. Recent developments in pure and applied mathematics have investigated the predictability of all kinds of Newtonian fluids whose dynamics are given by these equations from a myriad of perspectives. We will discuss control of various large-time quantities of interest in three broad categories. Firstly, control of relevant quantities atlarge time is used to prove global well-posedness of the relevant PDEs. Secondly, modeling of small-scale features in the turbulent (large-time) regime is achieved via large eddy simulation. The final category is the matching of large-time dynamics between two systems given partial observational data from one of those systems. An important theme will be the importance of the finite-dimensionality of the large-time behavior of the flows under consideration. Open questions will be discussed, and potential future directions in the field will be summarized.

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MS69

Asymptotic Expansions for the Navier-Stokes Equations

We study the three-dimensional Navier-Stokes equations in a periodic domain with the force decaying in time. Although the force has a certain coherent decay, as time tends to infinity, it can be too complicated for the previous theory of asymptotic expansions to be applicable. To deal with this issue, we systematically develop a new theory of asymptotic expansions containing the so-called subordinate variables which can be defined recursively. We apply it to obtain an asymptotic expansion for any Leray-Hopf weak solutions. The expansion, in fact, is constructed explicitly and the impact of the subordinate variables can be clearly specified. The complexifications of the Gevrey-Sobolev spaces, and of the Stokes and bilinear operators of the Navier-Stokes equations are utilized to facilitate such a construction.

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MS69

Velocity-Vorticity Reformulation in Fluid Dynamics: from Navier-Stokes to Mhd

In this talk, we propose the so-called velocity-vorticity-Voigt (VVV) model for the 3D Navier-Stokes system as well as the the Boussinesq systems. We briefly introduce the two fundamental models in fluid dynamics, and the Voigt regularization. Then, we outline the background and motivation of the model. In our work, we add a Voigt regularization term only to the momentum equation in velocity-vorticity formulation without regularizing the vorticity. We prove global well-posedness and regularity of this model along with an energy identity. We also show convergence of the model's velocity and vorticity to their counterparts in the 3D Navier-Stokes equations as the Voigt parameter tends to zero. Similar discussion will be given for the Boussinesq system with thermal fluctuation.

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MS69

Parameter Analysis in Continuous Data Assimilation for the Simplified Bardina Model

In this study, we conduct a parameter estimation on the data assimilation algorithm for the simplified Bardina model. Our approach involves creating an approximate solution for the simplified Bardina model using an interpolant operator derived from observational data of the system. The estimation will depend on the parameter alpha in the model. Some numerical simulation will also be provided.

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MS70

A Microscale Model of Neurotransmitter Diffusion Reveals How Astrocytes May Tune Neural Network Synchrony

Astrocytes are a type of glial cell that constitute 50% of brain volume, with each one wrapping around and ensheathing thousands of synapses. While abundant in the brain, their precise role in regulating synaptic and network dynamics is still under debate. Previous computational models have explored potential mechanisms governing synaptic interactions, focusing on calcium dynamics and neurotransmitter diffusion at the microscale. However, since it is computationally infeasible to include such intricate details in a network-scale mode, it has been challenging to investigate how these mechanisms enable astrocytes to influence spiking patterns and synchronization in larger networks. To address this challenge, we introduce an ”effective” astrocyte model that can be easily integrated into existing network frameworks. We demonstrate that the proximity of an astrocyte to a synapse makes synaptic transmission faster and weaker. Thus, our ”effective” astrocytes can be incorporated into spiking models by considering heterogeneous synaptic time constants, which are parametrized only by the degree of astrocytic proximity at that synapse. We apply this framework to a network of exponential integrate-and-fire neurons and show that astrocytes can drive the network towards synchronous activity and generate spatially correlated patterns, depending on factors such as the number of ensheathed synapses and the strength of ensheathment.

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MS70

Modeling Mechanisms of Microtubule Dynamics and Polarity in Neurons

In neurons, the polarity and stability of the microtubule cytoskeleton is required for long-range, sustained intracellular transport of cargo such as proteins and mRNA. In fruit fly neurons, the healthy microtubule cytoskeleton has a specific polarity, where depending on the region of the neuron, the microtubules are either all minus-end out or all plus-end out. However, these microtubules are dynamic and rearrange their orientation in the event of an injury. It is unknown how these mechanisms can maintain both dynamic rearrangement and sustained function. To better understand these mechanisms, we introduce a spatially-explicit mathematical model of microtubule growth and polarity using parameters informed by experimental data. We implement several mechanisms that control microtubule length using both a stochastic model and a continuous model, and validate such mechanisms with experimental data. In turn, we will discuss how the microtubule growth mechanisms can impact the overall polarity of the microtubule cytoskeleton, where we seek to understand how polarity can be maintained in healthy cells.

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MS70

Fast Intermittent Search Processes for Transcriptional Regulation

Many cellular processes rely on intricate temporal coordination to precisely regulate molecular events, such as neurotransmitter release, heart rhythmicity, and embryonic cell division. The apparent contradiction between the random molecular motion within cells and the observed temporal precision of cellular processes has intrigued molecular biologists for decades. One illustrative example of such processes is the widely-accepted mechanism for gene-regulation known as facilitated diffusion. In this process, transcription-factor (TF) proteins rapidly “search expansive DNA regions to bind to specific target sequences to consequently activate or inhibit gene transcription. Experimental observations indicate TF-DNA reaction events occur on the order of seconds, despite the outstanding difference in scale between a single TF protein and the vast domain of DNA through which it searches. In this talk, we employ stochastic modeling to investigate the facilitated diffusion mechanism, offering a resolution to discrepancies between prior models and experimentally-observed dynamics. Our model features a multiple-protein search process with time-delayed stochastic resetting events, and we analyze the “many-searcher asymptotic behavior of the extreme mean first passage time to DNA-binding for experimentally-informed parameter values. Our results provide a holistic interpretation of facilitated diffusion without introducing excessive biological complexity.

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MS70

Quantifying Microscopic Models of Biological Pattern Formation in Time

Pattern formation is present at many scales in biology, and here I will focus on the patterns formed by brightly colored pigment cells in zebrafish skin. Zebrafish are named for their dark and light stripes, but mutant fish feature other skin patterns, including spots and labyrinth curves. All of these patterns form as the fish grow due to the interactions of tens of thousands of pigment cells, making agent-based modeling a natural approach for describing pattern formation. Microscopic modeling involves many choices beyond specifying agent interactions and setting parameter values, such as deciding whether to implement cell behavior on or off lattice and to update agents synchronously or non-synchronously. Because comparing simulated patterns and biological images is often a qualitative process, this makes it challenging to broadly characterize the output of agent-based models and identify the role of modeling choices in predictions. To help address this challenge, here I will show how to apply methods from topological data analysis to quantify cell-based, time-dynamic systems.

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MS71

Nonlocal Approximations of Optimal Transport and Diffusion

Given a desired target distribution and an initial guess of its samples, what is the best way to evolve the locations of the samples so that they accurately represent the desired distribution? A classical solution to this problem is to evolve the samples according to Langevin dynamics, a stochastic particle method for the Fokker-Planck equation. In todays talk, I will contrast this classical approach with two novel deterministic approaches based on nonlocal particle methods: (1) a nonlocal approximation of dynamic optimal transport, with state and control constraints, and (2) a nonlocal approximation of general nonlinear diffusion equations. I will present recent work analyzing the convergence properties of each method, alongside numerical examples illustrating their behavior in practice. This is based on joint works with Karthik Elamvazhuthi, Matt Haberland, Matt Jacobs, Harlin Lee,and Olga Turanova.

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MS71

Fourier-Based Bounds for Wasserstein Distances and Their Applications in Data-Driven Problems

Optimal transport theory has gained substantial attention in the deep learning community, demonstrating promising outcomes in both theoretical frameworks and practical applications. Grounded in mathematics, optimal transport assumes a crucial role in diverse deep learning applications, including sampling, generation tasks, classification tasks, adversarial training, and domain adaptation, among others. The minisymposium aims to unite junior and senior researchers contributing to the intersection of optimal transport and deep learning, addressing both theoretical advancements and algorithmic developments.

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MS71

Monotone Generative Adversarial Network with a Geometry-Preserving Embedding Mapping

Generative Adversarial Networks (GANs) are powerful tools for creating new content, but they face challenges such as sensitivity to hyperparameter tuning and mode collapse. Existing strategies partially address these issues but may require careful architecture selection and empirical tuning. To address these issues, we propose a deep generative model that utilizes the Gromov-Monge embedding (GME). Our model identifies the low-dimensional structure of the underlying measure of the data and maps it into a measure in a low-dimensional latent space, which is then optimally transported to the reference measure. We guarantee that GME preserves the underlying geometry of the data. Furthermore, we show that the induced generative map exhibits c-cyclical monotonicity, where c is an intrinsic embedding cost employed by GME. This property lays the groundwork for better robustness to parameter initialization and mode collapse. Numerical experiments demonstrate the effectiveness of our approach in generating high-quality images, exhibiting robustness to hyperparameters and avoiding mode collapse.

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MS71

Enhancing Score-Based Generative Models Through Wasserstein Proximal Operator

In this presentation, I will discuss the essence of score-based generative models (SGMs) as entropically regularized Wasserstein proximal operators (WPO) for cross-entropy, elucidating this connection through mean-field games (MFG). The unique structure of SGM-MFG allows the HJB equation alone to characterize SGMs, demonstrated to be equivalent to an uncontrolled Fokker-Planck equation via a Cole-Hopf transform. Furthermore, leveraging the mathematical framework, we introduce an interpretable kernel-based model for the score functions, enhancing the performance of SGMs in terms of training samples and training time. The mathematical formulation of the new kernel-based models, in conjunction with the utilization of the terminal condition of the MFG, unveils novel insights into the manifold learning and generalization properties of SGMs.

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MS72

Novel Topological Measures of Multi-Chain Complexity in Biopolymers

Biopolymers live in crowded environments where they attain complex 3 dimensional conformations that are related to their sequence and function. To characterize the multi-component structure of biopolymers we employ methods from topology. A new framework in knot theory was introduced recently that enables one to characterize the complexity of collections of open curves in 3-space using the theory of knotoids and linkoids, which are equivalence classes of diagrams with open arcs. This gives rise to a collection of novel measures of entanglement of open curves in 3-space, which are continuous functions of the curve coordinates and tend to their corresponding classical invariants when the endpoints of the curves tend to coincide. In this talk, we show how knot theoretic measures, such as the Jones polynomial can be used to distinguish between systems of biopolymers and quantify the net entanglement present in such systems that is relevant to their function.

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MS72

Differential Geometry and Graph Theory-Based Machine-Learning Model for Drug Development

The fundamental step in the drug design and discovery process is understanding and accurately predicting the binding affinity between a drug candidate (ligand) and its receptor protein. Machine learning-based methods have become increasingly popular in this regard due to their efficiency and accuracy, as well as the growing availability of data on the structure and binding affinity of protein-ligand complexes. In mo-lecular and biomolecular studies, differential geometry and graph theory are widely used to analyze vast, diverse, and complex datasets. Using molecular surface representation, crucial chemical and biological data can be encoded in differentiable manifolds that can reduce dimensionality. Graph theory is extensively used in biomolecular research because molecules or molecular complexes can be naturally modeled as graphs where graph vertices typically represent atoms and graph edges represent possible interactions. Here, I will present several models based on differential geometry and graph theory that can be combined with advanced machine learning techniques to predict protein-ligand binding affinity with high accuracy. Our proposed models have demonstrated superior performance compared to numerous state-of-the-art models on established benchmark datasets.

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MS72

Computational Topology and Machine Learning: Discovering Sars-CoV-2 Evolution and Trans-Mission

In the fight against SARS-CoV-2, the rapid evolution of the virus presents a significant challenge for vaccine and antibody drug development. Frequent mutations across the virus's genome necessitate a swift and accurate understanding of their impacts, a task that proves both time-intensive and costly for traditional wet lab approaches. This talk delves into the innovative use of Computational Topology and Ma-chine Learning as powerful tools in this battle. Specifically, I will explore their role in predicting the bind-ing free energy (BFE) changes caused by mutations in the interaction between the virus's Spike protein and the human ACE2 receptor or antibodies. Such computational methods offer a faster, cost-effective alternative to traditional methods, enabling a deeper understanding of mutation-induced changes in infectivity and the effectiveness of antibody treatments. This research opens new pathways for the design of more precise and potent vaccines and antibody treatments, offering a glimpse into a future where technology and biology converge to combat viral threats more effectively

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MS73

Simulating Strongly Magnetized Charged Particle Dynamics by Nyström Type Exponential Integration

The main component of particle-in-cell (PIC) methods widely employed in plasma physics simulations is solution of a particle pushing problem. It is the model of a charged particle moving under the influence of electromagnetic fields which has to be solved for very large numbers of particles in PIC codes. When the plasma is strongly magnetized, this problem is computationally challenging due numerical stiffness arising from the wide disparity in time scales between fast scale, highly oscillatory gyromotion and slow scale, macroscopic behavior of the system. We explored an alternative to numerical particle pushing using exponential integration techniques that solve linear problems exactly, are capable of yielding oscillatory solutions, and are A-stable. In particular, we developed Nyström-type exponential integrators that exploit the mathematical structure of the Newtonian equations of motion. Our numerical experiments show that these exponential integrators yield computational savings compared to such widely used fast schemes as Boris and Buneman. Moreover, while Boris is known to artificially enlarge gyroradius when stepping over the gyroperiod for linear problems, the new exponential schemes preserve gyroradius accurately even with step sizes far exceeding the gyroperiod. We discuss the advantages of the new exponential schemes for particle pushing problems and outline research directions for further possible improvements to the methods.

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MS73

Approximation of the First P-Laplace Eigenpair on Surfaces

The p-Laplace operator appears in variety of applications including image processing, optimal transport, and distance approximation. We approximate the first eigenpair of the p-Laplace operator with zero Dirichlet boundary conditions using a surface 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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MS73

A Candidate Framework for Structure-Preserving Discretizations

In this talk, we present a possible general approach to structure-preserving discretizations and use it to study the approximation of differential structures defined by derivations. We determine the proper general setting in which one can expect convergence. It turns out that structure-preserving discretizations and their limits involving infinite dimensional operators should be looked through the lens of C^*-algebras. Indeed, it is only when a discretization is interpreted as a deformed structure from a C^*-algebra that one can understand the precise nature of the finite dimensional approximation and its limit as $n \to +\infty$. In fact, we show how the Berezin-Toeplitz quantization fits in naturally as a structure-preserving discretization of a differential algebra.

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MS73

Fully Discrete Energy Conserving and Entropy Dis-

sipative Particle Method for the Landau Equation

At the semi-discrete level, the recently proposed particle method to the Landau equation by Carrillo et al. conserves mass, momentum, energy, and has a decaying entropy. When this method is coupled with the standard time discretization such as forward Euler, not all the above properties can be maintained. In this work, we show that using a properly designed discrete gradient method, conservation of mass, momentum and energy along with the decay of entropy are guaranteed at the fully discrete level. Several numerical examples are given to validate these results.

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MS74

Solving Navier Stokes with Mimetic Operators

We present a new scheme for solving NavierStokes equations using mimetic difference operators. These operators can be constructed to high orders of accuracy and maintain the physical properties of the problem under consideration. We demonstrate the effectiveness of our scheme by modeling a lock release in 3D Cartesian coordinates, then extend our techniques to 3D curvilinear grids. The resulting scheme allows for simple and efficient computation of fluid processes on curvilinear grids, which allows us to solve problems in more complex regions while minimizing the restrictions of finite difference methods.

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MS74

Enhanced Parallel Solution of Diffusion-Like Problems in Two-Dimensions using UPC++ and MOLE

Solving diffusion-like problems is essential in various scientific and engineering applications. In this work, we present an innovative approach that leverages the power of UPC++ distributed objects and the Mimetic Operators Library Enhanced (MOLE) to efficiently address such problems. Our methodology combines the parallelism capabilities of UPC++ with MOLE's mimetic operators to approximate solutions to diffusion-like problems, showcasing a significant advancement in computational science. Through UPC++, we partition the domain into smaller, manageable regions, optimizing the use of available resources and achieving high-performance scalability. MOLE enhances the precision of our solution by ensuring that discretization maintains mathematical properties, improving accuracy, and simplifying boundary condition implementation. This study exemplifies the seamless integration of UPC++ and MOLE, highlighting their capacity to efficiently address real-world scientific and engineering challenges while laying the groundwork for continued progress in computational science.

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MS74

Mass Conservation of Mimetic Difference Schemes for Systems of Conservation Laws

Mimetic Differences tried to replicate in a discrete version properties of the continuum PDE solution, among them symmetries, conservation laws and others. In this talk the conservation of mass for systems of conservation laws is demonstrated and some numerical examples are given.

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MS74

A Mimetic-Machine Learning Framework For Turbulence Modeling Of The Burgers Equation

The modeling of the subgrid scale stress tensor closure term for turbulent flows is a challenge and is an area of active research. The underlying partial differential equations for turbulent flows contain nonlinear convective terms which can lead to aliasing errors, and requires special attention for spatial discretization. The mimetic methods are based on mimicking the fundamental vector calculus identities of div and grad, and possess a discrete equivalent of a global conservation law, thereby leading to accurate discretizations of the nonlinear convective terms. In this work, a machine learning based mimetic framework is proposed to uncover the subgrid scale stress tensor terms for modeling turbulence of the Burgers equation (i.e., Burgulence modeling). The one-dimensional nonlinear Burgers equation is used to evaluate the subgrid scale turbulence model of large eddy simulations. The numerical solution of the Burgers equation capturing all scales of motion is evaluated using direct numerical simulations (DNS) by implementing the high order Corbino-Castillo mimetic operators, along with the third order Runge Kutta temporal scheme. The filtered-DNS velocity profiles are then used as the ground truth in a priori testing for training a neural network to uncover turbulence modeling using a data-driven framework

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MS80

Probabilistic Measures for Ecological Resilience Through Adaptation

We propose an approach to quantifying ecological resilience, particularly focusing on noisy systems responding to episodic environmental disturbances with sudden physiological adaptations. Randomness plays a key role, accounting for model uncertainty and the inherent variability in the dynamical response among components of biological systems. Our measure of resilience is rooted in the probabilistic description of states within these systems, and is defined in terms of the dynamics of the ensemble average of a model-specific observable quantifying success or well-being. Our approach utilizes stochastic linear response theory to compute how the expected success of a system, originally in statistical equilibrium, dynamically changes in response to a environmental perturbation and a subsequent adaptation. The resulting mathematical derivations allow for the estimation of resilience in terms of ensemble averages of simulated or experimental data. Finally, through a simple but clear conceptual example, we illustrate how our resilience measure can be interpreted and compared to other existing frameworks in the literature.

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MS81

The Mean-Field Ensemble Kalman Filter: From Analysis to Algorithms

The ensemble Kalman methodology is an innovative and flexible set of tools which can be used for both state estimation in dynamical systems and parameter estimation for generic inverse problems. It has primarily been developed by practitioners in the geophysical sciences, yet, despite its widespread adoption in fields of application, firm theoretical foundations are only now starting to emerge. We consider a unifying approach to algorithms that rests on transport of measures and mean-field stochastic dynamical systems. The ensemble Kalman methods as implemented in practice rely on projections onto the space of Gaussian measures and particle approximations. With the goal of developing theoretical guarantees for the ensemble Kalman methodology applied to non-linear problems, we discuss the error analysis of the mean-field stochastic dynamical systems arising in ensemble Kalman filtering, along with Gaussian and particle approximations.

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MS81

Optimal Eddy Viscosity in Closure Models for Turbulent Flows

In this talk, we consider the question of fundamental limitations on the performance of eddy-viscosity closure models for turbulent flows, focusing on the Leith model for 2D Large-Eddy Simulation. Optimal eddy viscosities depending on the magnitude of the vorticity gradient are determined subject to minimum assumptions by solving PDE-constrained optimization problems defined such that the corresponding optimal Large-Eddy Simulation best matches the Direct Numerical Simulation. The main finding is that with a fixed cutoff wavenumber kc, the performance of the Large-Eddy Simulation systematically improves as the regularization in the solution of the optimization problem is reduced and this is achieved with the optimal eddy viscosities exhibiting increasingly irregular behavior with rapid oscillations. Since the optimal eddy viscosities do not converge to a well-defined limit as the regularization vanishes, we conclude that the problem of finding an optimal eddy viscosity does not in fact have a solution and is thus ill-posed. Moreover, while better behaved and hence practically more useful eddy viscosities can be obtained with stronger regularization, the corresponding Large-Eddy Simulations will not achieve their theoretical performance limits.

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MS81

Data Assimilation of the Navier-Stokes Equations Via Les with Observable Data

Integrating data assimilation with turbulence models presents a logical approach, yet it encounters immediate challenges. This is primarily due to the fact that observational data does not directly align with the model itself but rather with the underlying physical model, namely the Navier-Stokes Equations. In this talk, we will address and thoroughly investigate the mismatches between observational data and a turbulence model.

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MS81

Reduced-Order Models for Data Assimilation and Control of Multiscale Turbulent 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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MS83

True Random Number Generation Using Magnetic Tunnel Junctions in Dynamically Tuned Probability Trees

Perpendicular magnetic tunnel junction (pMTJ)-based true-random number generators (RNG) consume orders of magnitude less energy per bit than CMOS pseudo-RNG. We numerically investigate with a macrospin Landau-Lifshitz-Gilbert equation solver the use of pMTJs driven by spin-orbit torque to directly sample numbers from arbitrary probability distributions with the help of a tunable probability tree. The tree operates by dynamically biasing sequences of pMTJ relaxation events, called coinflips, via an additional applied spin-transfer-torque current. Using a single, ideal pMTJ device we successfully draw exponentially-distributed integer samples on the interval [0,255] based on p-value analysis. To investigate device-to-device variations, the thermal stability of the pMTJs are varied within manufacturing tolerances. We find that while repeatedly using a varied device inhibits ability to recover the probability distribution, the device variations average out when considering the entire set of devices as a bucket to draw random numbers from. Further, it is noted that the device variations most significantly impact the highest level of the probability tree, with diminishing errors at lower levels. The devices are then used to draw both uniformly and exponentially distributed numbers for the Monte Carlo computation of a problem from particle transport, showing excellent data fit with the analytical solution. Finally, the devices are benchmarked against CMOS and memristor RNG.

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MS83

Real-Time Analysis of Stochastic Bitstreams from Discrete Tunnel Diodes

Despite the generative capabilities of humans, we are limited in our ability to generate random numbers. When listing random numbers, one is predisposed to think of numbers that follow a pattern, creating trends or periodicity in the string. When faced with the same task, computers have similar difficulties. Pseudo random number generators (PRNGs) create strings that are seemingly random but are limited in length, deterministic, and predictable. Increasing randomness requires more hardware and complex algorithms that consume a lot of computational resources. True Random Number Generators (TRNGs) are therefore important for decreasing computational costs. TRNGs distill noise or inherently stochastic physical processes into bitstreams with a specific distribution. However, it is difficult to determine when a TRNG is truly random or if it has some dependence on a deterministic or predictable process that will limit its usefulness in important workloads, such as the simulation of particle accelerator physics. We will examine methods of analyzing bitstreams generated through operation of tunnel diodes as coinflip devices, stochastically producing high or low logic values. Through a series of statistically motivated tests, we can determine the quality of a bitstream as well as the dependence of tunnel diode outputs on previous outputs, proximally located tunnel diodes, or factors such as temperature. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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MS85

Optimal Algorithms for Large-Scale Elastic Shape Analysis

Shape analysis is a fundamental area of computer vision, critical to object recognition, classification, shape retrieval. Central to shape analysis is the definition of a shape space and efficient algorithms to compute the distance between the shape representations residing in the shape space. In this work, we adopt the square-root velocity functions (SRVF) of Srivastava et al. (PAMI, 2011) as the shape representation, and develop efficient optimization algorithms to compute the shape distance between 2d outlines/boundaries of objects. The shape distance computation is formulated as a high-dimensional minimization problem, in which the free variables are the starting point, the rotation angle, and the reparameterization function for optimal elastic matching of the SRVFs of the object boundaries. To solve this problem, we introduce compact discretizations of boundary curves, then develop novel optimization algorithms, by building on efficient solutions for the subproblems, i.e. FFT-based rigid alignment, linear-time dynamic programming and iterative optimization for reparameterization. We integrate these in a global optimization framework and obtain efficient algorithms that compute strong minima. We demonstrate their effectiveness with extensive numerical experiments, and find significant improvements compared to previous approaches. These enable an order of magnitude increase in size for large-scale analysis of shape datasets.

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MS85

Identifying Differential Equations with Weak Form and Frequency Domain

We consider identifying differential equation from one set of noisy observation. We assume that the governing equation can be expressed as a linear combination of different linear and nonlinear differential terms. This talk will discuss using weak form for ODE and PDE recovery and how identifying differential equation can be directly done in the Fourier domain. Fourier Ident shows robustness against complex dynamics and higher level of noise.

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MS85

Discrete Morse Theory, Persistent Homology and Forman-Ricci Curvature

It was observed experimentally that Persistent Homology of networks and hypernetworks schemes based on Forman's discrete Morse Theory and on the 1-dimensional version of Forman's Ricci curvature not only both perform well, but they also produce practically identical results. We show that this apparently paradoxical fact can be easily explained in terms of Banchoff's discrete Morse Theory. This allows us to prove that there exists a curvature-based, efficient Persistent Homology scheme for networks and hypernetworks. Moreover, we show that the proposed method can be broadened to include more general types of networks, by using Bloch's extension of Banchoff's work. We also point out a manner in which one can canonically associate a simplicial complex structure to a hypernetwork, directed or undirected. In particular, this allows for the extension and simplification of the geometric Persistent Homology methods of networks. Furthermore, such a construction allows for an easy investigation of the topological and geometric properties of hypergraphs.

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MS86

Convergence Rates for Deterministic Versions of Score Matching

Score matching is a popular method for generating new data from an unknown distribution given some samples. Score matching typically runs a stochastic differential equation on the sample particles and then uses the estimated score function to simulate the reverse process. Controlling the error between the unknown distribution and the result of the reverse process is extremely challenging, and often requires making assumptions that are unrealistic for applications. In this talk, I will consider a deterministic version of score matching, where the initial particles are evolved along the flow of a deterministic PDE (essentially the Porous Media Equation). An estimate of the velocity field along the flow is used to simulate the reverse process (by solving a continuity equation). Using recent results on Lagrangian flows for the Porous Media equation, we will give a bound on the error between the unknown distribution and the solution of the reversed flow at initial time in the Wasserstein distance. This gives a more natural control on the error compared to KL divergence bounds that are typically obtained in the stochastic case.

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MS86

Digital Computer Break the Curse of Dimensionality: Insights from Finite Geometry

Many of the foundations of machine learning rely on the idealized premise that all input and output spaces are infinite, e.g. $\mathbb{R}^d$. This core assumption is systematically violated in practice due to digital computing limitations from finite machine precision, rounding, and limited RAM. In short, digital computers operate on finite grids in $\mathbb{R}^d$. By exploiting these discrete structures, we show the curse of dimensionality in statistical learning is systematically broken when models are implemented on real computers. Consequentially, we obtain new generalization bounds with dimension-free rates for kernel and deep ReLU MLP regressors, which are implemented on real-world machines. Our results are derived using a new non-asymptotic concentration of measure result between a probability measure over any finite metric space and its empirical version associated with N i.i.d. samples when measured in the 1-Wasserstein distance. Unlike standard concentration of measure results, the concentration rates in our bounds do not hold uniformly for all sample sizes N; instead, our rates can adapt to any given N. This yields significantly tighter bounds for realistic sample sizes while achieving the optimal worst-case rate of $\mathcal{O}(1/N^{1/2})$ for massive. Our results are built on new techniques combining metric embedding theory with optimal transport.

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MS86

Probabilistic Takens Embedding Through the Wasserstein Tangent Space

In the theory of dynamical systems, Takens embedding theorem allows the reconstruction of the true underlying attractor from time series data with missing states. In particular, it proves that an embedding map exists between the two, which comes from the time delay of an observable. However, data measurements are often polluted by noise. Hence, we shift the paradigm from Lagrangian to Eulerian by looking at probability densities in the Wasserstein spaces and gradient flows. In this work, we generalize the Takens embedding theorem to the Eulerian framework by considering an embedding between Wasserstein spaces. We show that the classic delay embedding map as a push-forward map provides an embedding between Wasserstein spaces. We present theoretical guarantees for reconstructing the attractor from noisy data and when the dynamics are inherently stochastic. Moreover, the weaker condition we impose when learning the delay embedding map can help improve the algorithms stability.

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MS86

Optimal Transport Embeddings for Machine Learning

Modern machine learning techniques have evolved into a practical discipline enabling numerous advances in data analysis. Despite recent advances, difficulties with interpretability, stability, need for large training datasets, robustness to out of distribution examples, high computational and energy costs, remain. In this talk I will explain that in certain problems related to signal and image analysis and classification these difficulties can be ameliorated by adopting a physics-based model for how data classes are generated. We will explain a set of mathematical techniques for representing input data that can convexify input data classes and makes it possible to solve the classification problem using simple (e.g. linear) machine learning techniques. Based on the mathematics of optimal transport, the new representation techniques can be viewed as invertible transforms (representations, embeddings) for signal and image data. They have well-defined mathematical techniques and can convexify data classes emanating from certain physical situations. Computational examples relating to the classification of diverse signal and image databases, and comparison to other deep learning techniques, show these emerging transport representations/embeddings can classify data with the same or better accuracy but with significant benefits in terms of lower computational complexity, needing less training data, robustness to out of distribution examples, and interpretability.

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MS87

Thermo-Hydraulic-Mechanical Fracture Propagation by Employing Phase Field Approach

This work establishes a thermo-hydraulic-mechanical (THM) model for fracture propagation by utilizing a phase-field approach. The fluid-filled phase-field fractures (PFF) in porous media are solved with both physics-based discretizations and physics-based numerical solvers. In THM-PFF, four solution variables are of interest, namely displacements, phase-field, pressure, and temperature, which are determined by a vector-valued mechanics problem, a phase-field variational inequality, and scalar-valued pressure and temperature problems, respectively. The resulting overall problem is a coupled variational inequality system. The solution algorithm is based on an extension of the well-known fixed-stress algorithm in which displacements-phase-field, pressures, and temperatures are solved sequentially. The displacement-phase-field is solved in a quasi-monolithic fashion. For local mass conservation enriched Galerkin finite elements are employed for the pressure equation and similarly for the temperature equation. Local mesh adaptivity allows for small phase-field length-scale parameters and sufficient numerical accuracy while keeping the computational cost reasonable. Our new model and algorithmic developments have been substantiated with numerical tests.

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MS87

High-order Methods for Acoustic Wave Propagation

In this talk, we will present high-order methods for simulating acoustic wave propagation. The methods will combine high-order implicit time integrators with Fourier pseudospectral spatial approximations, aiming to resolve the dispersion errors with low sampling density. A modified Helmholtz equation will need to be solved at each time step, and will be solved efficiently by a well-designed iterative functional evalution method. Numerical examples will be presented to demonstrate the methods.

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MS87

Adaptivity for Computing Modes of Microstructured Optical Fibers and Their Confinement Losses

This paper presents the application of adaptivity techniques in the Finite Element Method (FEM) in the setting of microstructured fibers. Our goal is to compute the modes of different optical fibers of interest. It is of particular interest to capture the fine and highly oscillatory behavior of these modes on the fibers correctly. We discretize the time-harmonic hybrid Maxwell equations and employ the FEAST algorithm to solve the eigenvalue problem and we use the Dual Weighted Residual (DWR) error estimators for the adaptivity procedural. Our results display that the method captures the subtle oscillatory behavior present in the modes, that concentrate in specific portions of the different geometries of the fibers. We conclude this technique can be implemented in different geometries.

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MS88

A Unified Framework for the Analysis of Accuracy and Stability of a Class of Approximate Gaussian Filters for the Navier-Stokes Equations

Bayesian state estimation of a dynamical system utilising a stream of noisy measurements is important in many geophysical and engineering applications. We develop a unified framework for the analysis of several well-known and empirically efficient data assimilation (DA) techniques derived from various Gaussian approximations of the Bayesian filtering schemes for geophysical-type (infinite-dimensional) dissipative dynamics with quadratic nonlinearities. In particular, we consider the model dynamics governed by the two-dimensional incompressible Navier-Stokes equations and observations given by noisy measurements of averaged volume elements or spectral/modal observations of the velocity field. The DA algorithms include the Ensemble Kalman Filter (EnKF) and Ensemble Square Root Kalman Filter (EnSRKF). We establish rigorous results on (time-asymptotic) accuracy and stability of these algorithms with general covariance and observation operators. The derived bounds are given for the limit supremum of the expected value of the L^2 norm and of the $\mathbb{H}^1$ Sobolev norm of the difference between the approximating solution and the actual solution as the time tends to infinity. Our analysis reveals an interplay between the resolution of the observations associated with the observation operator underlying the DA algorithms and covariance inflation and localization which are employed in practice for improved filter performance.

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MS88

An Exact and Fully Nonlinear Generalization of the

Kalman Filter

The majority of data assimilation (DA) methods in the geosciences are based on Gaussian assumptions. While such approximations facilitate efficient algorithms, they cause analysis biases and subsequent forecast degradations. Non-parametric, particle-based DA algorithms have superior accuracy, but their application to high-dimensional models still poses operational challenges. Drawing inspiration from recent advances in the field of generative artificial intelligence (AI), this paper develops a new estimation theory which attempts to bridge the existing gap in DA methodology. Specifically, a Conjugate Transform Filter (CTF) is derived and shown to completely generalize the celebrated Kalman filter to arbitrarily non-Gaussian distributions. The new filter has several desirable properties, such as its ability to preserve statistical relationships in the prior state and convergence to highly accurate observations. An ensemble approximation of the new theory (ECTF) is also presented and validated through idealized statistical experiments. The numerical examples feature bounded quantities with non-Gaussian distributions, which is a typical challenge in Earth system models. Results indicate that the greatest benefits from ECTF occur when observation errors are small relative to the forecast uncertainty and when state variables exhibit strong nonlinear dependencies.

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MT1

Optimal Transport and Applications in Particle Physics and Machine Learning

This tutorial will provide background on the mathematical foundations of optimal transport and discuss applications to jet classification in high energy particle physics and machine learning.

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MT2

Mathematical Contributions to Weather and Climate Modelling

”Model hierarchies” will review reduced dynamical models which encapsulate essential physical feedbacks within the climate system, and have served as indispensable guardrails for building intuition and developing qualitative theoretical insights in this field.

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MT2

Mathematical Contributions to Weather and Climate Modelling Part 2

”Asymptotics for geophysical flows” systematizes this rich zoo of models from a unified mathematical perspective. By leveraging the power of multiscale techniques, detailed explanations of scale interactions emerge and quantitative accuracy becomes possible.

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MT3

Mathematical Contributions to Weather and Climate Modelling Part 4

”The role of data” addresses the all-important role of observational data in weather fore- casting and climate modelling and the related topics of data assimilation and data-based modelling.

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MT3

Mathematical Contributions to Weather and Climate Modelling Part 3

”PDE theory for atmosphere-ocean flows” summarizes selected rigorous results on some important geophysical flow models, such as the Boussinesq, anelastic/pseudo-incompressible, hydrostatic primitive, and quasi-geostropic equations.

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MP1

Choice of Model Error Covariances for Data Assimilation with the Transport Equation

The transport equation is used in the study of wildfire smoke transport. While it provides a strong foundation for estimating PM2.5 concentrations in wildfire smoke, modeling wildfire emissions poses challenges. Therefore, we assume the transport equation is inexact and employ weak constraint four-dimensional data assimilation to assimilate data and update PM2.5 concentration estimates. The choice of data and model error covariances significantly influence these estimates. We, therefore, use regularization methods to estimate these covariances.

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MP1

Sex Differences in Glutathione Metabolism and Their Consequences

Experiments show that females have higher glutathione (GSH) levels than males, which are caused by higher levels of estradiol. Understanding how hepatic GSH levels depend on estradiol is important since oxidative stress contributes to certain diseases, and oxidative stress is reduced by GSH. We use mathematical modeling to explain the causes of GSH differences in males and females and analyze the remarkable stability of GSH that arises during the menstrual cycle.

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MP1

An Inertial Iterative Scheme for Solving Variational Inclusion Problems with Applications

Developing iterative schemes for variational inclusion problems (VIP) is a dynamic research field. This presentation provides an overview of current VIP resolution algorithms. We introduce an efficient Mann-type algorithm with inertial extrapolation terms and selfadaptive step sizes, enhancing convergence without stringent conditions. The presented version is flexible, with easily implementable criteria for the inertial factor and relaxation parameter. Numerical experiments illustrate the practical implementation and performance of the proposed algorithm.

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MP1

Piecewise Smooth Solutions to Scalar Balance Laws with Singular Source Terms

We will present a local well-posed result for piecewise regular solutions with a single shock of scalar balance laws, with singular integral of convolution type kernels. In a neighborhood of the shock curve, a description of the solution is provided for a general class of initial data.

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MP1

Directional Derivative of Kemeny's Constant

In a connected graph G, Kemeny's constant gives the expected time for a random walk from an arbitrary vertex x to reach a randomly-chosen vertex y. Kemeny's constant is a measure of how well a graph is connected, and it is unknown how the addition or removal of edges will affect Kemeny's constant. Inspired by using the directional derivative of the normalized Laplacian as a centrality measure, we derive the directional derivative of Kemeny's constant for several graph families in this presentation. In addition, we find sharp bounds for the directional derivative of an eigenvalue of the normalized Laplacian and for the directional derivative of Kemeny's constant. We end with a discussion of some fun examples and pose some problems for future exploration. This is joint work with C. Albright, A. Holcombe Pomerance, J. Jeffries, K. Lorenzen, and A. Nix.

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MP1

Improving Digital Subtraction Angiography (dsa) Image Segmentation with Cnns

This poster introduces an innovative method for the segmentation of DSAimages, a critical task in medical image analysis. Using Convolutional Neural Networks (CNNs), our approach employs an iterative process to expand segmented regions in growing directions. A CNN predicts class probability scores within a small pixel neighborhood, determining pixel inclusion based on a threshold. The process continues iteratively until no new pixels qualify for inclusion. Our method achieves remarkable segmentation accuracy while preserving biological features.

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MP1

Automatic Complexity and Quantum Logic over Finite Fields

The automatic complexity of finite words was introduced by Shallit and Wang (2001). It measures the complexity of a word x as the minimum number of states of a finite automaton that uniquely accepts x. Here, an automaton M uniquely accepts a word x if x is the only word of length $|x|$ accepted by M. Via the digraph representation of automata we can view the computation of this number of states as a problem of extremal graph theory. A quantum version of automatic complexity was studied by Kjos-Hanssen (2017). We explore a finite field analogue of quantum automatic complexity, with particular attention to the subspace structure of the automata and the associated quantum logic.

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MP1

Sensitivity Analysis of a Permafrost Model Responding to Surface Temperature Variations in Variable Topography

We consider a computational model for energy equation in permafrost soils extending [Bigler, Peszynska, Vohra, 2022] using data and constitutive parameters from [Ling, Zhang' 2003]. Our focus is on the dependence of model results on several model parameters including the thermal conductivity, volumetric heat capacity, and the dependence of surface boundary conditions on the albedo which varies in various regions such as (lake, snow, vegetation, wildfire-affected vegetation). Next, we evaluate the response of the model to these parameters. To this end, we set up the sensitivity equation as well as Sobol indices sensitivity framework. Our results allow to assess the robustness of our computational model as well as to understand the uncertainty associated with the parameters and the model itself. Our simulations and analyses help to determine the response of the soils in the Arctic to the changing climate and to assess the reliability of the model.

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MP1

Parallel Recursive Skeletonization Solver for Dense Linear Systems on Gpu-Accelerated Computers

The dense linear systems in large-scale kernel approximation in machine learning, low-rank Schur complements of a large sparse matrix factorization, and discretization of boundary integral equations in physics and engineering often employ a multilevel structure of lowrank off-diagonal blocks. To solve such large systems efficiently, we present a GPU-based parallel recursive skeletonization solver utilizing batched dense linear algebra to allow for adjustable precision and achieve a linear rate with the matrix size given fixed ranks.

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MP1

From Observations to Theoretical Consistency: Decoder Recovery in Coded Aperture Imaging

Coded aperture imaging, crucial for low-light imaging in challenging conditions, requires specific decoders for image reconstruction. Our work introduces a one-layer CNN network for interpretable decoder recovery, without prior knowledge of encoding or decoding arrays. Using observed detector images, the network produces reconstructed images using a learned decoder. Promising results indicate the adaptability of the learned decoder to diverse encoded datasets, ensuring enhanced generalizability for coded aperture imaging applications in line with theoretical expectations.

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MP1

A Second-Order Partitioned Method for Fluid-Poroelastic Structure Interaction

This work focuses on the development of a novel, strongly-coupled partitioned method for fluid-poroelastic structure interaction. The time-dependent Stokes equations describe the fluid flow, and the Biot model describes the poroelastic material. A partitioned numerical method based on Robin interface conditions was developed, combined with the refactorization of Cauchys one-legged ?-like method. We prove the method is stable provided ??[1/2,1], and use numerical examples with finite element method spatial discretization to explore convergence rates.

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MP1

Accelerating the Computation of Tensor Z Eigenvalues

Efficient solvers for tensor eigenvalue problems are important tools for the analysis of higher-order data sets. We introduce, analyze and demonstrate an extrapolation method to accelerate the widely used shifted symmetric higher order power method for tensor Z- eigenvalue problems. We analyze the asymptotic convergence of the method, determining the range of extrapolation parameters that induce acceleration, as well as the parameter that gives the optimal convergence rate. We then introduce an automated method to dynamically approximate the optimal parameter, and demonstrate it's efficiency when the base iteration is run with either static or adaptively set shifts. Our numerical results on both even and odd order tensors demonstrate the theory and show we achieve our theoretically predicted acceleration.

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MP1

Closed-Loop Solute Transport in Blood Vessels

This work extends existing numerical models that solve for blood flow and concentration of oxygen in blood vessels from an open network of blood vessels to closed loops. Appropriate transmissibility conditions at each vessel junction and organ bed are constructed, that are based on balance laws. The class of interior penalty discontinuous Galerkin methods is used for the discretization of the models. Applications include treatment of hypoplastic left heart syndrome, a congenital heart disease.

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MP1

Efficiently Learning Models of Dynamic Networks

Many complex systems in science can be modeled by graphs which often possess uncertainty and temporal changes. Temporal Exponential Random Graph Models (TERGMs) have been introduced as a statistical model based on Markov property that facilitates the analysis of such networks. We discuss an efficient learning framework for TERGMs with a favorable sample complexity. This framework can be extended to applications such as hypergraph learning and graph prediction.

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MP1

Generalization of Sárközy's Theorem in Function Fields

Sárközy's theorem says that if $A \subset \mathbb{Z}$ is a dense subset, then there are distinct $a_1, a_2 \in A$ such that $a_1 - a_2$ is a perfect square. Using the Croot-Lev-Pach polynomial method, Green proved an $\mathbb{F}_q[t]$-analog of Sárközy's theorem with much stronger quantitative bounds. Using an idea of Bienvenu, we extend Green's result to accommodate expressions of the form $\Sigma_{i=1}^{r} c_i a_i^l$, where $a_i \in A$ and c_i are constants in $\mathbb{F}_q[t]$ adding up to 0.

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MP1

Efficient Generalized Exponential Integrator Scheme For Solving Non-Integer Order Differential Equations

Modeling real life phenomena using non-integer differential models has increasingly become the focus of many researchers in the areas of engineering, finance, physics, and so on. The aim of this study is to discuss the way in which Exponential Time Differencing methods can be generalized and applied for solving differential equations of fractional order. For efficient implementation, Real Distinct Pole (RDP) rational approximations of MittagLeffler functions are used and present some numerical examples to validate the theoretical findings.

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PP1

Higher Order Time Discretizations for Maxwell's Equations

In this poster presentation, we propose an energy-conserving higher-order time discretization for a system of Maxwell's equations. Our Maxwell's system consists of an electric pressure p, electric field density E and magnetic flux density H. The p variable allows for enforcement of divergence of E and also helps provide for a mixed finite element spatial discretization. Our time discretization is motivated by the higher-order, explicit leap frog scheme for a Maxwell's system consisting of E and H. In the extended system with p, this explicit leap frog scheme readily generalizes to a higher-order semi-explicit discretization for the (p, E, H)-system. We also then extend this to provide for a fully implicit leap-frog like discretization for the (p, E, H)-system. In both instances, we demonstrate that with appropriate energy definitions, the methods are stable and have a convergent error whose order depends on the order of the temporal discretization and the degree of the polynomial approximation for the spatial discretization. We also provide empirical validation of our results by showing computations on model problems in two and three spatial dimensions in conjunction with suitable higher order finite element spatial discretizations.

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PP1

Modeling Wildfire Smoke Transport with Data Assimilation

We estimate $PM_{2.5}$ concentrations from wildfire smoke by simulating the regional transport of wildfire smoke in the atmosphere. However, the transport processes are marred by errors attributed to parameterization and limited fundamental physics. We overcome this complexity by integrating error terms into model dynamics, observational data, and initial conditions. As a result, a cost functional associated with the errors evolves, leading to a system of coupled Euler-Lagrange (E-L) equations via the calculus of variations. The decomposition of the E-L system gives rise to two equations: a forward equation and a backward (adjoint) equation. The adjoint solution obtained by integrating backward in time is used in the forward problem, which uses representer functions to yield $PM_{2.5}$ estimates that match observations in an optimal sense. The representer functions are responses to unit impulses in space and time. We use dynamic adaptive mesh refinement, available in our computational model Smoke3d, to efficiently and accurately solve for the representer functions. We will describe how we use Smoke3d to solve for the representer functions. In particular, we discuss the representation of numerical Dirac delta functions and resulting accuracy.

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PP1

Sfd($\rtimes$): Finding Sparse Function Decomposition Via Orthogonal Transformation

High-dimensional real-world systems can be often well characterized by a small number of simultaneous low-complexity interactions. The analysis of variance (ANOVA) decomposition as well as the anchored decomposition provide a unique decompositions of a function into functions defined on an increasing number of variables. They are often sparse for real-world problems, i.e. most of the summands in the decomposition vanish. As the ANOVA and the anchored terms of the target function f are determined by its partial derivatives, the sparsity of the decomposition is equivalent to the fact that most mixed partial derivatives are zero. In this work, we introduce a technique that transforms the input of f such that in the new basis the ANOVA and anchored decompositions are sparse. Various numerical examples illustrate the reliability of the algorithm on clean and noisy data.

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PP1

Choice of Model Error Variance for Data Assimilation with the Transport Equation

The transport equation can be used to model a concentration profile and in this project, we use it to study wildfire smoke transport. Although the transport equation forms a strong foundation for estimating PM2.5 concentrations in wildfire smoke, it is challenging to model wildfire emissions since they vary significantly between fires due to biomass carbon densities, fuel quantity and condition, combustion efficiency, atmospheric interactions, etc. Therefore, we assume the transport equation is inexact and employ weak constraint four-dimensional variational data assimilation (4D-Var) to assimilate data and update PM2.5 concentration estimates. These PM2.5 estimates can vary significantly depending on the choice of data and model error covariances. Rather than use heuristics to estimate prior errors, we use regularization methods, such as the Chi-square method, L-curve, and generalized cross-validation, to specify the error covariances. These methods involve calculating the model misfit and the data residual, and the representer method presents a mathematically elegant and efficient way to calculate them. We will show 4D-Var data assimilation results from the 1D transport equation when using simulated data.

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PP1

Building Towards a Multiphase Model of Thrombosis on Moving Structures

Thrombosis is a complex phenomenon that involves the interplay between biochemistry and fluid-structure interaction. Platelet activation and aggregation involves dozens of chemical reactions both near the subendothelium and along the edge of the thrombus. Hydrodynamic forces play a large role on the stability of the clot, and flow mediated transport is necessary to bring platelets close enough to initiate thrombosis. Here, we present a multiphase model of thrombosis on a moving surface that incorporates both platelet aggregation and relative motion between the blood and the thrombus. We discuss both the modeling and the numerical challenges that result from this kind of system.

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PP1

Approximation of Current Density Modeling Skin and Proximity Effects

In engineering processes, alternating currents may be sent through process material to control and optimize natural phenomena. We discuss a numerical method that approximates the alternating current density modeled using the time harmonic Maxwell equations and address preliminary efforts accounting for the skin effect and proximity effect.

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PP1

Generative Modeling of Turbulent Combustion

Generative machine learning models, such as the denoising diffusion probabilistic model, have advanced rapidly in the field of computer vision recently where they have been used to learn complex distributions, such as natural images. In this work, we first build a large dataset of turbulent combusting flows in a laser ignited rocket combustor using a sixth-order TENO scheme for the multi-component Navier-Stokes equations. In order to mollify the large computational cost of learning the reverse diffusion process in 3D, we propose an approach in which the diffusion process is conducted in a low dimensional latent space, which is then lifted to 3D. The turbulent statistics and conservation errors of the model are analyzed. This model facilitates uncertainty quantification, low-dimensional representation, and inference of hidden state based on partial measurements (such as density from Schlieren images).

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PP1

Useful: a Python Framework for Anomaly Detection in Etl

In big data contexts, ETL processes can be fraught with errors: whether data sources have erroneous entries, bugs are introduced in code, or system failures cause partial data corruption. Here, we introduce a python framework called *useful* that automatically manages anomaly detection. This framework can track important statistical properties within data flows over time and report on unusual or possibly errant values. It also can correspond changes to possible sources of error, like specific commits in git history. Integration requires writing a single decorator on an existing function and latency is minor. In this poster, we demonstrate how to use useful and why its, well, useful.

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PP1

Life Beneath the Ice: Antarctic Microbial Mat Morphology and Spatial Ecology

In the ice-covered lakes of Antarcticas dry valleys, benthic microbial communities are the dominant life forms. The communities, largely composed of cyanobacteria, form mats of combined biological material and sediment that build up over time. A key structure present in the mats topography are pinnacles. Video data taken from a variety of sites in the lake spanning a distribution of environmental conditions allows us to examine how pinnacle spatial patterning varies along these environmental gradients. I have analyzed the topography of these microbial mats by using video data of the mats to create photogrammetric models. Spatial statistical metrics of the 3-D point clouds, including Voronoi diagrams, Ripleys L, and Clark-Evans R-index of dispersion, can help better understand the distribution of pinnacles. We observe clustered, regularly spaced, and randomly distributed spatial patterning at different sites, although the causes of these variations have not been identified. Future work will allow us to understand if and how these variations are caused by environmental changes. By investigating modern mat formation and the connection between morphology and environment, we also aim to better understand how polar ecosystems are impacted by changing environments.

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PP1

Preventing Ankle Twists: An Analysis of Lateral Transient Stability in the Human Lower Limb

Maintaining dynamic stability poses a significant challenge during the evolution from quadrupedal to bipedal locomotion in humans. Unlike our ancestors and primate relatives with flat feet, humans have evolved a unique foot arch structure that is known to enable running and jumping by providing foot stiffness. However, its contribution to stability, especially lateral dynamic (transient) stability relating to ankle twists, remains uncertain. To quantify this lateral stability, we introduced a novel, straightforward dimensionless indicator for lower limb stability, named transient postural stability, representing the maximum perturbation that can be resisted without losing stability. This indicator is derived from a nonlinear multi-Degree-of-Freedom mechanical model that incorporates actual unstable scenarios and employs an energy approach. We show that modern humans possess an optimized foot arch height, which offers superior lateral stability compared to those with flat or high arches during locomotion. By contrast, high-arch foot is inept in handling inclinations; whereas flat foot resists inclination but lacks stability at high landing speeds. The generalizable nonlinear mathematical model and transient stability indicator for the lower limb have the potential to assist in identifying individuals at a high risk of ankle injuries, informing the design of footwear and robotic feet, and inspiring further research into postural stability.

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PP1

Directional Derivative of Kemeny's Constant

In a connected graph G, Kemeny's constant gives the expected time for a random walk from an arbitrary vertex x to reach a randomly-chosen vertex y. Kemeny's constant is a measure of how well a graph is connected, and it is unknown how the addition or removal of edges affects Kemeny's constant. Inspired by using the directional derivative of the normalized Laplacian as a centrality measure, we derive the directional derivative of Kemeny's constant for several graph families in this presentation. In addition, we find sharp bounds for the directional derivative of an eigenvalue of the normalized Laplacian and for the directional derivative of Kemeny's constant. We end with a discussion of some fun examples and pose some problems for future exploration.

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PP1

Integration of the Douglas-Rachford Splitting Method with a 1D Linear Advection Equation Solver

In this poster, we present a modified Douglas-Rachford (DR) Splitting Method applied to the 1D linear advection equation solver. Our adaptation, inspired by 'A simple and efficient convex optimization based bound-preserving high order accurate limiter for Cahn-Hilliard-Navier-Stokes system' [Liu et al., 2023], improves stability and precision, particularly within challenging boundary conditions, and delivers a modest but meaningful accuracy increase. The DR method's integration marks a significant advancement in numerical PDE solving, reinforcing the importance of solver fidelity. Error analyses illustrate improved consistency at various mesh refinements, indicating the method's potential for intricate simulations. We will elucidate the DR method's modifications and their impact on solver performance, highlighting our active research aimed at refining computational accuracy and expanding scientific applica-

tions.

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PP1

An Ode-Based Framework of Experience-Belief Dynamics

As information of all types becomes more readily available, the manner in which ideas spread and are retained becomes more important to understand. While someone may hear an idea or experience something new, their opinion about the topic may not change at the same frequency. Inspired by the SIR framework, three variants of an ODE system to model these interactions using fast-slow dynamics are presented: experience-belief, memory, and memory-belief. The models are simple in conception, but display some complicated behavior with the potential to encapsulate the essential components of these dynamic real-world systems.

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PP1

Learning Partial Differential Equations Using Occupation Kernel Functions

Using data, we are interested in learning non-parametric maps from real-valued functions to real-valued functions. These real-valued functions are the boundaries for a first-order partial differential equation (PDE). Employing the method of characteristics, we transition from a PDE to a system of ordinary differential equations (ODEs). Our goal is then to learn these ODEs. The objective function is derived by leveraging the fundamental theorem of calculus. Reproducing Kernel Hilbert Spaces (RKHS) is a fundamental concept in functional analysis, particularly in machine learning. Along with RKHS theory, the approach utilizes the occupation kernel method (OCK). The learned non-parametric maps, which minimize the objective function, are then represented using a finite linear combination of occupation kernel functions.

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PP1

Social Network Dynamics: Addressing Aggregation Challenges in School Friendship Networks

A key challenge of performing inference and other statistical analyses on social networks is limited data availability. One approach for addressing this problem is to gather data from several similarly situated communities in an attempt to study the aggregate properties of the networks. For example, researchers interested in school children may collect network data from several classrooms within the same school to study the relationship between network effects and learning outcomes. However, this aggregation approach introduces its own challenges, as the distributions of network metrics and dependent variables of interest may not be heterogeneously distributed. In this talk, I present methodological and theoretical analysis of this problem, motivated by real-world data collected to measure language development by Broda et al. (2023), including a multilevel model approach (Chow, 2022) for centrality scores and a related sensitivity analysis addressing the consistency of aggregation results. I will also discuss an extension that incorporates network embeddings, using spectral and graph-based neural network outputs as covariates to predict language development outcomes.

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PP1

Data-Driven Evaluation of ML/DL Performance for Timely and Precise Fault Identification in Automotive Cyber-Physical Systems

Multivariate time series classification (TSC) plays a crucial role in diverse real-world applications, from finance to vehicle diagnostics. In automotive diagnostics, TSC can be used for fault detection—a critical component of modern automotive diagnostic frameworks, where accurate and timely identification of anomalies is paramount. This study introduces a supervised learning benchmark for fault detection in automotive systems using Controller Area Network (CAN) data, leveraging the first publicly available dataset of its kind containing simulated faults. We employ a data-driven approach to capture the complex temporal dependencies inherent in high-dimensional CAN data. The proposed benchmark provides a robust analytical basis for model comparison among traditional ML/DL techniques, highlighting the effectiveness of each technique in discerning subtle system faults and demonstrating their capability for rapid and precise fault identification (exceeding 98% accuracy). We delve into the nuances of algorithmic performance under the data-driven paradigm, highlighting strengths and limitations of each approach by evaluating model robustness against the complexities inherent in TSC and analyze advanced performance metrics providing a comprehensive evaluation of model capabilities. Unveiling the potential of ML/DL methods in diverse diagnostic scenarios, this study paves the way for reliable system monitoring across cyber-physical systems.

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PP1

Revisiting the NGM Method in the Case of Extended SVIR Models

This study seeks to investigate the use of the Next Generation Matrix (NGM) method [Diekmann et al., 1990 and van den Driessche and Watmough, 2002] in formulating the vaccinated reproduction number ($\mathcal{R}_v$) of extended SIR models with imperfect vaccination. We consider two extended versions of SIR models, where the infected individuals are subdivided based on vaccination status and differential morbidity. In these models, vaccinated individuals could acquire infection, and then transition to a separate class compared to the non-vaccinated infected individuals. Our results indicate that the eigenvalues of the Jacobian matrix resulting from the NGM method are extremely long bulk expressions comprised of the model parameters. However, we use algebraic simplifications and MATLAB computations to simplify the spectral radius to a considerable extent, which enables us to express $\mathcal{R}_v$ in terms of $\mathcal{R}_0$. It is still very difficult to obtain a pragmatic expression to draw useful conclusions based on $\mathcal{R}_v$. As such, we emphasize the lack of usefulness of the results generated by the NGM method in a model of the said structure, as well as the need for an alternative approach in that regard.

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PP1

Improving Dsa Image Segmentation with Cnns

This poster introduces an innovative method for segmenting Digital Subtraction Angiography (DSA) images, a critical task in medical image analysis. Using Convolutional Neural Networks (CNNs), our approach employs an iterative process to expand segmented regions in growing directions. A CNN predicts class probability scores within a small pixel neighborhood, determining pixel inclusion based on a threshold. The process continues iteratively until no new pixels qualify for inclusion. Our method achieves remarkable segmentation accuracy while preserving biological features. This project aims to improve the accuracy of predictions of the DSA images. The combination of precision and preservation capabilities distinguishes our method, marking a notable advancement in the field of DSA image segmentation.

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PP1

Modulational Instability in the Ostrovsky Equation and Related Models

We study the modulational instability of small-amplitude periodic traveling wave solutions in a generalized Ostrovsky equation. Specifically, we investigate the invertibility of the associated linearized operator in the vicinity of the origin and derive a modulational instability index that depends on the dispersion and nonlinearity. We then show that the small-amplitude periodic traveling waves of the Ostrovsky equation exhibit modulational instability if the wavenumber is greater than a critical value which agrees with previously found numerical results both qualitatively and quantitatively. We also study the effects of surface tension on modulational instability using the index.

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PP1

Quantum-Powered Computational Multiphysics and Multiscale Modeling and Simulation

The emergence of quantum computing technology has opened up new avenues in modeling and simulation in science and engineering. Traditional computational models and simulations have limitations in terms of accuracy, speed, and complexity. In this session, we discuss the potential of quantum computing in addressing these limitations, primarily from a computational science and engineering perspective, including computational fluid dynamics, finite element analysis, combustion modeling, fluid-structure interaction, and computational aero-acoustics. In this contribution, we highlight how quantum computing, combined with appropriate algorithms, can help us achieve unprecedented accuracy, speed, and complexity in simulations, eventually enabling significant progress in the design, testing, and development of complex engineered systems such as airplanes, spacecraft, cars, and machines. Our research and scientific computing software propose a paradigm shift in R&D and engineering, bringing them more within the digital scope and realizing a significant speed-up in the design and development process of complex engineered systems and the simulation of multiphysics phenomena. Overall, this work demonstrates the transformative potential of quantum computing in computational modeling and engineering and multiphysics and multiscale simulation.

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PP1

Interaction Measures, Partition Lattices and Kernel Tests for High-Order Interactions

Models that rely solely on pairwise relationships often fail to capture the complete statistical structure of the complex multivariate data found in diverse domains, such as socioeconomic, ecological, or biomedical systems. Non-trivial dependencies between groups of more than two variables can play a significant role in the analysis and modelling of such systems, yet extracting such high-order interactions from data remains challenging. Here, we introduce a hierarchy of d-order ($d \geq 2$) interaction measures, increasingly inclusive of possible factorisations of the joint probability distribution, and define non-parametric, kernel-based tests to establish systematically the statistical significance of d-order interactions. We also establish mathematical links with lattice theory, which elucidate the derivation of the interaction measures and their composite permutation tests; clarify the connection of simplicial complexes with kernel matrix centring; and provide a means to enhance computational efficiency. We illustrate our results numerically with validations on synthetic data, and through an application to neuroimaging data.

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PP1

Bystander Effect As An Emergent Property of Individual Psychological Prospects

The bystander effect is a sociological phenomenon in which individuals are less likely to help a person in need if there are others present. Sociologists and psychologists have proposed multiple plausible reasons for the bystander effect, from ambiguity and group cohesiveness to diffusion of responsibility and mutual denial. We build a dynamical systems model based on these sociological and psychological hypotheses, along with ideas borrowed from behavioral economics; in particular, we use prospect theory to predict an individuals decision to take action or not. With this model, we find the conditions under which a bystander effect emerges from these individual decisions.

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PP1

Modeling the Long-Distance Effects of Predation

In population dynamics and ecological studies, predator-prey interaction occupies a prominent place. We construct an agent-based patch model to demonstrate the effects of predation at distances. We vary the strength of such parameters as, predator abundance, predator ferocity, predator lethality, and anti-predator defenses, to see how these characteristics affect distance prey dynamics.

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PP1

Evolution Conditions for Eradicating Drug-Resistance Population

The evolution of drug resistance in bacteria is a complex process influenced by several factors. Initially, bacteria may acquire resistance through genetic mutations or by acquiring resistance genes from other bacteria through horizontal gene transfer. The treatment of infectious diseases has become increasingly challenging due to the emergence of the prevalence of drug-resistant bacteria. The use of antibiotics kills sensitive strains but leaves behind resistant ones, which multiply and spread. In this research, we abstract in a switched linear system the evolution aspects driven by the use of antibiotics in a population. We study the biological conditions such as proliferation, death rate, and mutation rate under which a switched system will be stable by applying the concept of Lyapunov theory. Our findings will provide insights into how sequential drug use can enhance treatment outcomes and reduce the prevalence of drug-resistant infections.

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PP1

Extension of Mechanosensitive Piezo1 Hodgkin-Huxley Model for Midrange Pressures

Mechanosensitive ion channels expressed on neurons contribute to varying currents as a function of mechanical forces such as pressure. The traditional Hodgkin-Huxley model features voltage-sensitive gating mechanisms without accounting for other mechanisms. We develop a Hodgkin-Huxley-type differential equation model for the mechanosensitive ion channel Piezo1 combining pressure- and voltage-sensitive gating mechanisms to calculate the resulting current given varying pressure over the entire relevant range. This model extends a previous triple-gate model for the Piezo1 channel that was formulated for responses to saturating (70 mmHg) and no (0 mmHg) pressure (Zhang and Zou, 2022). Using the pressure-dependent open probability of the channel, we develop an interpolation of the gating parameters for pressures ranging from 0 to 70 mmHg. We confirm the sensitivity and thresholding behavior of our model by replicating published experimental results from Lewis and Grandl (2015) of current traces of single Piezo1 channels on excised cells clamped at various voltages. Distribution Statement A (Approved for Public Release, Distribution Unlimited)

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PP1

On the Potential Benefits of Simulation-Based Inference and Data Fusion for Enhancing Interferometric Visibility Measurements Through a Turbulent Atmosphere

Flow-induced optical distortions in airborne environments, as well as inside the domes of large telescopes, are limiting factors on observation quality. In this work, we ask whether interferometric off-axis measurements can, in principle, provide incremental information that enhances observations. To address the question, we consider a simple simulated model of a turbulent flow with an unknown Fried parameter and wind speed over an optical setup consisting of two interferometers. Our goal is to use side-channel information from an off-axis interferometer to improve the estimation error of the main channels visibility. To avoid overspecialization, we formulate the task of inferring the main channels visibility as a general statistical problem, which we tackle from the perspective of multi-source simulation-based inference with probabilistic neural networks. Accordingly, we train Bayesian heteroskedastic neural estimators on simulated data and demonstrate their utility in terms of efficiency, accuracy, and uncertainty calibration in a series of numerical experiments. Our experiments highlight the benefits of data fusion as well as potential limitations on estimation quality.

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PP1

Statistical Modeling of Quantify the Uncertainty of FoldX-Predicted Protein Folding and Binding Stability

Computational methods of predicting protein stability changes upon mutations are invaluable tools in studying large numbers of protein variants. However, they are limited by a wide variation in accuracy and difficulty of assessing prediction uncertainty. Using a popular computational tool, FoldX, we develop a statistical framework that quantifies the uncertainty of predicted changes in protein stability. We show that multiple linear regression models can be used to quantify the uncertainty associated with FoldX prediction for individual mutations. Comparing the performance among models with varying degrees of complexity, we find that the model precision improves significantly when we utilize molecular dynamics simulation. Based on the model that incorporates information from molecular dynamics, biochemical properties, as well as FoldX energy terms, we can generally expect upper bounds on the uncertainty of folding stability predictions of 2.9 kcal/mol and 3.5 kcal/mol for binding stability predictions. The uncertainty for individual mutations varies; our model estimates it using FoldX energy terms, biochemical properties of the mutated residue, as well as the variability among snapshots from molecular dynamics simulation. Using a linear regression framework, we construct models to predict the uncertainty associated with FoldX prediction of stability changes upon mutation. This technique is straightforward and can be extended to other computational methods as well.

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PP1

Accelerating the Computation of Tensor Z-Eigenvalues

Efficient solvers for tensor eigenvalue problems are important tools for the analysis of higher-order data sets. We are proposing extrapolation methods to accelerate the widely used shifted symmetric higher order power method for tensor Z-eigenvalue problems. We analyze the asymptotic convergence of the method, determining the range of extrapolation parameters that induce acceleration, as well as the parameter that gives the optimal convergence rate. We then introduce an automated method to dynamically approximate the optimal parameter, and demonstrate it's efficiency when the base iteration is run with either static or adaptively set shifts.

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PP1

Closed-Loop Solute Transport in Blood Vessels

Hypoplastic left heart syndrome (HLHS) is a congenital heart disease that accounts for 2-3% of congenital heart diseases in the United States and 40% of all neonatal cardiac deaths. HLHS causes oxygenated blood to mix with deoxygenated blood, resulting in death. This raises a critical need to accurately model the transport of oxygen in blood vessels and organs throughout the human body to improve outcomes in patients with HLHS. Previously, numerical reduced models have been created to solve for blood flow and concentration of one solute. These models reduce the dimensions of the vessels and organs to improve computational efficiency. Our work extends the models from open network of blood vessels to closed loops. Appropriate transmissibility conditions at each vessel junction and organ bed are constructed, that are based on balance laws. The class of interior penalty discontinuous Galerkin methods is used for the discretization of the models.

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PP1

Extending Statistics-Informed Neural Network to Multidimensional Stochastic Processes

The statistics-informed neural network (SINN) has been proposed as a machine-learning-based stochastic trajectory generator. SINN is built on a deterministic recurrent neural network that takes an input stream of white noise sequences to generate an ensemble of stochastic trajectories that has statistical properties similar to the original stochastic dynamics. While the capabilities of SINN have been demonstrated using various one-dimensional non-Markovian processes, for this methodology to be a promising tool for real applications (e.g., via surrogate modeling), it is required to extend SINN to reproduce multidimensional stochastic processes. In this presentation, we present our efforts in this regard. First, since many cross terms are to be included in the total loss function to capture the complex statistical properties of a multidi-

mensional process, we employ a self-adaptive loss-balanced technique to effectively balance various loss terms. Second, since the estimation of a multidimensional probability density function (PDF) is computationally inefficient, instead of adding these to the total loss function, we include a set of one-dimensional PDFs of some linear combinations of component processes. Third, we investigate the impact of the dimensionality of the input white noise sequence on the performance of SINN. Lastly, we perform simulation studies using the Langevin dynamics of the Fermi-Pasta-Ulam chain and the kinetic Monte Carlo simulation of surface chemistry.

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PP1

Computational Methods for Multi-Physics Simulation of Melting in Steelmaking

Iron and steel production accounts for approximately 8% of global carbon dioxide (CO_2) emissions. There are pathways to decarbonize these processes, including replacing fossil fuels in iron ore reduction and electrifying other steelmaking process parts. Iron pellets produced using hydrogen, or Hydrogen Direct Reduced Iron (HDRI), have property differences from those produced using conventional DRI processes. These differences may impact melting in electric arc furnaces (EAF) and other downstream processes. The physical properties of iron pellets vary significantly with temperature during heating, complicating predictions of their behavior. In this project, we seek to develop an integrated simulation, including the fluid flow and convective thermal transport around the pellet particle. We also examine conduction and phase changes within the particle as they impact the melting process. We use adaptive mesh refinement (AMR) to resolve both the changing size of the particle and the complex physics of the interaction between the pellet and the surrounding fluid. We base our simulations on the AMReX-incflo module, which allows large-scale Navier-Stokes simulation while resolving the changing particle size during melting. As we advance our numerical tools, we anticipate an improved understanding of the dynamics of HDRI melting, which will, in turn, accelerate the adoption of low-carbon technologies in the steelmaking industry.

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PP1

Using a Fast Adaptive Function Approximator to Calculate Protein-Filament Binding Kinetics

The cytoskeleton, consisting of biopolymer filaments, molecular motors, and passive crosslinking proteins, provides the internal structure of cells that facilitate movement, growth, and cell division. Understanding the microscopic motor-filament kinetics and dynamics is essential for comprehending macroscopic behaviors of reconstituted cytoskeletal assemblies, such as self-organized flow and active stress. In this study, we employ an adaptive fast Chebyshev approximation based on tree search alongside parallel computing to accurately recover the equilibrium distribution of crosslinking proteins, thus satisfying detailed balance in binding through kinetic Monte Carlo sampling, while maintaining cost-effectiveness. Additionally, we offer expandable features, including segregating the simulation process via pre-building and allowing the free-loading of different explicit formulations of the motor's potential energy. This research has the potential to better describe the evolution of cytoskeletal active matter.

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PP1

Detecting and Resetting Tipping Points to Create More Hiv Post-Treatment Controllers with Bifurcation and Sensitivity Analysis

The existence of HIV post-treatment controllers (PTCs) gives a hope for HIV functional cure. Understanding the critical mechanisms underlying PTCs represents a key step toward this goal. The critical mechanisms are represented by parameters and initial conditions that mostly affect the tipping points of the qualitatively different dynamics. For the tipping points in parameter space, we develop a sensitivity analysis of the threshold conditions of the associated bifurcations. Our results suggest that the infected cell death rate and the saturation parameter for CTL proliferation most significantly affect the post-treatment control. We further unfold the disease dynamics through codimension one and two bifurcation analyses, which include the derivations of the parameter-dependent center manifolds and normal forms. For the tipping points in state space of initial conditions, we first investigate the saddle-type viral set point to identify its stable manifold, which delimits different trapping regions of viral set points. In addition, we identify that a homoclinic cycle bifurcated

from Bogdanov-Takens bifurcation serves another threshold for HIV control. The identified stable manifold and homoclinic cycle serves as a guide for the count of immune cells and HIV virus at the time of therapy termination.

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IP1

Critical Transitions in Complex Systems: Theory and Applications to Climate and Ecosystem Dynamics

Many systems in nature are characterized by the coexistence of different stable states for a given set of environmental parameters and external forcing. Examples for such behavior can be found in different fields of science ranging from mechanical or chemical systems to ecosystem and climate dynamics. As a consequence of the coexistence of a multitude of stable states, the final state of the system depends strongly on the initial condition. Perturbations, applied to those natural systems can lead to a critical transition from one stable state to another. Those transitions are called tipping phenomena in climate science, regime shifts in ecology or phase transitions in physics. Such critical transitions can happen in various ways: (1) due to bifurcations, i.e. changes in the dynamics when external forcing or parameters are varied extremely slow (2) due to fluctuations which are always inevitable in natural systems, (3) due to rate-induced transitions, i.e. when external forcing changes on characteristic time scale comparable to the time scale of the considered dynamical system and (4) due to shocks or extreme events. We discuss these critical transitions and their characteristics and illustrate them with various examples from climate and ecosystem dynamics.

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IP2

Learning the Solution Operators of Forward and Inverse Problems for Pdes

Given the very high computational cost of numerically simulating PDEs, there is an increasing interest in learning the underlying PDE solution operator from data. We review the emerging field of operator learning by laying out its mathematical foundations and discussing different architectures ranging from neural operators to transformers. Both mathematical results and extensive numerical experiments will presented in the talk to compare different operator learning models. Downstream applications to Inverse Problems for PDEs will also be presented.

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IP3

Sampling and Generative Modeling Using Dynamical Representations of Transport

Drawing samples from a probability distribution is a central task in applied mathematics, statistics, and machine learning—with applications ranging from Bayesian computation to computational chemistry and generative modeling. Many powerful tools for sampling employ transportation of measure, where the essential idea is to couple the target probability distribution with a simple, tractable reference' distribution, and to use this coupling (which may be deterministic or stochastic) to generate new samples. Within this broad area, an emerging class of methods use dynamics to define a transport incrementally, e.g., via the flow map induced by trajectories of an ODE or the stochastic mapping induced by sample paths of an SDE. These methods have shown great empirical success, but their consistency and convergence properties, and the ways in which they can exploit structure in the underlying distributions, are less well understood. We will discuss properties and theoretical underpinnings of these new dynamical approaches to transport. In particular, we will discuss the statistical convergence of generative models based on neural ODEs and flow matching. We will also present two new, contrasting, dynamical constructions of transport: a gradient-free method that avoids complex training procedures by instead evolving an interacting particle system that approximates a Fisher–Rao gradient flow; and a discrete-time dynamical system based on an infinite-dimensional Newton iteration, which involves successively solving linear PDEs. We will attempt to illuminate the relative advantages and pitfalls of these dynamical methods.

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IP4

Formulating Effective Models, Methods, and Conceptual Frameworks for the Geosciences

Can waves transport significant amounts of ocean heat and tracers great distances, thus affecting Earths climate? This question was the basis for a project which culminated in the wave-driven circulation model and a concrete answer to how this process takes place. Moreover, the project also showed that wave-generated transport was most intense in the nearshore, leading to an examination of the impact of wave-generated transport on important nearshore processes, such as movement of ocean pollution and nutrients in coastal areas. In my talk, I will describe how the vortex-force conceptualization led to the formulation of the model and a theoretical basis for how waves and currents interact at scales larger than the wave scales. The ever-present noise in natural processes and in the instruments used to measure them motivated me to create computational methods that could combine models, such as the wave circulation model and models for climate and weather, and observations in a probabilistic framework to make better predictions. While optimal estimate methods for linear problems existed, the focus of my work was instead on developing algorithms that could handle the more common noisy nonlinear processes in the geosciences. I will detail some of the strategies I used to create methods and algorithms that assimilate observations, rational models, and machine-learned data-driven constructs to improve forecasts in time-dependent problems, arising in the geosciences and beyond. Finally, I will discuss my more recent work, which employs mathematical arguments to guide in quantifying and understanding resilience in the context of a changing climate and biological systems response via adaptation to stresses.

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IP5

Gradient Flows, Non-Smooth Kernels and Generative Models for Posterior Sampling in Inverse Problems

This talk is concerned with inverse problems in imaging from a Bayesian point of view, i.e. we want to sample from the posterior given noisy measurement. We tackle the problem by studying gradient flows of particles in high dimensions. More precisely, we analyze Wasserstein gradient flows of maximum mean discrepancies defined with respect to different kernels, including non-smooth ones. In high dimensions, we propose the efficient flow computation via Radon transform (slicing) and subsequent sorting or Fourier transform at nonequispaced knots. Special attention is paid to non-smooth Riesz kernels. We will see that Wasserstein gradient flows of corresponding maximum mean discrepancies have a rich structure. In particular, singular measures can become absolutely continuous ones and conversely. Finally, we approximate our particle flows by conditional generative neural networks and apply them for conditional image generation and in inverse image restoration problems like computerized tomography and superresolution. This is joint work with Johannes Hertrich (UCL) and Paul Hagemann, Fabian Altekruger, Robert Beinert, Jannis Chemseddine, Manuel Graf, Christian Wald (TU Berlin).

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SP1

W. T. and Idalia Reid Prize Lecture: 100 Years of Traffic Models: From Road Tolls to Autonomy

In 1924, on The Quarterly Journal of Economics, Frank H. Knight debated on social costs using an example of two roads, which was the base of the Wardrops principle. The author suggested the use of road tolls and it was probably the first traffic model ever. Few other milestones of a long history include the traffic measurements by Greenshields in 1934, the Lighthill-Whitham-Richards model in late 1950s and follow-the-leader microscopic models. After describing some of these milestones, we will turn to modern theory of conservation laws on topological graphs with application to traffic monitoring. The theory required advance mathematics such BV spaces and Finsler-type metrics on L1. In late 2000s, this theory was combined with Kalman filtering to deal with traffic monitoring using data from cell phones and other devices. Then we will turn to measure-theoretic approaches for multi-agent system, which encompass follow-the-leader-type models. Tools from optimal transport allows to deal with the mean-field limit of controlled equations, representing the action of autonomous vehicles. We will conclude discussing how autonomy can dissipate traffic waves and reduce fuel consumption, then illustrating the results of a 2022 experiment with 100 autonomous vehicles on an open highway in Nashville.

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SP2

I. E. Block Community Lecture: Go Boldly Where No Math Has Gone Before

The role of mathematics in the worlds greatest discoveries and inventions is often overlooked or unappreciated by the general public. What we remember about maths in school might amount to prime numbers or finding the length of hypotenuse, both of which may appear to have no relevance to our everyday lives. How many of us will recall words like polynomial and integral and appreciate the applications of these fundamental mathematical concepts? Can we easily name the many mathematicians who have pioneered world-changing scientific breakthroughs? This talk aims to change all of that. I will bring you on a journey of mathematical progress and share with you the reasons why I believe that maths is important, exciting and innovative. You will learn about the multitude of ways that maths has helped to solve the worlds greatest challenges, and the scientists who championed these innovations. The journey will continue into modern times, where maths is being used to tackle important unsolved issues affecting us now and dictating our future. The final stop will bring us to space where I will describe my role as a mathematician taking on the future of space sustainability.

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SP3

Theodore Von Krmn Prize Lecture: From Reduced-Order Modeling to Scientific Machine Learning

Reduced-order models play a critical role in achieving design, control and uncertainty quantification for complex systems. They are also a key enabling technology for predictive digital twins. Our Operator Inference approach combines classical theory of projection-based reduced-order modeling with a modern algorithmic perspective from data-driven scientific machine learning. The result is a scalable, non-intrusive, physics-informed approach to deriving surrogate models that embed structure dictated by the underlying physics. An attractive property of the approach is its flexibility in expressing the reduced-order model in a linear subspace or a nonlinear (polynomial) manifold. Operator Inference is shown to be successful in achieving predictive reduced-order models for challenging engineering problems where training data are sparse and expensive to acquire.

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SP4

John Von Neumann Lecture: Exploring the Mysteries of Deep Neural Network Optimization

In 1961, Minsky perceived a fundamental flaw within the burgeoning field of artificial neural networks. He doubted that such a nonlinear system could be effectively trained using gradient methods, because unless the structure of the search space is special, the optimization may do more harm than good. Fast forward to today, and we observe deep neural networks far more complex than those envisioned at the field's inception being successfully trained with methods akin to gradient descent. It has, indeed, become evident that the objective function displays a highly benign structure that we are only starting to comprehend. In this lecture, I aim to summarize our current understanding of this enigmatic optimization process. I will explore a diverse array of themes, including intrinsic dimensionality, the optimization landscape, and implicit regularization, and I will highlight key open questions, all within the context of residual networks and generative models.

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JP1

Joint Plenary with the Siam Conference on Applied Mathematics Education (ed24): Signals of a Critical Transition in Inclusive Stem Education

In the last few years, we have experienced several external shocks to our educational system, such as COVID-19 and renewed critical conversations about racism in higher education. How is the mathematics community responding? I will highlight a few efforts across the math institutes and in classrooms to confront inequity and rehumanize mathematics education. I will also explore how complex systems theory and computational approaches can be used to understand how our educational system is changing. In a recent study, we conducted a computational text analysis of educational journal articles in postsecondary biology education to understand how attention to topics in social justice, equity, diversity and inclusion have evolved over time. We found a rapid shift in attention to inclusive teaching occurs between 2018 and 2019, marked by an increase in section length, increased use of inclusive teaching keywords, and an increase in complexity of ideas in the semantic network. Some effect is associated with structured authoring resources and support. However, this alone is not enough to explain the observed shift, suggesting that many other structures, conversations, and investments are already providing the fertile ground that is advancing educational equity in STEM education.

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CP1

Fixed Points and Stability in Nonlinear Fractional and Delay Differential Equations

In this paper we study the stability properties of nonlinear differential equations with variable delays and give conditions to ensure that the zero solution is asymptotically stable by applying Fixed Point Theorems. These conditions do not require the boundedness of delays, nor do they ask for a fixed sign on the coefficient functions. An asymptotic stability theorem with a necessary and sufficient condition is proved. The same technique is also applied to some nonlinear fractional differential equations of Caputo type. In this case, we first convert the fractional differential equation as an integral equation with a singular kernel by applying the variation of parameters formula in terms of Mittag-Leffler functions that are completely monotone. This allows us to define a mapping function by the right-hand side of the integral equation. We show that this function has a fixed point that is a solution of the original differential equation tending to zero as time approaches infinity. Stability and asymptotic stability theorems are proved.

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CP2

On-Demand Significance Testing Using Monte Carlo Simulation

In the realm of econometrics, statistics, psychometrics, and other diverse research domains, a plethora of significance tests is available, ranging from conventional t-tests applicable in Ordinary Least Square regression models to more intricate tests for autocorrelation, homoskedasticity, and others. However, researchers often encounter situations where established tests are absent, rendering traditional approaches impractical. This paper introduces a method for conducting on-demand significance tests tailored for such scenarios. Leveraging Monte Carlo simulation and drawing insights from various fields, this approach ensures methodologically sound randomization. The methodology is firstly illustrated through the application to the Difference-in-Difference (DD) coefficient, a frequently used model in epidemiology and policy evaluation. Subsequently, the procedure is employed to assess the significance of dependency on irrelevant alternatives within Thurstone's method for paired comparisonsa widely utilized technique in psychometry, survey research, and marketing. The paper concludes with an evaluation of the advantages and disadvantages inherent in this approach. This research contributes to the methodological toolkit of researchers fostering a more nuanced approach to significance testing.

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CP2

On the Potential Benefits of Simulation-Based Inference and Data Fusion for Enhancing Interferometric Visibility Measurements Through a Turbulent Atmosphere

Flow-induced optical distortions in airborne environments, as well as inside the domes of large telescopes, are limiting factors on observation quality. In this work, we ask whether interferometric off-axis measurements can, in principle, provide incremental information that enhances observations. To address the question, we consider a simple simulated model of a turbulent flow with an unknown Fried parameter and wind speed over an optical setup consisting of two interferometers. Our goal is to use side-channel information from an off-axis interferometer to improve the estimation error of the main channel's visibility. To avoid overspecialization, we formulate the task of inferring the main channels visibility as a general statistical problem, which we tackle from the perspective of multi-source simulation-based inference with probabilistic neural networks. Accordingly, we train Bayesian heteroskedastic neural estimators on simulated data and demonstrate their utility in terms of efficiency, accuracy, and uncertainty calibration in a series of numerical experiments. Our experiments highlight the benefits of data fusion as well as potential limitations on estimation quality.

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CP2

Data Assimilation Modeling of An Electrohydrodynamic Flow

In this work, we explore the potential application of data assimilation technique in computational electrohydrodynamics. Data assimilation, i.e., the optimal combination of simulation results and measurement data, has been essential to numerical weather forecast and not yet been widely used to model electrohydrodynamic flow phenomena. Therefore, we study the flow driven by electrical corona discharge in air between a needle tip (high voltage) and a planar electrode (ground). The currents at the two electrodes are monitored. During the first 0.5 ms, at each preset time interval, the simulation results are assimilated to the measurements using ensemble Kalman filtering. It is found that, after data assimilation, the model prediction of currents for the next 0.5 ms agrees better with the experimental results. In general, assimilating averaged quantities over the time interval produces better results than assimilating instantaneous values, while the effect of the time interval is still inconclusive, which might be due to the lack of spatially-resolved measurement data.

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CP3

A Principled Pattern Recurrence Method for Multiscale Time Series Analysis

Time series from complex nonlinear systems often exhibit recurring patterns at multiple temporal scales, and those recurrences can give insight on the underlying physical processes. In this work, we propose a principled and robust method to define recurrences in time series using local minima of the 1-Wasserstein distance function between subsets of one-dimensional signals. A statistical test based on the distribution of distances between such patterns in Brownian motion provides an additional criterion to define recurrences. This method is particularly fit to study phenomena that occur, and most importantly recur, over many different time scales, alike climate, biological and financial time series. We show analytical and numerical results on time scale invariance for the 1-Wasserstein distance distribution between patterns in Brownian motion, for which other common metrics' performance vary with time scale and sampling density. This new way to define recurrences is applied to detect natural time scales in palaeoclimate time series through dominant recurrence time intervals, as well as studying combination of events happening over different time scales, and their implication for regimes shifts and abrupt changes in the last 800,000 years.

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CP3

Reduced Order Modeling Approach for Radiation Source Identification and Localization

This work presents a Reduced order modeling based approach for radiation source detection when only a limited number of sensors are available in a radiation field. The reduced order modeling approach consists of two major procedures;online and offline. The offline procedure is used to create a spatial-energetic basis for representing the radiation field for a range of possible source compositions and locations. The online procedure is used to reconstruct the entire radiation field using data from a few detectors. Probabilistic principal component analysis is used to find the spatial-energetic basis functions and Bayesian parameter estimation with a Gaussian prior is used to estimate the latent variables that depend on the source scenerio. The reconstruction procedure is illustrated for a simple benchmark problem using a sparse set of noisy data. Here we discussed the noise impact of trial data on the performance of reduced order model. Moreover, the results are validated using a terrestrial radiation detection scenario. We showed that the ROM approach can be used to localize and detect energy spectra of a mixed radiation source, which is composed with individual radiation sources, given noisy simulation data at a limited number of sensor locations.

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CP3

Mathematical Modeling and Analysis of Cd200-Cd200r in Cancer Treatment

The CD200-CD200R complex is formed by a cell membrane protein CD200 expressed on tumor cells and its receptor CD200R expressed on immune cells. CD200 positive tumor cells inhibit cellular functions of M1 and M2 macrophages and dendritic cells (DCs) through the CD200-CD200R complex, resulting in downregulation of Interleukine-10 and Interleukine-12 and affecting the activation of T cells. Our work provides two ODE models, a complete and simplified model, to investigate how the binding affinities of CD200R and the populations of M1 and M2 macrophages affect the functions of CD200-CD200R complex in tumor growth. Our simulations show that the tumor loads depend on the relation of the CD200R binding affinity between M2 macrophages and DCs. We observed that CD200-CD200R blockade would be an efficient treatment when the CD200R binding affinity of M1 macrophages or DCs is strong. The simplified model shows that the population of macrophages only affects the treatment efficacy when the binding affinities of CD200R on M1 and M2 macrophages are close. Investigating the dynamics of the equilibria of the simplified model, we found that the CD200 positive tumor load is higher than the CD200 deficient case when the M1 macrophages dominate the population, and the tumor load goes from eradication to persistence to oscillation, as the tumor growth rate increases.

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CP3

A Probabilistic Approach to Detect Intermolecular Interactions in Single-Molecule Localization Microscopy

Interactions between biological macromolecules mediate all cellular processes. Single-molecule localization microscopy (SMLM) provides a way to directly visualize molecular positions by fluorescently labeling two presumed interaction partners and localizing them with nanoscale precision. However, to infer coupling from noisy measurements of molecular positions, a few important questions must be answered. For example, if two molecules are detected in proximity (with arbitrary localization precision), what is the probability that they are indeed coupled? Also, if multiple choices are available for selecting sets of interacting pairs in a dense image, which choice should we pick? And how should we account for colocalization events that occur by random chance rather than bona fide coupling? Here we developed a probabilistic approach that addresses these questions and allows determining the fraction of coupled molecular pairs from two-color SMLM datasets. The approach is robust across a range of molecular densities and localization precisions. We have demonstrated the utility of our theoretical framework using simulations and experiments of equilibrium and dynamic biochemical reactions.

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CP3

Parallel Sparse Skew-Symmetric Matrix-Vector Multiplication with Reverse Cuthill-McKee Reordering

Sparse matrices, prevalent in various application areas of scientific computing, persist as a bottleneck in parallel computing. We effectively use Reverse Cuthill-McKee (RCM) reordering algorithm to transform sparse skew-symmetric matrices into a band form, then efficiently parallelize it by splitting the band matrix into 3 different parts by considering amounts of sparsity. Our proposed method, Parallel 3-Way Banded Skew-Symmetric Sparse Matrix-Vector multiplication (SS-SpMV) with RCM, is novel in the sense that it is the first implementation of parallel processed skew-symmetric SpMV kernels. We note that since a skew-symmetric matrix is structurally symmetric with just signs of the elements are flipped, our work also improves parallel symmetric SpMV kernels from a different perspective than the common trends in literature, as to manipulating the form of matrix in a preprocessing step to accelerate the repeated computations in iterative solvers. This work and its findings naturally apply to parallel sparse symmetric SpMVs as well. Our parallel implementation achieves a significant strong scaling of up to 19 over serial kernel and performs better than the prevalent approach of involving synchronization phases [Elafrou, Goumas, and Koziris, 2019] into parallel symmetric SpMVs.

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CP4

The Strict Superlinear Order can be Faster Than the Infinite Order

The sequences with strict superlinear convergence are the output of numerous algorithms; such speed is clearly much faster than linear, but is it also slower than, say, quadratic? We show that actually there are four distinct classes of strict superlinear order: “weak’, “medium’, “strong’ and “mixed’. The speed of the sequences from the first three classes is increasingly much faster (term-by-term big Oh, i.e., $|x^* - x_k| = \mathcal{O}(|y^* - y_k|^\alpha)$, as $k \to \infty, \forall \alpha > 1$ given), whereas the speed of the “mixed’ class cannot be assessed. We prove that the speed of the sequences from the “medium’ and “weak’ classes is term-by-term slower than the speed of the sequences with high classical C-orders $p > 1$ (in the sense of big Oh above), while an example shows that certain sequences from the “mixed’ class may be term-by-term faster than some sequences with infinite C-order. We also show that for a given sequence with strict superlinear convergence, one can evaluate numerically to which class it belongs. Some recent results of Rodomanov and Nesterov (2022), resp. Qi et al. (2023) show that certain classical quasi-Newton methods (DFP, BFGS and SR1) belong to the “weak’ class.

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CP4

Learning Decentralized Partially Observable Mean Field Control for Artificial Collective Behavior

Recent reinforcement learning (RL) methods have achieved success in various domains. However, multi-agent RL (MARL) remains a challenge in terms of decentralization, partial observability and scalability to many agents. Meanwhile, collective behavior requires resolution of the aforementioned challenges, with application in active matter physics, self-organizing systems, opinion dynamics, and biological or robotic swarms. MARL via mean field control (MFC) offers a solution to scalability, but fails to consider decentralized and partially observable systems. We enable decentralized behavior of agents under partial information by proposing novel models for decentralized partially observable MFC (Dec-POMFC), a broad class of problems with permutation-invariant agents allowing for reduction to tractable single-agent systems. We provide a theoretical basis, including a dynamic programming principle, together with optimality guarantees for Dec-POMFC solutions applied to finite swarms of interest. Algorithmically, we propose Dec-POMFC-based policy gradient methods for MARL via centralized training and decentralized execution, together with gradient approximation guarantees. In addition, we improve upon histogram-based MFC by kernel methods. We evaluate numerically on collective behavior tasks such as adapted Kuramoto and Vicsek swarming models, being on par with state-of-the-art MARL. Overall, our framework takes a step towards RL-based engineering of artificial collective behavior.

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CP4

Learning Mean Field Games on Sparse Graphs: A Hybrid Graphex Approach

Learning the behavior of large agent populations is important in numerous research areas. Although multi-agent reinforcement learning (MARL) has made progress in solving these systems, solutions for many agents often remain computationally infeasible and lack theoretical guarantees. Mean Field Games (MFGs) address both issues and can be extended to Graphon MFGs (GMFGs) to include agent network structures. The applicability of GMFGs is limited by graphons only capturing dense graphs since most empirically observed networks show some degree of sparsity. Thus, we introduce the novel concept of Graphex MFGs (GXMFGs). Graphexes are the graph theoretical limiting objects to sparse graph sequences that also have other desirable features such as the small world property. Learning equilibria in these games is challenging due to the rich and sparse structure of the underlying graphs. To tackle these challenges, we design a new learning algorithm for the GXMFG setup. This hybrid graphex learning approach leverages that the system mainly consists of a highly connected core and a sparse periphery. After defining the system and giving theoretical results, we state our learning approach and demonstrate its capabilities on synthetic graphs and real-world networks. This comparison shows that our GXMFG learning algorithm successfully extends MFGs to a highly relevant class of hard, realistic learning problems that are not accurately addressed by current MARL and MFG methods.

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CP4

An Investigation into the Correlation between Wastewater Virus Levels and Underreported Positive Cases of COVID-19

This paper introduces a Bayesian spatial-temporal underreporting model, utilizing wastewater data to explore the correlation between normalized wastewater virus levels and actual positive COVID-19 cases. The model takes into account spatial and temporal dynamics, effectively addressing underreporting concerns and offering precise predictions for proactive outbreak management. By analyzing wastewater samples and integrating closely monitored demographic information, a minimum virus concentration linked to the presence of at least one COVID-19 case is identified, serving as a dependable early detection indicator. These findings contribute to the formulation of guidelines and early warning systems based on wastewater surveillance, enabling targeted resource allocation and the implementation of effective public health measures for controlling COVID-19 transmission.

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CP4

Vector Field Model of Chronic Kidney Disease Stage Enables Accurate Renal Prognosis Prediction

Chronic kidney disease (CKD) is the cause of end-stage kidney disease (ESKD), cardiovascular disease, and death, and is categorized into 18 stages on the basis of the estimated glomerular filtration rate (eGFR) and proteinuria. It is difficult to accurately predict CKD progression, because CKD stage cannot be mathematically analyzed in terms of scale and cut-off values. In this study, we determined whether CKD stage transformed into a vector field accurately predicts ESKD risk (CKD vector field model). The distance from stage G1 A1 to a patient's current stage in terms of on eGFR and proteinuria was defined, r. The model was constructed to reflect ESKD risk on the basis of r and validated using data from a cohort study of CKD patients in Japan followed up for three years (n=1,564). Moreover, the directional derivative of the model was developed as an index of CKD progression velocity. Cox proportional hazards models showed the exponential association between r and ESKD risk ($p < 0.0001$). The CKD potential model more accurately predicted ESKD with the areas under the receiver operating characteristic curves adjusted for baseline characteristics 0.81 (95% CI 0.76, 0.87) than CKD stage 0.59 (95% CI 0.54, 0.63) ($p < 0.0001$). Moreover, the directional derivative of the model better predicted the ESKD risk than eGFR slope ($p < 0.0001$). Those results indicated that the vector field model enables the accurate estimation of ESKD risk and CKD progression.

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CP4

Solution of Linear Ill-Posed Problems by Modified Truncated Singular Value Expansion

The numerical solution of linear ill-posed problems generally requires incorporation of regularization to yield a meaningful approximate solution. A common approach to compute a regularized approximate solution is to apply the truncated singular value expansion of the operator. A modification of the truncated singular value expansion for linear discrete ill-posed problems in finite dimensions has been described in [1], and was shown to furnish approximate solutions of higher quality than the standard truncated singular value expansion. This paper extends the modified singular value expansion to ill-posed problems in a Hilbert space setting. REFERENCES [1] S. Noschese and L. Reichel, A modified TSVD method for discrete ill-posed problems, Numerical Linear Algebra with Applications, 21

(2014), pp. 813822.

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CP5

Optimal Control for Coupled Sweeping Process under Minimal Assumptions

In this talk, we launch the study of nonsmooth optimal control problems involving a controlled sweeping process governed by a nonsmooth time-dependent sweeping set and coupled with controlled differential equations and having joint endpoints constraints. This general model incorporates different controlled submodels as a particular case including second order sweeping processes, a subclass of integro-differential sweeping processes, evolution variational inequalities (EVI), and dynamical variational inequalities (DVI). Essentially, after establishing the existence of optimal solutions for our general fixed time Mayer problem, we shall establish the full form of the nonsmooth Pontryagin maximum principle. This will be accomplished via a modification of the exponential-penalty approximation method and by using advanced tools from nonsmooth and variational analysis. The utility of the theoretical results will be illustrated with a numerical application.

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CP5

Multiphysics Time-Integration for Turbulent Combustion at the Exascale

Turbulent reacting flow systems are often modeled with coupled time-dependent partial differential equations (PDEs). Solving such equations can easily tax the worlds largest supercomputers. One pragmatic strategy for attacking such problems is to split the PDEs into components that can more easily be solved in isolation. This generic operator-splitting strategy leads to a set of ordinary differential equations (ODEs) that need to be solved as part of an outer-loop time-stepping approach. In many combustion applications, the ODEs to be solved can be very stiff, exhibiting timescales that span many orders of magnitude. The SUNDIALS library provides a plethora of robust time integration algorithms for solving these ODEs on exascale-capable computing hardware, yet for many complex applications (such multicomponent fuels or emissions predictions), the chemical models remain too complex to solve using reasonable resources. The Quasi-Steady State Approximation (QSSA) can be an effective tool for reducing the size and stiffness of the simulations. In this talk, I will discuss the use of the SUDIALS library of ODE solvers together with automatic code generation tools to solve complex turbulent reacting flow problems using QSSA models.

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CP5

Boundary Null Controllability of a Heat Equation with Two Nonlinearities and a Fourier-Type Boundary

In this presentation, we study the null controllability of a nonlinear heat equation with control contained in nonlinear Fourier-type boundary conditions. We demonstrate that, given appropriate assumptions on the data, and when the nonlinearities are of class $\mathcal{C}^2$ among others conditions, the system can be brought to rest at time T. To this end, we establish new Carleman estimates and use an observability inequality to discuss the null controllability of the linearized system. Finally, we prove the null controllability of the nonlinear problem through the application of Leray-Schauders fixed-point Theorem.

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CP5

Designing Quantum Gates Using High Order Hermite Methods

We seek to improve upon recent work in quantum optimal control by using a discrete adjoint approach with higher order numerical integrators. This can result in fewer timesteps being needed to evolve Schrodinger's equation accurately, which can decrease the cost of computing the gradient of the objective function. This decreases the cost of each iteration of the optimization process, reducing the time needed to find an 'optimal' gate. The main challenge in using the discrete adjoint approach with high-order numerical integrators is that the expressions used to timestep Schrodinger's equation become more complicated, which makes it even more complicated to find a choice of Lagrange multiplier which cancels out computationally expensive terms, which is an essential aspect of keeping the gradient computation inexpensive. By using implicit Taylor series methods based on Hermite quadrature, we can timestep Shcrodinger's equation with an arbitrarily high order of accuracy and still use the discrete adjoint approach to compute the gradient, which is then used to perform a second-order optimization via a quasi-Newton method. This method is implemented in the QuantumGateDesign.jl package.

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CP5

Phosphoev: Predicting Sites of Phosphorylation of

Proteins Using Enhancement Value Methodologies

Phosphorylation is a common type of post-translational modifications. Many types of machine learning methods, such as SVM, random forests and neural networks, have been constructed to predict phosphorylation sites. Here, we generated position-specific enhancement values (EV) using nearby amino acid sequences, 10 amino acids surrounding a site of interest. These values are calculated by taking the ratio of amino acids of the positive only locations to all potential phosphorylation sites and placed them in a lookup table. For cases where an amino acid is not present for a given position, a value of 1 is used within the table. Using this information, the enhancement value product (EVP) was calculated to determine the propensity of a site to be modified, a value greater than 1 being positive with higher values more likely. We performed the training and testing on Serine, Threonine or combination of both sites with negative sites chosen from the proteins containing at least one phosphorylation site on it. Accuracy values ranged from 70 to 84% depending on the value of the cutoff and number of amino acids to be included in calculation of the EVP. This method is being expanded to include other features, such as information on disorder content and secondary structure, to increase the accuracy of the method. The PhosPhoEV program will allow for researchers to see which features modify the EVP the most and can be used to determine effects of mutations surrounding sites of interest.

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CP5

Backprogation and Adjoint Differentiation of Chaos

Computing the linear response, or the derivative of long-time-averaged observables with respect to system parameters, is a central problem for statistics and engineering. Conventionally, there are three straight-forward formulas for the linear response: the pathwise perturbation (including the backpropagation method), the divergence, and the kernel differentiation formula. We shall explain why none works for the general case, which is typically chaotic, high-dimensional, and small-noise. We present the fast response formula, which is an 'ergodic-theorem' for the linear response of hyperbolic chaos. It is the average of some function of u-many vectors over an orbit, where u is the unstable dimension, and those vectors can be computed recursively. Then we discuss how to further incorporate the kernel differentiation trick to overcome non-hyperbolicity.

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MS1

Residual Alignment: The Key to Deciphering Layer-Wise Neural Collapse?

The ResNet architecture has been widely adopted in deep learning due to its significant boost to performance through the use of simple skip connections, yet the underlying mechanisms leading to its success remain largely unknown. In this talk, I will discuss a recently discovered phenomenon called Residual Alignment (RA) characterized by four properties that emerge when training ResNets: (RA1) intermediate representations of a given input are equispaced on a line, embedded in high dimensional space; (RA2) top left and right singular vectors of Residual Jacobians align with each other and across different depths; (RA3) Residual Jacobians are at most rank C for fully-connected ResNets, where C is the number of classes; and (RA4) top singular values of Residual Jacobians scale inversely with depth. RA consistently occurs in models that generalize well, in both fully-connected and convolutional architectures, across various depths and widths, for varying numbers of classes, on all tested benchmark datasets, but ceases to occur once the skip connections are removed. This phenomenon reveals a strong alignment between residual branches of a ResNet (RA2+4), imparting a highly rigid geometric structure to the intermediate representations as they progress linearly through the network (RA1) up to the final layer, where they undergo Neural Collapse.

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MS1

The Emergence of Reproducibility and Consistency in Diffusion Models

Recently, diffusion models have emerged as powerful deep generative models, showcasing cutting-edge performance across various applications. In this work, we uncover a distinct and prevalent phenomenon within diffusion models in contrast to most other generative models, which we refer to as "consistent model reproducibility'. To elaborate, our extensive experiments have consistently shown that when starting with the same initial noise input and sampling with a deterministic solver, diffusion models tend to produce nearly identical output content. This consistency holds true regardless of the choices of model architectures and training procedures. Additionally, our research has unveiled that this exceptional model reproducibility manifests in two distinct training regimes: (i) "memorization regime,' characterized by a significantly overparameterized model which attains reproducibility mainly by memorizing the training data; (ii) "generalization regime,' in which the model is trained on an extensive dataset, and its reproducibility emerges with the model's generalization capabilities. Our analysis provides theoretical justification for the model reproducibility in "memorization regime'. Moreover, our research reveals that this valuable property generalizes to many variants of diffusion models, including conditional diffusion models, diffusion models for solving inverse problems, and fine-tuned diffusion models.

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MS1

A Fractal Perspective on Scaling Laws of Large Language Models

Scaling laws provide a quantitative approach to understanding the relationship between the performance of large language models and the scale of computational resources and model size. This talk introduces a phenomenological theory that elucidates this quantitative aspect of large language models. A key feature of our theory is its adaptability in modeling real-world data through the application of fractal theory, yielding predictions that align with experimental observations.

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MS1

Anchor Function: A Benchmark Function for Studying Language Models

Understanding transformer-based language models is becoming increasingly crucial, particularly as they play pivotal roles in advancing towards artificial general intelligence. However, language model research faces significant challenges, especially for academic research groups with constrained resources. These challenges include complex data structures, unknown target functions, high computational costs and memory requirements, and a lack of interpretability in the inference process, etc. Drawing a parallel to the use of simple models in scientific research, we propose the concept of an anchor function. This is a type of benchmark function designed for studying language models in learning tasks that follow an “anchor-key’ pattern. By utilizing the concept of an anchor function, we can construct a series of functions to simulate various language tasks. The anchor function plays a role analogous to that of mice in diabetes research, particularly suitable for academic research. We demonstrate the utility of the anchor function with an example, revealing two basic operations by attention structures in language models: shifting tokens and broadcasting one token from one position to many positions. These operations are also commonly observed in large language models. The anchor function framework, therefore, opens up a series of valuable and accessible research questions for further exploration, especially for theoretical study.

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MS2

Where Can Advanced Optimization Methods Help in Deep Learning?

Modern neural network models are trained using fairly standard stochastic gradient optimizers, sometimes employing mild preconditioners. A natural question to ask is whether significant improvements in training speed can be obtained through the development of better optimizers. In this talk I will argue that this is impossible in the large majority of cases, which explains why this area of research has stagnated. I will go on to identify several situations where improved preconditioners can still deliver significant speedups, including exotic architectures and loss functions, and large batch training.

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MS2

Deep Neural Network Initialisation: Nonlinear Activations Impact on the Gaussian Process

Randomly initialised deep neural networks are known to generate a Gaussian process for their pre-activation intermediate layers. We will review this line of research with extensions to deep networks having structured random entries such as block-sparse or low-rank weight matrices. We will then discuss how the choice of nonlinear activations impacts the evolution of the Gaussian process. Specifically we will discuss why sparsifying nonlinear activations such as soft thresholding are unstable, we will show conditions to overcome such issues, and we will show how non-sparsifying activations can be improved to be more stable when acting on a data manifold. This work is joint with Michael Murray (UCLA), Vinayak Abrol (IIIT Delhi), Ilan Price (DeepMind), and from Oxford: Alireza Naderi, Thiziri Nait Saada, Nicholas Daultry Ball, Adam C. Jones, and Samuel C.H. Lam.

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MS2

Beyond Backpropagation: a Lifted Bregman Formulation of Training Neural Networks

We introduce a novel mathematical formulation for the training of neural networks with (potentially non-smooth) proximal maps as activation functions. This formulation is based on Bregman distances and a key advantage is the simplicity of its partial derivatives with respect to the networks parameters. We investigate the use of non-smooth first-order optimization methods in parameter estimation, which exploits the specific structure of this formulation. In addition, we showcase an example where this framework is adapted to the regularized inversion of deep neural networks. We propose a family of variational regularizations based on these Bregman distances. Theoretical results as well as numerical results are presented to support the effectiveness of this framework on practical applications.

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MS3

Adapting Properties of Matrix Rank to the Ranks of Tensors

The notion of rank on matrices has been generalised in several different ways to notions of rank on higher-order tensors. Which of these notions is the most useful depends on the context and problem at hand, and none of them is viewed as the single canonical generalisation of matrix rank. We will review several of these notions as well as why they were introduced, and then discuss how various properties of matrix rank extend to them once suitable adaptations are made.

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MS3

Polynomial Codes and Tensor Decompositions

I will talk about a few recent and not-so-recent results which yield interesting consequences for polynomial codes by studying related basic combinatorial and geometric questions about tensors.

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MS3

Discreteness of Asymptotic Tensor Ranks

Several recent works have investigated and showed properties of the images of asymptotic ranks for 3-tensors in some regimes. Blatter, Draisma and Rupniewski showed they are well-ordered over finite fields (under some conditions for the ranks); Christandl, Vrana and Zuiddam showed a characterisation of asymptotic slice-rank over the complex numbers which implies its image is countable; and Blatter, Draisma and Rupniewski extended this to show it holds for any rank measure that is algebraic (that is invariant under any automorphism of the complex numbers). The question of whether the image, as a countable set, contains points that accumulate, meaning that converge to a limit, remained open even over finite fields (a well ordered set can still contain such points, if the points converge to a limit from below). We show for a family of measures, including the asymptotic rank, asymptotic subrank and asymptotic slice-rank, that for every fixed set of coefficients that is finite (e.g. a finite field), their image over all 3-tensors with these coefficients is discrete, i.e. has no such converging sequences. We also show the same for the asymptotic slice-rank over all of the complex numbers (without fixing a finite set). Our results rests mainly on a new type of lower bounds for the asymptotic subrank, merely by the dimensions of the three ambient spaces (for concise tensors) and by considering the maximal and minimal ranks of matrices spanned by the slices of any tensor.

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MS3

Tensor Ranks and the Fine-Grained Complexity of Dynamic Programming

Generalizing work of Knnemann, Paturi, and Schneider [ICALP 2017], we study a wide class of high-dimensional dynamic programming (DP) problems in which one must find the shortest path between two points in a high-dimensional grid given a tensor of transition costs between nodes in the grid. This captures many classical problems which are solved using DP such as the knapsack problem, the airplane refueling problem, and the minimal-weight polygon triangulation problem. We observe that for many of these problems, the tensor naturally has low tensor rank or low slice rank. We then give new algorithms and a web of fine-grained reductions to tightly determine the complexity of these problems. For instance, we show that a polynomial speedup over the DP algorithm is possible when the tensor rank is a constant or the slice rank is 1, but that such a speedup is impossible if the tensor rank is slightly super-constant (assuming SETH) or the slice rank is at least 3 (assuming the APSP conjecture). We find that this characterizes the known complexities for many of these problems, and in some cases leads to new faster algorithms.

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MS4

Stability of Nematic State in Periodically Modulated Nematic Phases

Nematic liquid crystals composed of bent-core molecules may exhibit periodically modulated structure. One of these phases is the twist bend nematic phase where the molecules are arranged in a heliconical structure with a nanoscale pitch. This can be characterized when the bend elastic constant is much smaller than both splay and twist elastic ones. We study the model of the twist bend nematic phase that allows the bend elastic constant to be small but in the positive range and attain its minimizer in one dimensional setting. We also characterize the parameter regime for the stability of the global and local minimizers of the nematic phase under the homeotropic boundary condition. Numerical simulations based on the constrained minimization is used to illustrate the predictions of the analysis. This is a joint work with C. Garcia-Cervera, T. Giorgi, and Z. Li.

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MS4

Multi-Block Copolymers: Decorated Phases

Energies governing the behavior of copolymers are often made of a local term, plus a long range interaction. The former generally has a coagulating effect, favoring fewer but bigger components, while the latter has a splitting effect, favoring smaller, more numerous components. Therefore, optimal configurations must arrange themselves to strike a balance between those two competing forces. In this talk, we will present some recent results in this direction.

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MS4

Nonlocal Effects on a Generalized OhtaKawasaki Model and Its Asymptotically Compatible Scheme

We propose a generalized OhtaKawasaki model to study the nonlocal effect on the pattern formation of some binary systems with general long-range interaction.By performing Fourier analysis in the 1D case, we find that the optimal number of bubbles for the generalized model may have an upper bound no matter how large the repulsive strength is. The existence of such an upper bound is characterized by the eigenvalues of the nonlocal kernels. Additionally, we explore the conditions under which the nonlocal horizon parameter may promote or demote the bubble splitting, and apply the analysis framework to several case studies for various nonlocal operators. Meanwhile, we study its asymptotical compatibility of the Fourier spectral method in multidimensional space. We show that the asymptotical compatibility holds in 2D and 3D over a periodic domain by introducing the Fourier collocation discretization, and adopt the second-order backward differentiation formula (BDF) method in time which inherits the energy dissipation law. In the numerical experiments, we verify the asymptotical compatibility, the second-order temporal convergence rate, and the energy stability of the proposed schemes. More importantly, we discover a novel square lattice pattern when certain nonlocal kernel are applied in the model. In addition, the experiments confirm the existence of an upper bound for the optimal number of bubbles in 2D for some specific nonlocal kernels.

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MS4

A New Proof of the Number of Steady Solutions to a 2D Smoluchowski Equation

In this paper, we re-examine a 2D Smoluchowski equation employed for modeling nematic liquid crystalline polymers. Specifically, we provide a novel proof concerning the investigation of steady-state solutions to the 2D Smoluchowski equation. We establish that when the intensity constant is less than or equal to 4, a unique (trivial) solution exists. Conversely, when the intensity constant exceeds 4, precisely two solutions emerge, corresponding to the isotropic and nematic phases, respectively. Notably, the proof relies solely on calculus, rendering it more transparent and accessible.

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MS5

Analyzing the Loss Landscape of Mildly Overparameterized Neural Networks

In this talk I'll discuss techniques for analyzing the loss landscape of both shallow and deep, mildly overparameterized ReLU networks with width growing as $\Omega(n\log(n))$ where n is the size of the training set. For a generic, finite input dataset and the squared error loss we show both by count and volume that most activation patterns correspond to parameter regions with no bad local minima. Furthermore, for one-dimensional input data, we show most activation regions realizable by the network contain a high dimensional set of global minima and no bad local minima. We experimentally confirm these results by finding a phase transition from most regions having full rank Jacobian to many regions having deficient rank depending on the amount of overparameterization. Recent extensions to understanding the conditioning of the NTK will also be discussed. Joint work with Kedar Karhadkar, Hanna Tseran and Guido Montfar.

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MS5

Achieving Acceleration Despite Very Noisy Gradients

We consider accelerated first-order optimization methods for smooth convex problems with noisy gradients where the noise intensity is proportional to the magnitude of the gradient. We show that Nesterov's accelerated gradient descent does not converge under this noise model if the ratio between the variance and the gradient norm exceeds one. We propose a new method (AGNES) which fixes this deficiency and provably achieves an accelerated convergence rate no matter how small the signal to noise ratio in the gradient estimate is, and compare AGNES with existing methods in the literature. Finally, we test the efficacy of AGNES for the training of CNNs.

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MS5

Proximal Mean Field Learning in Shallow Neural Networks

We propose a custom learning algorithm for shallow overparameterized neural networks, i.e., networks with single hidden layer having infinite width. The infinite width of the hidden layer serves as an abstraction for the overparameterization. Building on the recent mean field interpretations of learning dynamics in shallow neural networks, we realize mean field learning as a computational algorithm, rather than as an analytical tool. Specifically, we design a Sinkhorn regularized proximal algorithm to approximate the distributional flow for the learning dynamics over weighted point clouds. In this setting, a contractive fixed point recursion computes the time-varying weights, numerically realizing the interacting Wasserstein gradient flow of the parameter distribution supported over the neuronal ensemble. An appealing aspect of the proposed algorithm is that the measure-valued recursions allow meshless computation. We demonstrate the proposed computational framework of interacting weighted particle evolution on binary and multi-class classification. Our algorithm performs gradient descent of the free energy associated with the risk functional.

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MS5

Neural Network Approaches for Parametric Optimal Control

In this talk, we explore numerical approaches for deterministic, finite-dimensional optimal control problems with dynamics dependent on unknown or uncertain parameters. Our aim is to streamline the solution process over a set of relevant parameters offline, facilitating swift decision-making and adaptability to parameter changes online. To address the curse of dimensionality inherent in high-dimensional state and/or parameter spaces, we employ neural networks to represent the policy. We compare two training strategies: Firstly, our model-based approach utilizes the problem dynamics and objective function definition to learn the value function and derive the policy through feedback. Secondly, we employ actor-critic reinforcement learning to approximate the policy through data-driven methods. Using an example involving a two-dimensional convection-diffusion equation, which features high-dimensional state and parameter spaces, we investigate the accuracy and efficiency of both training paradigms. While both paradigms lead to a reasonable approximation of the policy, the model-based approach is more accurate and considerably reduces the number of PDE solves.

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MS6

Stochastic Population Dynamics in Discrete Time

We present a general theory for coexistence and extinction of ecological communities that are influenced by stochastic temporal environmental fluctuations. The results apply to discrete time stochastic difference equations and we can also include in the dynamics auxiliary variables that model environmental fluctuations, population structure, eco-environmental feedbacks or other internal or external factors. Using the general theory, we work out several examples including the Ricker model, Log-normally distributed offspring models, lottery models, discrete Lotka-Volterra models as well as models of perennial and annual organisms.

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MS6

Stochastic Nutrient-Plankton Models

We analyze plankton-nutrient food chain models composed of phytoplankton, herbivorous zooplankton and a limiting nutrient. These models have played a key role in understanding the dynamics of plankton in the oceanic layer. Given the strong environmental and seasonal fluctuations that are present in the oceanic layer, we propose a stochastic model for which we are able to fully classify the longterm behavior of the dynamics. In order to achieve this we had to develop new analytical techniques, as the system does not satisfy the regular disspativity conditions and the analysis is more subtle than in other population dynamics models.

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MS6

Large Timescale Diffusion Approximation in Stochastic Logistic Models

It is well known that diffusion approximations of birth-and-death processes (BDP) give rise to stochastic differential equations (SDE) generating absorbed singular diffusions. Such approximation procedures are usually derived only over a finite time interval. It is interesting to compare the dynamics of the BDP and SDE models during a larger timescale. In this talk, we will discuss this issue by comparing the long transient dynamics and quasi-stationary distributions of these two models.

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MS6

WKB Approximation of Quasi-stationary Distributions with Applications

Quasi-stationary distribution (QSD) is a powerful tool in characterizing the local dynamics of a dynamical system under noise perturbations. Its WKB approximation can be used to extract essential dissipative and conservative structures, thus aiding in gaining a clearer understanding of the local dynamics. This talk is dedicated to discussing recent mathematical advancements surrounding the WKB approximation of QSDs and their applications.

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MS7

Gamma Convergence for the De Gennes-Cahn-Hilliard Energy

The degenerate de Gennes-Cahn-Hilliard (dGCH) equation is a model for phase separation which may more closely approximate surface diffusion than others in the limit when the thickness of the transition layer approaches zero. As a first step to understand the limiting behavior, we present the Gammalimit of the dGCH energy. We find that its Gammalimit is a constant multiple of the interface area, where the constant is determined by the de Gennes coefficient together with the double well potential. In contrast, the transition layer profile is solely determined by the double well potential. We will also present results about the classification of minimizers for the dGCH energy.

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MS7

A Discontinuous Galerkin Method for the Allen-Cahn Equation

We present an energy-stable hybridizable interior penalty discontinuous Galerkin method for the Allen-Cahn equation. To obtain an unconditionally energy stable scheme, the energy potential is split into a sum of a convex and concave function. Energy stability for the proposed scheme is proven to hold for arbitrary time. Existence and uniqueness for the scheme is also established. Under standard assumptions on the energy potential (Lipschitz continuity), we demonstrate rigorously that the method converges optimally for symmetric schemes, and sub optimally for nonsymmetric schemes.

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MS7

Unconditionally Stable Numerical Methods for Cahn-Hilliard-Navier-Stokes-Darcy System with Different Densities and Viscosities

In this presentation, we consider the numerical modeling and simulation via the phase field approach for coupled two-phase free flow and two-phase porous media flow of different densities and viscosities. The model consists of the Cahn-Hilliard-Navier-Stokes equations in the free flow region and the Cahn-Hilliard-Darcy equations in porous media that are coupled by several domain interface conditions. It is showed that the coupled model satisfies an energy law. Then we first propose a coupled unconditionally stable finite element method for solving this model and analyze the energy stability for this method. Furthermore, based on the ideas of pressure stabilization and artificial compressibility, we propose an unconditionally stable time stepping method that decouples the computation of the phase field variable, the velocity and pressure of free flow, the velocity and pressure of porous media, hence significantly reduces the computational cost. The energy stability of this decoupled scheme with the finite element spatial discretization is rigorously established. We verify numerically that our schemes are convergent and energy-law preserving. Numerical experiments are also performed to illustrate the features of two-phase flows in the coupled free flow and porous media setting.

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MS7

Dynamics of Non-Conservative Phase Field Models

Phase field models describe dynamics of complex systems in many settings. This includes the classic Cahn-Hilliard equation for binary mixtures of liquid metals and the unstable thin film equation for dewetting of viscous fluids on hydrophobic substrates. These models are given by fourth-order nonlinear parabolic partial differential equations whose solutions conserve mass and evolve according to gradient flows dissipating an energy functional. To model applications like tumor growth in biology or evaporation and condensation of fluid drops, non-conservative forms of these equations have been studied. Long-time coarsening dynamics in these models can require different analytical approaches. When the equations also no longer follow gradient flows, then dramatically more complicated dynamics (including finite time singularities and limit-cycle oscillations) can occur in the weakly conservative limit.

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MS8

On a Geometric Partitioning Problem with Both Finite and Infinite Area Constraints

We consider the problem of partitioning the plane into three disjoint domains, one having unit area and the remaining two having infinite area, for which perimeter is minimized. We show that the only solution, up to rigid motions of the plane, is a lens cluster consisting of circular arcs containing the finite area region, attached to a single axis, with two triple junctions where the arcs meet at 120 degree angles. In particular, we show that such a configuration is a local minimizer of the total perimeter functional, and on the other hand any local minimizer of perimeter among clusters with the given area constraints must coincide with a lens cluster having this geometry. Some known results and conjectures on similar problems with both finite and infinite area constraints are also presented. Improper partitioning problems of this type arise in the study of phase separation in models of triblock copolymers.

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MS8

Rigidity of the Eikonal Equation with L^p Entropies

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

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MS8

Negative Power of Laplacian As a Long Range Force in Growth and Inhibition Systems

A geometric variational problem is proposed 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, $(-\Delta)^{-s}$, provides an inhibitory force. It is shown that when $s \in (\frac{1}{2}, \frac{d}{2}]$, where $d = 2$ or 3 is the dimension of the space, neither the growth force nor the inhibition force dominates the system. The two forces still compete and compromise if $d = 3$ and $s = 2$. However, if $d = 2$ and $s = 2$, the growth tendency may overwhelm the inhibition force. Another discussed property for $s \in (\frac{1}{2}, \frac{d}{2}]$ is coarsening: large components grow larger while small components shrink and disappear.

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MS8

A Phase Field Approximation of a Degenerate Ohta-Kawasaki Energy

We study the minimizers of a degenerate case of the Ohta-Kawasaki energy, defined as the sum of the perimeter and a Coulombic nonlocal term. We investigate radially symmetric candidates which give us insights into the asymptotic behaviors of energy minimizers in the large mass limit. In order to numerically study the energy, we propose a phase-field reformulation which is shown to Gamma-converge to the original model in the sharp interface limit. Our phase-field simulations and asymptotic results suggest that the energy minimizers exhibit behaviors similar to the self-assembly of amphiphiles, including the formation of lipid bilayer membranes.

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MS9

How to Learn from Data in Optimal Harvesting Problems - An Approach Based on Statistics

Theoretical solutions to many stochastic control problems, such as optimal harvesting problems, are well known, but their practical applicability often suffers from the assumption of known dynamics of the underlying stochastic process. This leads to the statistical challenge of developing purely data-driven controls in a non-parametric framework. In this talk, we discuss how to bring together stochastic control and statistics, which we explore for ergodic singular control problems and underlying one- and multi-dimensional diffusions. Among others, they include classic models for optimal resource management. The exploration vs. exploitation dilemma plays an essential role in the considerations. We find exact rates of convergence of sublinear order for the regret and compare the results with those of deep Q-learning algorithms.

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MS9

Bridging Adaptive Management and Reinforcement Learning for More Robust Decisions

Control problems involving complex systems of interacting populations are widespread in environmental science. In this talk, we focus on a classic example of such a proble: fishery management. Specifically, we our problem is the following: how does one adaptively establish fishery quotas in a way that allows long-term sustainable fishing and avoids population crashes? We explore the application of reinforcement learning (RL) to this question. Our results indicate that RL can provide advantages over standard fishery management strategies such as maximum sustainable yield and constant escapement. The key to our result is RL's flexibility to accommodate model complexity, something that optimal control approaches have a hard time with. By using rich observation and action spaces, RL-derived policies can be more responsive to fluctuations in the environment, leading to a more robust management of the fishery. Finally, we will discuss new applications of this framework to different environmental management problems such as biodiversity conservation and invasive species management.

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MS9

The Tempo and Mode of Environmental Fluctuations Matter for Population Growth

Populations consist of individuals living in different states and experiencing temporally varying environmental conditions. Individuals may differ in their geographic location, stage of development (e.g. juvenile versus adult), or physiological state (infected or susceptible). Environmental conditions may vary due to abiotic (e.g. temperature) or biotic (e.g. resource availability) factors. As survival, growth, and reproduction of individuals depend on their state and the environmental conditions, environmental fluctuations often impact population growth. Here, we examine to what extent the tempo and mode (i.e. periodic versus random) of these fluctuations matter for population growth. To this end, we model population growth for a population with m individual states and experiencing n different environmental states. The models are switching, linear ordinary differential equations $x'(t) = A(\sigma(t/\omega))x(t)$ where $x(t) = (x_1(t), \dots, x_m(t))$ corresponds to the population densities in the m individual states, $\sigma(t)$ is a piecewise constant function representing the fluctuations in the environmental states $1, \dots, n$, ω is the frequency of the environmental fluctuations, and $A(1), \dots, A(n)$ are Metzler matrices representing the population dynamics in the environmental states $1, \dots, n$. $\sigma(t)$ can either be a periodic function or a continuous-time Markov chain. Under suitable conditions, there exists a Lyapunov exponent $\Lambda(\omega)$ such that $\lim_{t \to \infty} \frac{1}{t} \log \sum_i x_i(t) = \Lambda(\omega)$ for all nonnegative, non-zero initial conditions $x(0)$ (with probability one in the random case). For both the random and deterministic models, we derive analytical first-order and second-order approximations of $\Lambda(\omega)$ in the limits of slow $(\omega \to 0)$ and fast $(\omega \to \infty)$ environmental fluctuations. These approximations show that typically the long-term population growth rate $\Lambda(\omega)$ depends both on the tempo (ω) and mode (random versus deterministic) of the environmental fluctuations. Applications to stage-structured and spatially-structured models will be used to illustrate this conclusion.

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MS9

Harvesting of a Stochastic Population Under a Mixed Regular-Singular Control Formulation

This talk focuses on optimal harvesting-renewing for a stochastic population. A mixed regular-singular control formulation with a state constraint and regime switching is introduced. The decision-makers either harvest or renew at finite or infinite harvesting/renewing rates. The payoff functions depend on the harvesting and renewing rates. Several properties of the value function are established. The limiting value function as the white noise intensity approaches infinity is identified. The Markov chain approximation method is used to find numerical approximations of the value function and optimal strategies.

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MS10

Iterative Slicing-and-Matching Schemes for Measure Transport

We study iterative schemes for measure transfer and approximation problems, which are defined through a slicing-and-matching procedure. Similar to the sliced Wasserstein distance, these schemes benefit from the availability of closed-form solutions for the one-dimensional optimal transport problem and the associated computational advantages. While such schemes have already been successfully utilized in data science applications, not too many results on their convergence are available. Our main contribution is an almost sure convergence proof for stochastic slicing-and-matching schemes. The proof builds on an interpretation as a stochastic gradient descent scheme on the Wasserstein space. Numerical examples on step-wise image morphing are demonstrated as well.

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MS11

Reconstructing Transition Dynamics from Static Single-Cell Genomic Data

Recently, single-cell transcriptomics has provided a powerful approach to investigate cellular properties in unprecedented resolution. However, given a small number of temporal snapshots of single-cell transcriptomics, how to connect them to obtain their collective dynamical information remains an unexplored area. One major challenge to connecting temporal snapshots is that cells measured at one temporal point may divide at the next temporal point, leading to growth and differentiation in the system. Its increasingly clear that without incorporating cellular growth dynamics, the inferred dynamics often becomes incomplete and less accurate. To fill these gaps, we present a novel method to reconstruct the growth and dynamic trajectory simultaneously as well as the underlying gene regulatory networks. A deep learning-based dynamic unbalanced optimal transport is developed to infer interpretable dynamics from high-dimensional datasets.?

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MS11

Unraveling Cellular Dynamics and Protein Folding with Optimal Transport and Language Models

Recent advancements in machine learning have revolutionized our ability to model and analyze complex spatiotemporal systems. In this talk, we will present several novel approaches that leverage optimal transport, transformers, operator learning, and language models to tackle fundamental challenges in this domain. First, we introduce CINEMA-OT, a causal-inference-based approach to single-cell perturbation analysis that employs optimal transport to match counterfactual cell pairs. We demonstrate CINEMA-OT's superior performance on various datasets, including airway antiviral response and immune cell recruitment. Next, we present the Continuous Spatiotemporal Transformer (CST), a new transformer architecture designed for modeling continuous systems. By optimizing in Sobolev space, CST guarantees continuous and smooth outputs, overcoming limitations of traditional transformers. We then discuss Neural Integral Equations (NIE), a method that learns unknown integral operators from data. This approach models spatiotemporal systems with non-local dependencies with wide-ranging applications in the sciences. Finally, we introduce CaLMFlow, a novel flow matching method based on Volterra integral equations and causal language models. We apply CaLMFlow to predict single-cell perturbation responses and protein backbone generation. These advancements offer powerful tools for modeling and understanding continuous spatiotemporal systems, with impact across many scientific domains.

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MS12

Effects of Dispersal on Population Dynamics under Stochastic Environment

We study the dynamics of a species whose population is scattered between n patches, and individuals disperse between these patches. In the discrete case we consider the Beverton-Holt model, with a small random perturbation in the intrinsic growth, $r_i = \overline{r}_i + \rho\xi(t)$ and show that we can estimate the mean and covariance of the total population in terms of the parameter ρ. For the continuous time setting we consider SDE version of the ODE model given in Grumbach et al JOMB '23, and show when we get extinction, or when the total population converges to nonatomic stationary distribution. We also consider models where there is noise, and/or random switching between finitely many states, where we show that a piecewise deterministic Markov process (PDMP) can be approximated by an ODE, as the rate of switching increases to infinity, and an SSDE will become an SDE, while if the noise parameter goes to zero an SSDE will become a PDMP, and an SDE will become an ODE.

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MS12

Optimal Control by Deep Learning Techniques and Its Applications on Epidemic Models

Neural networks, though called as black-box uniform approximator and difficult to interpret, have an unreasonable effectiveness in learning unknown mechanisms with bless of dimensionality, and have lots of applications. In this talk, I will introduce a recent state-of-the-art universal differential equation method that embeds neural networks into differential equations. Three applications will be shown. (1) Using deep learning techniques to estimate effective reproduction number and compared with EpiEstim and EpiNow2 method. (2) Discovering unknown human behavior change mechanisms in transmission dynamics. (3) Using deep learning techniques to solve optimal control problems by representing optimal control function as neural networks, and compared with traditional direct, indirect, and dynamic programming methods.

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MS12

Square Root Identities for the Harvested Beverton-Holt Model

We study the effects of a periodically varying environment on a harvested discrete logistic model. This leads to the formulation of three square root identities that identify economically and sustainably favored harvest levels. We then include uncertainty in a populations proliferation rate, which sparks a risk sensitivity analysis regarding the probability of populations falling below an unsustainable threshold. Corresponding risk sensitivity plots reveal risk bow ties.

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MS12

Optimal Harvesting of Stochastic Populations - Theoretical Results and Numerical Methods

We consider the problem of harvesting from a stochastic population while avoiding extinction. Using ergodic optimal control, we find the optimal harvesting strategy which maximizes the asymptotic yield of harvested individuals. When the benefit is linear in the harvested amount, we find that a bang-bang strategy is optimal under very general conditions. The effects of parameter changes are explored. More realistic environments have very complex stochasticity. On top of the usual white-noise environmental variation, there can be seasonal variation, and the environment can suffer from large but random changes. It is likely impossible to explicitly solve complex models with many layers of stochasticity, but numerical methods can help and therefore the models are useful. We find theoretical results that justify the use of the Markov chain approximation method, developed by Kushner Martins (1991) and Kushner Dupuis (1992), in finding numerical approximations of the optimal strategies and value functions in a very large class of models. These models can have general cost functions of harvesting or seeding, price functions reactive to market conditions and random fluctuations, seasonal fluctuations, and large-scale random fluctuations. The numerical methods are used to explore for interesting intuitions and unusual findings, which would not have been available theoretically.

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MS13

Multi-Layer Neural Networks as Trainable Ladders of Hilbert Spaces

An important aspect of deep learning theory is to characterize the space of functions explored by neural networks (NNs). Prior works have studied the function space and training dynamics of shallow (one-hidden-layer) NNs by representing them as integrals over probability measures. In this talk, I will present an extension of such a distributional perspective to the analysis of deeper NNs, which has been challenging previously. In this view, a multi-layer NN corresponds to a ladder of kernel functions and reproducing kernel Hilbert spaces (RKHSs) that can evolve through training, allowing us to define a function space and a complexity measure with theoretical properties and implications that we examine in several aspects. First, the complexity measure controls both the approximation and the generalization errors for learning functions in this space. Second, corresponding to the training of multi-layer NNs in the infinite-width mean-field limit, we characterize the evolution of the ladder of RKHSs as the dynamics of multiple random fields with global convergence guarantees in certain cases. Third, we show examples of depth separation where increasing the model depth expands the corresponding function space.

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MS13

Revisiting Neural Network Approximation Theory in the Age of Generative AI

Textbooks on deep learning theory primarily perceive neural networks as universal function approximators. While this classical viewpoint is fundamental, it inadequately explains the impressive capabilities of modern generative AI models such as language models and diffusion models. This talk puts forth a refined perspective: neural networks often serve as algorithm approximators, going beyond mere function approximation. I will explain how this refined perspective offers a deeper insight into the success of modern generative AI models.

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MS13

Aligning with Local Landscape: Theoretical Insights into the Structure of Sgd Noise

In this paper, we provide a theoretical study of noise geometry for minibatch stochastic gradient descent (SGD), a phenomenon where noise aligns favorably with the geometry of local landscape. We propose two metrics, derived from analyzing how noise influences the loss and subspace projection dynamics, to quantify the alignment strength. We show that for (over-parameterized) linear models and two-layer nonlinear networks, when measured by these metrics, the alignment can be provably guaranteed under conditions independent of the degree of over-parameterization. To showcase the utility of our noise geometry characterizations, we present a refined analysis of the mechanism by which SGD escapes from sharp minima. We reveal that unlike gradient descent (GD), which escapes along the sharpest directions, SGD tends to escape from flatter directions and cyclical learning rates can exploit this SGD characteristic to navigate more effectively towards flatter regions. Lastly, extensive experiments are provided to support our theoretical findings.

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MS13

Local Linear Recovery Guarantee of Deep Neural Networks at Overparameterization

Determining whether deep neural network (DNN) models can reliably recover target functions at overparameterization is a critical yet complex issue in the theory of deep learning. To advance understanding in this area, this talk introduces a concept we term “local linear recovery’ (LLR), a weaker form of target function recovery that renders the problem more amenable to theoretical analysis. In the sense of LLR, functions expressible by narrower DNNs are guaranteed to be recoverable from fewer samples than model parameters. We will provide upper bounds on the optimistic sample sizes, defined as the smallest sample size necessary to guarantee LLR, for functions in the space of a given DNN. These upper bounds are achieved in the case of two-layer tanh neural networks. Our results lay a solid ground to future investigations into the recovery capabilities of DNNs in overparameterized scenarios.

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MS14

An ADMM-LAP Method for Total Variation Myopic Deconvolution of Adaptive Optics Retinal Images

Adaptive optics corrected flood imaging of the retina is a popular technique for studying the retinal structure and function in the living eye. However, the raw retinal images are usually of poor contrast and the interpretation of such images requires image deconvolution. Different from standard deconvolution problems where the point spread function (PSF) is completely known, the PSF in these retinal imaging problems is only partially known which leads to the more complicated myopic (mildly blind) deconvolution problem. We propose an efficient numerical scheme for solving this myopic deconvolution problem with total variational (TV) regularization. First, we apply the alternating direction method of multipliers (ADMM) to tackle the TV regularizer. Specifically, we reformulate the TV problem as an equivalent equality constrained problem where the objective function is separable, and then minimize the augmented Lagrangian function by alternating between two (separated) blocks of unknowns to obtain the solution. Due to the structure of the retinal images, the subproblems with respect to the fidelity term appearing within each ADMM iteration are tightly coupled and a variation of the linearize and project method is designed to solve these subproblems efficiently. The proposed method is called the ADMM-LAP method. Theoretically, we establish the subsequence convergence of the ADMM-LAP method to a stationary point.

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MS14

New Methods for Nonstationary Anisotropic Tikhonov Regularization

Regularization techniques are necessary to compute meaningful solutions to discrete ill-posed inverse problems. The well-known Tikhonov regularization method equipped with a discretization of the gradient operator as regularization operator penalizes large gradient components of the solution to overcome instabilities. However, this method is homogeneous, i.e., it does not take into account the structure of the regularized solution and therefore tends to smooth the desired structures and discontinuities, which often contain important information. A possible way to overcome this issue is to implement local anisotropic regularization by penalizing weighted directional derivatives, which requires prior knowledge of the local orientation field of the solution. This talk introduces two new methods that automatically and simultaneously recover the regularized solution and the local orientation parameters for the novel anisotropic regularization term by either applying an alternating minimization scheme or by solving a bilevel optimization problem. Application of the proposed algorithms to the denoising of various synthetic and real data with complex structures shows their effectiveness and robustness; their performance is also successfully demonstrated on linear inverse problems in geophysics, tomography and image restoration.

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MS15

Features of the Geometry of Loss Landscapes

Today, training neural networks is accomplished by using a gradient based algorithm to minimize the loss function L of the neural network. Therefore, the underlying geometry of L is of interest. While much remains unknown, in this talk we will discuss some features that have been studied in recent years.

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MS15

Structure and Gradient Dynamics Near Global Minima of Deep Neural Networks

In this talk, we will present new results on the structure of global minima of two-layer neural networks. This structure is hierachical, and different level may have different ability for generalization. In particular, we determine the set of parameters which give perfect generalization and fully characterize the gradient flows around it. With novel techniques, our work uncovers some simple aspects of the complicated loss landscape and reveals how model, target function, samples and initialization affect the training dynamics differently. Based on these results, we also explain why (overparametrized) neural networks could generalize well.

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MS15

Why is Adam Better than SGD on Transformers?

Adam is the default algorithm for training large foundation models. In this talk, we aim to understand why Adam is better than SGD on training large foundation models, and propose a memory-efficient alternative called Adam-mini. First, we provide an explanation of the failure of SGD on transformer: (i) Transformers are "heterogeneous": the Hessian spectrum across parameter blocks vary dramatically; (ii) Heterogeneity hampers SGD: SGD performs badly on problems with block heterogeneity. Second, motivated by this finding, we introduce Adam-mini, which partitions the parameters according to the Hessian structure and assigns a single second momentum term to all weights in a block. We empirically show that Adam-mini saves 45-50% memory over Adam without compromising performance, on various models including 7B-size language models and ViT.

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MS16

Learning Deep Linear Neural Networks: Riemannian Gradient Flows and Convergence to Global Minimizers

We study the convergence of gradient flows related to learning deep linear neural networks (where the activation function is the identity map) from data. In this case the composition of the network layers amounts to simply multiplying the weight matrices of all layers together resulting in an overparameterized problem. The gradient flow with respect to these factors can be re-interpreted as a Riemannian gradient flow on the manifold of rank-r matrices endowed with a suitable Rie- mannian metric. We show that the flow always converges to a critical point of the underlying functional. Moreover we establish that for almost all initializations the flow converges to a global minimum on the manifold of rank matrices for some k =¡ r.

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MS16

Recent Advances in Riemannian Optimization for Deep Learning

Past years have seen several attempts to exploit Riemannian optimization to handle constraints/invariances in neural networks, for example when imposing low-rankness or orthogonality constraints on the weights of the model. This talk will present recent progress along these research direction.

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MS16

Efficient Training of Deep Neural Networks with Gauss-Newton-Like Methods

Deep neural networks (DNNs) have achieved inarguable success as high-dimensional function approximators in countless fields, including numerous scientific applications such as surrogate modeling, operator learning, and model discovery. However, this success comes at significant hidden costs, notably a long training time. Typically, training is posed as a stochastic optimization problem to learn the DNN weights. However, we can interpret training as solving a high-dimensional, nonlinear data fitting problem for which Gauss-Newton has traditionally been the go-to optimization strategy. Despite this tradition, Gauss-Newton has not gained widespread use for DNN training, often due to computational bottlenecks. In this talk, we propose a memory and computationally efficient Gauss-Newton implementation that can solve the training problem well and learn weights that generalize. We will describe how we obtain this efficiency by approximating the Jacobian with only a few additional passes through the network. We will outline how our optimizer reliably solves the training problem using a trust-region method. We will demonstrate the computational advantages of our approach over traditional stochastic optimizers on several benchmark deep learning tasks

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MS16

Implicit Bias of Gradient Descent for Learning Neural Networks

Deep neural networks are usually trained by minimizing a non-convex loss functional via (stochastic) gradient descent methods. A puzzling empirical observation is that learning neural networks with a number of parameters exceeding the number of training examples often leads to zero loss, i.e., the network exactly interpolates the data. Nevertheless, it generalizes very well to unseen data, which is in stark contrast to intuition from classical statistics which would predict a scenario of overfitting. A current working hypothesis is that the chosen optimization algorithm has a significant influence on the selection of the learned network. In fact, in this overparameterized context there are many global minimizers so that the optimization method induces an implicit bias on the computed solution. It seems that gradient descent methods and their stochastic variants favor networks of low complexity (in a suitable sense to be understood), and, hence, appear to be very well suited for large classes of real data. Initial attempts in understanding the implicit bias phenomenon considers the simplified setting of linear networks, i.e., (deep) factorizations of matrices. This has revealed a surprising relation to the field of low rank matrix recovery in the sense that gradient descent favors low rank matrices in certain situations. Moreover, restricting further to diagonal matrices shows connection to compressive sensing and l1-minimization.

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MS17

Structured Fista for L1-Regularized Optimization Model in Image Restoration

In this paper, we propose an efficient numerical algorithm for large-scale ill-posed linear inverse problems arising from image restoration. To enhance computational speed, we extend the structured fast iterative shrinkage-thresholding algorithm (sFISTA) to solve the corresponding l_1-regularized minimization problem by leveraging two hidden structures. Firstly, we approximate the coefficient matrix as a sum of a small number of Kronecker products, which not only introduces an additional level of parallelism into the computation but also enables the subsequent optimization procedure to utilize computationally intensive matrix-matrix multiplications. Secondly, since all matrices in the Kronecker product approximation are structured matrices (such as Toeplitz and Hankel), fast matrix-vector multiplication algorithms can be employed at each iteration. Consequently, our proposed algorithm is referred to as structured FISTA for l_1-regularized optimization model (sFISTA-l_1). The l_1-regularized optimization model is nonsmooth, which poses challenges in analyzing convergence results. However, this paper proves that sFISTA-l_1 exhibits similar convergence properties to sFISTA and provides a proof approach applicable to any nonsmooth convex regularization term. Finally, numerical experiments are conducted to validate the efficiency of sFISTA-l_1.

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MS17

Effective Approximate Preconditioners for Linear Inverse Problems

Many problems in science and engineering give rise to linear systems of equations that are commonly referred to as large-scale linear discrete ill-posed problems. These problems arise for instance, from the discretization of Fredholm integral equations of the first kind. The matrices that define these problems are typically severely ill-conditioned and may be rank deficient. Because of this, the solution of linear discrete ill-posed problems may not exist or be extremely sensitive to perturbations caused by error in the available data. These difficulties can be reduced by applying regularization to iterative refinement type methods which may be viewed as a preconditioned Landweber method. Using a filter factor analysis, we demonstrate that low precision matrix approximants can be useful in the construction of these preconditioners.

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MS17

A Scale-Invariant Relaxation in Low-Rank Tensor Recovery

In this talk, we consider a low-rank tensor recovery problem. Based on the tensor singular value decomposition (t-SVD), we propose the ratio of the tensor nuclear norm and the tensor Frobenius norm (TNF) as a novel nonconvex surrogate of the tensor's tubal rank. The rationale of the proposed model for enforcing a low-rank structure is analyzed as its theoretical properties. Specifically, we introduce a null space property (NSP) type condition, under which a low-rank tensor is a local minimum for the proposed TNF recovery model. Numerically, we consider a low-rank tensor completion problem as a specific application of tensor recovery and employ the alternating direction method of multipliers (ADMM) to secure a model solution with guaranteed subsequential convergence under mild conditions. Extensive experiments demonstrate the superiority of our proposed model over state-of-the-art methods.

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MS17

A Surrogate Hyperplane Bregman-Kaczmarz Method for Solving Linear Inverse Problems

Linear inverse problems arise in many practical applications. In the present work, we propose a residual-based surrogate hyperplane Bregman-Kaczmarz method (RSHBK) for solving this kind of problems. The convergence theory of the proposed method is investigated detailedly. When the data is contaminated by the independent noise, an adaptive version of our RSHBK method is developed. An adaptive relaxation parameter is derived for optimizing the bound on the expectation error. It is proved that our adaptive RSHBK method converges to the true solution through the utilization of Lambert-W function. We demonstrate the efficiency of our proposed methods for both noise-free and independent noise problems by comparing with other state-of-the-art Kaczmarz methods in terms of computation time and convergence rate through synthetic experiments and real-world applications.

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MS18

Ultra-Marginal Feature Importance: Learning from Data with Causal Guarantees

Scientists frequently prioritize learning from data rather than training the best possible model; however, research in machine learning often prioritizes the latter. Marginal contribution feature importance (MCI) was developed to break this trend by providing a useful framework for quantifying the relationships in data. In this work, we aim to improve upon the theoretical properties, performance, and runtime of MCI by introducing ultra-marginal feature importance (UMFI), which uses dependence removal techniques from the AI fairness literature as its foundation. We first propose axioms for feature importance methods that seek to explain the causal and associative relationships in data, and we prove that UMFI satisfies these axioms under basic assumptions. We then show on real and simulated data that UMFI performs better than MCI, especially in the presence of correlated interactions and unrelated features, while partially learning the structure of the causal graph and reducing the exponential runtime of MCI to superlinear.

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MS18

The Dependency Diagram: A New Method of Understanding Interdependence in Multivariate Distributions

Determining the interdependence structure of an arbitrary probability distributions remains an unsolved problem. Among the difficulties in doing so include no operationally motivated method of quantifying multivariate mutual information, and furthermore the existence of qualitatively distinct probability distributions whose entropies, joint entropies, and mutual informations are identical despite one consisting of only dyadic (pairwise) interactions while the other consists of triadic interactions. Here, we make steps toward further understanding the dependence structure of an arbitrary discrete probability distribution. This method leverages *dependency decomposition* lattice of split distributions and derives a Venn-like diagram quantifying how each statistical dependency relates to the others in the distribution. We then close by demonstrating the diagrams usefulness by considering a variety of examples.

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MS18

Causal Feature Selection in the Era of Big Data

The era of big data is marked by an unprecedented deluge of information, fueling the exponential growth of machine learning algorithms as they harness this wealth of data to uncover valuable insights and drive innovation. The surge of machine learning underscores the imperative for responsible ML practices, as ethical considerations become paramount in ensuring the interpretability, fairness, adversarial robustness, and generalization of these models. Feature selection plays a pivotal role in the responsible ML tasks. However, building upon statistical correlations between variables can lead to spurious patterns with biases and compromised performance. In this talk, I will elaborate on the current study of causal feature selection: what it is and how it can reinforce the four aspects of responsible ML. By identifying features with causal impacts on outcomes and distinguishing causality from correlation, causal feature selection is posited as a unique approach to ensuring ML models are ethically and socially responsible in high-stakes applications.

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MS18

Quantifying Information Flow and Information Interaction in Neural Circuits

Inspired by problems in neuroscience, we explore how one might formally define a meaningful notion of information flow about a specific message within a neural circuit. Here, a neural circuit is assumed to consist of a network of computational nodes, with transmissions (modeled as random variables) being sent between these nodes over time. We show that obvious measures of information flow based on mutual information fail, and that obtaining a definition capable of identifying paths along which information flows is non-trivial. We explore a measure based on counterfactual causal influence (CCI), to serve as a theoretical north star in the search for observational definitions. If time permits, the talk will also cover a related question of quantifying information interactions between three random variables, a problem that sits at the heart of defining information flow. Using the framework of partial information decomposition, we will provide an explanation of how interactions might be defined and estimated, and what kinds of insights these measures could yield.

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MS19

Causal Learning in Stochastic Processes: A Graphical Framework Using Local Independence

Local independence is an asymmetric notion of independence which describes how a system of stochastic processes (e.g., point processes or diffusions) evolves over time. In short, a process B is locally independent of a process A given a process C if knowing the past of A and C is not more informative about the present of B than knowing the past of C only. Directed graphs may represent local independence structure using a separation criterion which is analogous to d-separation. We discuss how one can use tests of local independence to learn the underlying causal structure from observations of multivariate stochastic processes. If some processes are unobserved, one can use directed mixed graphs (DMGs) to describe the local independence structure of the observed processes. Several DMGs may describe the same local independencies, and therefore we wish to characterize such Markov equivalence classes (MECs) of DMGs. It turns out that DMGs satisfy a maximality property allowing us to construct a simple graphical representation of an entire MEC. This is convenient as the MEC can be learned from data, and its graphical representation concisely describes which underlying structures could have generated the observations. Deciding Markov equivalence of DMGs is computationally hard, and we introduce a new class of weak equivalence relations. Weak equivalence classes enjoy properties similar to those of MECs, and they provide a computationally feasible framework for causal learning.

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MS19

Learning Linear Non-Gaussian Cyclic Causal Models via Algebraic Constraints

One of the main tasks of causal inference is to learn direct causal relationships among observed random variables. These relationships are usually depicted via a directed graph whose vertices are the variables of interest and whose edges represent direct causal effects. In this talk we will discuss the problem of learning such a directed graph for a linear causal model. We will specifically address the cases where the graph may have directed cycles or there might be hidden variables. In general, the causal graph cannot be learned uniquely from observational data. However, in the special case of linear non-Gaussian acyclic causal models, the directed graph can be found uniquely. When cycles are allowed the graph can be learned up to an equivalence class. We characterize the equivalence classes of such cyclic graphs and we propose algorithms for causal discovery. Our methods are based on using specific polynomial relationships which hold among the 2nd and higher order moments of the random vector and which can help identify the graph.

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MS19

Causal Inference in Directed, Possibly Cyclic, Graphical Models

We consider the problem of learning a directed graph $G^\star$ from observational data. We assume that the distribution which gives rise to the samples is Markov and faithful to the graph $G^\star$ and that there are no unobserved variables. We do not rely on any further assumptions regarding the graph or the distribution of the variables. In particular, we allow for directed cycles in $G^\star$ and work in the fully nonparametric setting. Given the set of conditional independence statements satisfied by the distribution, we aim to find a directed graph which satisfies the same d-separation statements as $G^\star$. We propose a hybrid approach consisting of two steps. We first find a *partially ordered partition* of the vertices of $G^\star$ by optimizing a certain score in a greedy fashion. We prove that any optimal partition uniquely characterizes the Markov equivalence class of $G^\star$. Given an optimal partition, we propose an algorithm for constructing a graph in the Markov equivalence class of $G^\star$ whose strongly connected components correspond to the elements of the partition, and which are partially ordered according to the partial order of the partition. Our algorithm comes in two versions – one which is provably correct and another one which performs fast in practice.

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MS20

Analysis of Tumor Microenvironment in Breast Cancer: Feature Extraction and Comparison Between Racial Groups

It is seen that the mortality rate for Black women diagnosed with breast cancer is 42% higher than the comparable rate for White women. Previously, this disparity was believed to be caused by external factors such as financial and environmental conditions. However, recent findings have revealed a biological difference between the two racial groups that contribute to this difference in mortality rate. This research project aims to analyze disparities in the effects of breast cancer on Black and White women using data science techniques. This is done by initially defining tumor microenvironment (TME) features, some of which are spatial features derived from a Delaunay Triangulation plot. The dataset provided includes histological labels and corresponding spatial coordinates for various tissue types from Piedmont Hospital in Georgia. By examining the extracted TME features using statistical tests such as the T-test, the study aims to uncover variations in the impact of breast cancer across racial groups. Significant differences between the features were identified among various racial and socioeconomic demographics. Addressing these variations is crucial for promoting equitable healthcare outcomes for all women affected by breast cancer.

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MS20

Assessing the Random Walk Model for 1D Vertical Tracer Transport in the North-West Pacific Ocean

”The Lagrangian model in case of a space-varying diffusivity is considered and the random walk model is applied on an idealized test problem with known solutions. Numerical schemes are utilized to simulate stochastic differential equations (SDEs), including methods such as Euler, Milsteins, and Ito-backward, to accurately capture diffusive processes. The findings and algorithms derived from this ideal model are then applied to real-world data, where discrete diffusivity is tackled through interpolation techniques. Stochastic Numerical Schemes and their distributions are assessed, alongside the estimation and analysis of Theoretical Expectations. Additionally, residence times for particles are computed for both cases, offering a better understanding of particle behavior. Moreover, the paper introduces the concept of kernel density estimation for constructing probability density functions from simulated particle movements, providing insights into diffusive transport modeling. Furthermore, it evaluates the probability distribution of chlorophyll in the North-West Pacific Ocean at coordinates (50N, 149W).”

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MS20

DeepFake Technology for Bid Data Generation Using Autoencoders and Deep Neural Networks

In the emerging field of radiogenomics, the primary challenge is the high cost of genetic testing, which restricts access to large, paired datasets of imaging and genetic information. Such datasets are essential for the effective training of machine learning algorithms in radiogenomic analyses. This research aims to bridge the gap between gene expression in tumors and their morphological representation in MRI scans of breast cancer patients. In this work an advanced autoencoder for processing gene expression data, and the derived weights from this autoencoder utilized were then employed to initialize a supervised Deep Neural Network (DNN). This network extracted distinct morphological markers from each MRI scan. This study introduces an innovative approach that utilizes deepfake technology, employing dual Generative Adversarial Networks (GANs) to generate synthetic imaging data from a radiogenomic dataset. This synthetic data, nearly indistinguishable from real data, is produced using a supervised neural network and is aimed at enhancing breast cancer diagnostics. Notably, the proposed neural network, when enhanced with an autoencoder and dropout techniques, demonstrated superior predictive accuracy over linear regression models. Specifically, it reduced errors by an average of 1.8% in mean absolute percent error. These findings underscore that the images generated by the proposed model are virtually indistinguishable from authentic images and exhibit high reliability in applications through the PyTorch framework. The results of this study underscore the potential of the proposed methodology to significantly contribute to advancements in breast cancer diagnostics.

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MS20

A Simplified Mathematical Model for Cell Proliferation in a Tissue-Engineering Scaffold

While the effects of external factors like fluid mechanical forces and scaffold geometry on tissue growth have been extensively studied, the influence of cell behavior particularly nutrient consumption and depletion within the scaffold has received less attention. Incorporating such factors into mathematical models allows for a more comprehensive understanding of tissue-engineering processes. This work presents a comprehensive continuum model for cell proliferation within two-dimensional tissue-engineering scaffolds. Through mathematical modeling and asymptotic analysis based on the small aspect ratio of the scaffolds, the study aims to reduce computational burdens and solve mathematical models for tissue growth within porous scaffolds. The model incorporates fluid dynamics of nutrient feed flow, nutrient transport, cell concentration, and tissue growth, considering the evolving scaffold porosity due to cell proliferation, with the crux of the work establishing the ideal pore shape for channels within the tissue-engineering scaffold to obtain the maximum tissue growth. We investigate scaffolds with specific two-dimensional initial porosity profiles, and our results show that scaffolds which are uniformly graded in porosity throughout their depth promote more tissue growth.

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MS21

Fractal Density Concept in Calculating the Returns of the Omniscient, Yet Lazy, Investor

”Fractal geometry has found its use in various subfields, distant from theoretical mathematics, including technical analysis. This work will expand on this theme, by introducing new applications of fractals to the theory of investing, especially optimization of trading bots. In the introduction, crucial to the work aspects of fractal geometry will be outlined along with to-date applications of fractals in technical analysis. It will be argued that any market chart can be imagined as a fractal. With such assumption, the concepts of fractal dimension and density can be utilized to calculate the time complexity of such graphs. For better understanding of real-world application of this method, it will be shown on the example of hypothetical Omniscient Investor, that his returns can be represented as a two-dimensional function of frequency in which he opens / closes positions and his laziness. Then it will be argued that it can be directly translated to optimizing the returns of trading bots with regard to cost of raising the investing frequency and spread by calculating the local maxima of the adjusted before mentioned two-dimensional function.”

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MS21

A *Light* Intro into a New Type of Riemannian Submersion

Submersion theory persists as a rich subject of differential geometry with many applications to real world systems. Here, we provide brief examples of such applications, and cover the basics of differential geometry needed to get a glimpse into modern theory. Then, we present an example of the pointwise bi-slant Riemannian submersion, our new mapping generalizing the notion of the slant, semi-slant, pointwise semi-slant, and bi-slant submersions.

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MS21

The Classification of Internet Memes Through Supervised and Unsupervised Machine Learning Algorithms

”Memes, those captivating internet phenomena, effortlessly deliver online entertainment. By leveraging time-series data from Google Trends, we can vividly illustrate and dissect the dynamic trends in meme popularity. Previous studies have discerned four distinct post-peak popularity patterns ””smoothly decaying,”” ””spikey decaying,”” ””leveling off,”” and ””long-term growth””and elegantly modeled these using ordinary differential equations. This research introduces a programmatic approach that harnesses both supervised and unsupervised machine learning algorithms. The dataset, now expanded to over 2000 elements, becomes the canvas for exploration. The K-means algorithm identifies clusters, which then serve as labels for the supervised SVC algorithm. The overarching goal is to achieve accurate classification of meme popularity patterns. Concurrently, each meme in the dataset will be categorized, such as catchphrase or viral video, facilitating an insightful analysis into the intriguing relationship between meme category and its distinctive popularity trajectory.”

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MS21

A Simplified Mathematical Model for Erosion and Deposition in a Porous Medium

In this paper, we investigate the dynamic processes of erosion and deposition in a porous medium that occur when the solid internal morphology of the porous medium interacts with fluids at its contact interface. These phenomena are encountered both in natural settings, such as soil erosion, and in various industrial applications, like water-filtration devices. The focus of our research is to develop a comprehensive two-dimensional continuum model that accurately describes how erosion and deposition influence the internal morphology of the porous medium under a fluid flow. To achieve this goal, we utilize first-principle equations, including the Darcy and continuity equations, to model the fluid flow. The Navier-Cauchy equations are adapted to describe the deformation of the elastic porous medium due to the flow shear stress. Further, we incorporate the advection-diffusion-reaction equation to study the mass transport of particles within the porous medium. By integrating an erosion and deposition evolution model, we effectively monitor how particle concentration of the fluid and porosity of the porous medium evolve together. To simplify our model, we employ asymptotic analysis, based on the porous medium small aspect ration, to derive a reduced model. As a result of the erosion and deposition model, the porous medium expands and shrinks due to erosion and deposition, respectively.

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MT1

Mathematical Contributions to Weather and Climate Modelling Part 2

”Asymptotics for geophysical flows” systematizes this rich zoo of models from a unified mathematical perspective. By leveraging the power of multiscale techniques, detailed explanations of scale interactions emerge and quantitative accuracy becomes possible.

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MT2

Optimal Transport and Applications in Particle Physics and Machine Learning

This tutorial will provide background on the mathematical foundations of optimal transport and discuss applications to jet classification in high energy particle physics and machine learning.

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MT3

Mathematical Contributions to Weather and Climate Modelling Part 4

”The role of data” addresses the all-important role of observational data in weather fore- casting and climate modelling and the related topics of data assimilation and data-based modelling.

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MT3

Mathematical Contributions to Weather and Climate Modelling Part 3

”PDE theory for atmosphere-ocean flows” summarizes selected rigorous results on some important geophysical flow models, such as the Boussinesq, anelastic/pseudo-incompressible, hydrostatic primitive, and quasi-geostropic equations.

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