54th Barrett Memorial Lectures Schedule

Unless stated otherwise, events will be in the SERF building, **room 307.**
Breakfast and coffee will be provided each morning during registration.

Monday, May 18, 2026

- 07:30-08:45 — Registration, Breakfast & Coffee
- 08:45-09:00 — Welcome
- 09:00-10:00 — George Yin
- 10:00-10:30 — Coffee Break
- 10:30-11:30 — Yulong Lu
- 11:30-12:30 — Tan Bui
- 12:30-14:00 — Lunch (Ayres Hall, 4th floor)
- 14:00-15:00 — Yue Yu
- 15:00-16:00 — Konstantinos Spiliopoulos
- 16:00-16:30 — Coffee Break
- 16:30-17:30 — Ekaterina Rapinchhuk
- 17:30-18:30 — Poster Session and Refreshments (Ayres Hall, 4th floor)

Tuesday, May 19, 2026

- 07:30-09:00 — Registration, Breakfast & Coffee
- 09:00-10:00 — Tamar Schlick
- 10:00-10:30 — Group Photo (Ayres Hall) & Coffee Break
- 10:30-11:30 — Lars Ruthotto
- 11:30-12:30 — Zixuan Cang
- 12:30-14:00 — Lunch (Ayres Hall, 4th floor)
- 14:00-15:00 — Emilie Purvine
- 15:00-16:00 — Haizhao Yang
- 16:00-16:30 — Coffee Break
- 16:30-17:30 — Wenrui Hao
- 17:30-18:30 — Open Discussion Session
- 18:30 — Banquet (Hilton Knoxville)

Wednesday, May 20, 2026: Special Session in Memory of Professor Tim Schulze

- 07:30-08:45 — Registration, Breakfast & Coffee
- 08:45-09:00 — Special Remarks
- 09:00-10:00 — Russell Caflisch
- 10:00-10:30 — Coffee Break
- 10:30-11:30 — Hamza Ruzayqat
- 11:30-12:30 — Daniel Anderson
- 12:30-14:00 — Lunch (Ayres Hall, 4th floor)

- 14:00-15:00 — Christian Ratsch
- 15:00-16:00 — Petr Plechac
- 16:00-16:30 — Coffee Break
- 16:30-17:30 — Christopher Raymond
- 17:30-18:30 — Closing Remarks

Monday, May 18, 2026

09:00-10:00 — George Yin, University of Connecticut

Title: Deep Filtering and Related Problems

Abstract: In this talk, we will review some of our recent work on using machine learning to treat nonlinear filtering and problems arising in control and optimization. Nonlinear filtering is a fundamental problem in signal processing, information theory, communication, control and optimization, and systems theory. Instead of using stochastic partial differential equations for obtaining the conditional distribution, we construct finite-dimensional approximations using deep neural networks for the optimal weights. Problems involving classification of states will also be mentioned.

10:30-11:30 — Yulong Lu, University of Minnesota Twin Cities

Title: In-Context Learning in Scientific Computing

Abstract: Transformer-based foundation models, pre-trained on large datasets spanning a wide range of tasks, have shown remarkable adaptability to diverse downstream applications—even in low-data regimes. A particularly striking capability is in-context learning (ICL): when given a prompt containing a few examples from a new task alongside a query, these models can produce accurate predictions without any parameter updates. This emergent behavior is often viewed as a paradigm shift for transformers, yet its theoretical foundations remain only partially understood. In this talk, I will present recent theoretical progress toward understanding ICL in scientific computing. I will focus on understanding how transformer architectures can implicitly perform task adaptation in three representative problem classes: learning solution operators of PDEs, dynamical system prediction and generative modeling.

11:30-12:30 — Tan Bui, The University of Texas at Austin

Title: Rigorous Model-Constrained Scientific Machine Learning for Digital Twins: A Computational Mathematics Perspective

Abstract: Digital twins (DTs) are high-fidelity virtual representations of physical systems and processes. At their foundation lie mathematical and physical models that describe system behavior across multiple spatial and temporal scales. A central purpose of DTs is to enable “what-if” analyses through hypothetical simulations, supporting lifecycle monitoring,

parameter calibration against observational data, and systematic uncertainty quantification (UQ). For DTs to serve as a reliable basis for real-time forecasting, optimization, and decision-making, they must reconcile two traditionally competing requirements: mathematical rigor and physical fidelity, and computational efficiency at scale. This has motivated a new generation of approaches that combine classical tools from numerical analysis, partial differential equations, inverse problems, and optimization with the expressive power of Scientific Machine Learning (SciML). In this talk, I will outline a principled pathway from traditional computational mathematics to rigorously grounded SciML. I will then present recent Scientific Deep Learning (SciDL) methods for forward modeling, inverse and calibration problems, and uncertainty quantification, emphasizing mathematical structure, stability, and generalization. Both theoretical results and numerical demonstrations will be shown for representative problems governed by transport, heat, Burgers, Euler (including transonic and hypersonic regimes), and Navier–Stokes equations.

14:00-15:00 — Yue Yu, Lehigh University

Title: Learning Nonlocal Neural Operators

Abstract: During the last 20 years there has been a lot of progress in applying neural networks (NNs) to many machine learning tasks. However, their employment in scientific machine learning with the purpose of learning complex responses of physical systems from experimental measurements has been explored much less. In this talk, we will consider learning of heterogeneous material responses as an exemplar problem to investigate automated physical model discovery from experimental data. In particular, we propose to parameterize the mapping between excitation and corresponding system responses in the form of nonlocal neural operators, and infer the neural network parameters from experimental measurements. As such, the model is built as mappings between infinite-dimensional function spaces, and the learnt network parameters are resolution-agnostic. Moreover, the nonlocal operator architecture also allows the incorporation of fundamental mathematical and physics knowledge. Both properties improve the learning efficacy and robustness from scarse and noisy measurements.

To demonstrate the applicability of our nonlocal operator learning framework, two typical scenarios will be discussed: (1) learning of a material-specific constitutive law, (2) development of a foundation constitutive law across multiple materials. As an application, we learn material models directly from digital image correlation (DIC) displacement tracking measurements on a porcine tricuspid valve leaflet tissue, and we will show that the learnt model substantially outperforms conventional constitutive models.

15:00-16:00 — Konstantinos Spiliopoulos, Boston University

Title: Scaling Effects and Efficiency in Deep Learning Algorithms

Abstract: We are interested in the design of provably-efficient (both statistically and computationally) deep learning algorithms. The cornerstone of our approach is to view the neural network output as a stochastic process, i.e., a random object evolving over time. In

this talk, I will present our recent work on studying the effect of scaling in the statistical behavior (such as bias and variance) of deep neural networks as well as on the test accuracy and generalization properties of the given architecture. We find that in terms of variance reduction of the neural network's output and increased test accuracy the best choice is to choose the scaling of the hidden layers to correspond to the so-called mean-field scaling. We also find that this is particularly true for the outer layer, in that the neural network's behavior is more sensitive to the scaling of the outer layer as opposed to the scaling of the inner layers. The mechanism for the mathematical analysis is an asymptotic expansion for the neural network's output yielding a clean bias-variance decomposition. An important practical consequence of the analysis is that it provides a systematic and mathematically informed way to choose hyperparameters (such as learning rates) and to compare different architectures leading to provably-efficient and stable algorithms. Such choices guarantee that the resulting neural network architectures behave in statistically robust ways during training. I will discuss applications of these ideas to the design of deep learning algorithms for scientific problems including solving high dimensional partial differential equations (PDEs), closure of dynamical systems (like PDEs, moment equations etc.) and reinforcement learning with applications to financial engineering, turbulence, computational biology. I will conclude by presenting an overview of our research program, aimed at advancing foundational understanding to develop efficient and reliable artificial intelligence.

16:30-17:30 — Ekaterina Rapinchuk, Michigan State University

Title: Multistage Active Learning with Auction Dynamics on Graphs

Abstract: The success behind machine learning is dependent upon a sufficient amount of labeled samples. In addition, the choice of training points often has a significant impact on the performance of a machine learning model. Active learning is a sub-field of machine learning that helps to improve the performance of underlying machine learning methods by carefully selecting unlabeled points to be labeled, using human or oracle input in the loop. Moreover, semi-supervised learning techniques take advantage of the information in the usually abundant unlabeled data in addition to the often scarce labeled data. We propose a multistage semi-supervised active learning framework utilizing graph-based auction dynamics that first explores and then exploits the input data space while selecting unlabeled points to be labeled. In particular, we design a novel active learning acquisition function to measure uncertainty. The overall algorithm is very useful for common scenarios of limited labeled samples.

Tuesday, May 19, 2026

09:00-10:00 — Tamar Schlick, NYU

Title: Adventures with RNA Graphs: from Euler to Viruses

Abstract: Development of our RNA As Graphs (RAG) resource for modeling RNA secondary structures will be described, leading to many practical applications to RNA structure analysis and design. Recent work on viral frameshifting mechanisms will be highlighted, in

particular transition path sampling simulations of a large-scale conformational transition between two pseudoknots and its biological significance. The research highlights the connection between basic and applied research, and the strong impact that theoretical mathematics (topology and knot theory) can have on biology, medicine, and technology.

Yan S, Schlick T. Heterogeneous and multiple conformational transition pathways between pseudoknots of the SARS-CoV-2 frameshift element. Proc Natl Acad Sci U S A. 2025 Jan 28;122(4):e2417479122. doi: 10.1073/pnas.2417479122. Epub 2025 Jan 24. PMID: 39854230; PMCID: PMC11789066.

10:30-11:30 — Lars Ruthotto, Emory University

Title: Continuous-Time Deep Learning for Generative AI and High-Dimensional PDEs

Abstract: Continuous-time differential equation models have become an important mathematical tool in modern AI. In this lecture, I will show how ODEs, SDEs, and PDEs provide a unifying framework that connects deep learning architectures in applications such as generative modeling, optimal transport, and stochastic control. Starting from the interpretation of residual networks as discretized ODEs, I will trace a path through neural ODEs and the optimal control view of training, to stochastic extensions via Fokker-Planck equations and density evolution. I will present a high-dimensional PDE perspective that unifies generative modeling approaches including continuous normalizing flows, flow matching, and score-based diffusion models and builds bridges to dynamic optimal transport. I will close with applications in stochastic optimal control and mean-field games, and highlight open problems where the probability and PDE communities can make fundamental contributions.

11:30-12:30 — Zixuan Cang, North Carolina State University

Title: Optimal Transport in Single-Cell and Spatial Biology

Abstract: Single-cell and spatial omics technologies now make it possible to measure cellular states, molecular signals, and tissue organization at unprecedented resolution. These data raise a range of questions: how can we compare cell populations, align tissues or modalities, infer developmental dynamics, and quantify spatial interactions among cells? Optimal transport provides a flexible framework for addressing these problems by constructing couplings between distributions while incorporating geometry, constraints, and biological structure. This talk will highlight how optimal transport has become a useful mathematical language for studying cellular systems across scales, from cell-state variation to spatial organization and dynamic biological processes. Examples from single-cell and spatial biology will illustrate how transport-based models can integrate heterogeneous measurements, encode biological constraints, and produce interpretable descriptions of tissue structure, cellular communication, and developmental change. Together, these ideas show how optimal transport can help transform high-dimensional biological data into quantitative models of biological organization and function.

14:00-15:00 — Emilie Purvine, Pacific Northwest National Laboratory

Title: Scientific discovery through complex structure modeling and analysis

Abstract: Real-world systems often exhibit complex structures that are large, heterogeneous, high dimensional, and deeply interconnected. Central to understanding such systems is careful selection of mathematical models and algorithms tailored to the domain-relevant questions at stake. This presentation explores how graph, hypergraph, and geometric and topological frameworks drive scientific discovery across diverse domains such as biology, chemistry, and cybersecurity. In particular, we see how hypergraph centrality rankings reveal meaningful correlations with key genes in biological systems and topological signatures capture anomalous patterns within dynamic systems. Additionally, this work introduces an evolving software package designed to augment and transform data using geometric and topological techniques, offering new capabilities for machine learning pipelines. Together, these examples highlight the power of mathematically principled approaches to unlocking insights in complex, data-driven discovery.

15:00-16:00 — Haizhao Yang, University of Maryland College Park

Title: Modeling and Computation in the Space of Language: Symbolic and LLM-Based Approaches

Abstract: Scientific modeling and computation traditionally rely on structured mathematics and hand-designed algorithms. In this talk, I propose a new perspective: treating both modeling and computation as processes operating within the space of natural language. I will introduce two complementary approaches that realize this vision. The first uses symbolic learning based on tree structures to generate mathematical expressions, where modeling is performed by constructing symbolic trees and computation is governed by operator rules. The Finite Expression Method (FEX) exemplifies this approach by discovering interpretable, high-accuracy solutions to PDEs and physical systems. The second approach employs large language models (LLMs) for automatic code generation and reasoning to translate scientific problem descriptions into formal mathematical models and executable solvers to solve these problems. As an example, the OptimAI framework demonstrates how multi-agent LLM collaboration enables reliable end-to-end optimization problem modeling and solving. Together, these methods point toward a unified paradigm where symbolic and language models form the foundation for interpretable, scalable scientific discovery and computation.

16:30-17:30 — Wenrui Hao, Penn State

Title: Parameter Identifiability in Data-Driven Modeling and Its Applications in Federated Learning with Heterogeneous Data

Abstract: Parameter identifiability is a fundamental challenge in data-driven modeling, particularly for complex, nonlinear systems arising in biological and biomedical applications. In many real-world settings, including multi-institutional clinical studies, data

are inherently heterogeneous, distributed, and privacy-sensitive, rendering centralized model calibration infeasible. This work investigates parameter identifiability within the framework of data-driven modeling and explores its implications for federated learning with heterogeneous data sources.

We establish a computational foundation for practical identifiability by leveraging the Fisher Information Matrix (FIM) and its theoretical connections to coordinate identifiability. Based on this foundation, we develop an efficient approach for identifiability assessment that scales to high-dimensional models. To address non-identifiable or weakly identifiable parameters, we introduce regularization-based strategies that improve model stability, enhance interpretability, and enable robust uncertainty quantification.

Building on these advances, we propose identifiability-based federated training strategies that adaptively integrate information across distributed clients. To further address data heterogeneity, we incorporate zentropy-based formulations, bridging thermodynamic principles with information theory to better quantify and reconcile discrepancies across datasets.

Wednesday, May 20, 2026

Special Session in Memory of Professor Tim Schulze

09:00-10:00 — Russell Caflisch, Courant Institute, NYU

Title: An Adjoint Method for Optimization of the Boltzmann Equation

Abstract: We present an adjoint method for optimization of the Boltzmann equation for rarefied gas dynamics. The adjoint method is derived using a ""discretize then optimize"" approach. Discretization (in time and velocity) is via the Direct Simulation Monte Carlo (DSMC) method, and adjoint equations are derived from an augmented Lagrangian. After a forward (in time) solution of DSMC, the adjoint variables are found by a backwards solver. They are equal to velocity derivatives of an objective function, and are used for optimization of the Boltzmann equation. For general collision models, DSMC requires the use of a rejection sampling step, which involves discontinuities that lead to a new term, involving a ""score function"". This is joint work with Yunan Yang (Cornell) and Denis Silantyev (U Colorado, Colorado Springs)."

10:30-11:30 — Hamza Ruzayqat, King Abdullah University of Science and Technology

Title: Sequential Markov Chain Monte Carlo and Localization Strategies for Data Assimilation

Abstract: High-dimensional nonlinear filtering remains one of the central challenges in Bayesian data assimilation, as the computational cost of sequential inference grows rapidly with dimension and standard particle filters often suffer from severe weight degeneracy. This talk begins with a brief review of filtering theory and particle filtering, highlighting the

main difficulties associated with high-dimensional state spaces and expensive likelihood evaluations. We then introduce Sequential Markov Chain Monte Carlo (SMCMC) methods as a weight-free alternative for approximating the filtering distribution through direct sampling. To further improve scalability, we discuss localization strategies that exploit the spatial structure of the problem and significantly reduce computational cost while preserving accuracy. In the linear-Gaussian observation setting, the proposed approximation leads to a Gaussian mixture representation of the filtering density, from which independent samples can be drawn exactly; for nonlinear or non-Gaussian observations, MCMC kernels are used instead. Numerical experiments on high-dimensional linear and nonlinear geophysical models demonstrate that the proposed localized SMCMC framework provides accurate and efficient filtering, with strong robustness under sparse observations and non-Gaussian noise.

11:30-12:30 — Daniel Anderson, George Mason University

Title: Primarily Mush, A Side of KMC, and a Poker Irregularity To Go

Abstract: I will describe three topics that, while seemingly disconnected, have been informed by, inspired by, or otherwise influenced by Tim Schulze. I will first describe convective instabilities in mushy layers, where Tim's modeling and computational contributions, which began in the 1990s, have helped shape the current understanding of so-called chimney formation and mushy layer dynamics, impacting fields from metallurgy to climate dynamics. Second, on KMC, Tim taught me everything I know about the subject, which is still a tiny fraction of the body of work he and his colleagues amassed in this area. Nonetheless it was enough for me to inspire a group of graduate students in 2008 to explore KMC dynamics in an industrial modeling project on battery dynamics. Third, I had little trouble rousing Tim's interest in 2022 regarding a non-standard poker probability problem for which he quickly provided a proof that appeared in our recreational math publication in 2024. I will describe some simple calculations and some explanations."

14:00-15:00 — Christian Ratsch, UCLA

Title: KMC simulations for Epitaxial Growth of Quantum Dots

Abstract: TBA

15:00-16:00 — Petr Plechac, University of Delaware

Title: TBA

Abstract: TBA

16:30-17:30 — Christopher Raymond, University of Delaware

Title: TBA

Abstract: TBA

Poster

Trung Nguyen, University of Tennessee, Knoxville

Title: Multi-level, multi-color mathematical graph neural networks for molecular property prediction

Abstract: Graph Neural Networks (GNNs) have demonstrated significant potential in molecular property prediction. However, current GNN architectures mostly rely on standard node or edge features that overlook the complex, multi-scale interactions between atoms in small molecules. This research introduces a mathematics-driven approach that integrates concepts from Geometric Graph Learning (GGL) and Algebraic Graph Learning (AGL) to enhance molecular representations. Drawing upon GGL principles, we construct

multi-color molecular graphs where nodes represent atoms and edges are weighted based on both spatial distances and local geometric features, such as curvatures derived from differential geometry applied to atomic interactions. Furthermore, we encode high-dimensional atomic interactions through the spectral properties of algebraic subgraphs, such as the Laplacian and adjacency matrices derived from these geometric graphs. The construction of these multi-level graphs and their connectivity follow the principles of Persistent Spectral Graph Theory, where a filtration process generates a family of graphs across different scales, capturing both topological persistence and geometric evolution of atomic relationships. This integrated approach enables reliable and robust molecular representations by incorporating both short- and long-range dependencies, thereby surpassing the limitations of conventional GNNs. Our approach significantly improves predictive performance in molecular property prediction tasks and provides a reliable framework to advance drug discovery and materials science applications.

Alireza Shahi, University of Tennessee, Knoxville

Title: Comparing Geometric Representations for Binding Affinity Prediction: From Shape Descriptors to Interaction Manifolds.

Abstract: Binding affinity prediction is a fundamental challenge in structure-based drug design. In this work, we present a comparative study of geometric representations, ranging from global shape descriptors to interaction-aware differential geometry models. We introduce the Element Interaction Manifold (EIM), which encodes protein–ligand interactions using element-specific manifolds capturing curvature, surface area, and volumetric features.

We evaluate multiple EIM configurations (global, local, hybrid, and multi-kernel) alongside established methods, including Surface 3D Zernike Descriptors (3DZD), Element-Pair 3DZD (EP-3DZD), and interaction-based baselines. On the CASF-2016 benchmark, the Hybrid EIM achieves strong performance (Pearson $R = 0.808$), outperforming traditional geometric and learning-based approaches. Although combining EIM with EP-3DZD yields a slightly higher correlation ($R = 0.811$), the improvement is marginal relative to the increased feature dimensionality.

These results demonstrate that multi-scale differential geometry provides an efficient and interpretable framework for capturing protein–ligand interactions and predicting binding affinity.

Lane H. Rogers, University of Tennessee, Knoxville

Title: An Improvement to AFL-EAT-Score Using Hypergraph Modeling

Abstract: A persistent problem in molecular biochemistry is predicting protein-ligand binding affinity (pK). Accurate prediction of pK is useful in the design of molecules that will bind effectively to a target site. Computational methods of predicting pK are often intractable, so the adoption of machine learning techniques is a standard approach to the

task. Previous efforts have sought to use simple graph models of protein-ligand complexes in order to generate features for a suitable machine learning process. The metric of algebraic graph learning on extended atom types (AGL-EAT-)Score has shown particularly impressive performance. The novel contribution offered by the present work is a segue to modeling protein-ligand complexes as hypergraphs, rather than simple graphs, in an attempt to capture more subtle structural properties of the underlying complex in the features of the machine learning process. Our results find that rudimentary hypergraph methods slightly exceed the performance of state-of-the-art simple graph methods, but with a considerable amount of added computational overhead. Further methods may seek to incorporate a number of sophistications to the hypergraph method in order to achieve enhanced performance and efficiency.

Luis Carlos Picon Nunez, University of Tennessee, Knoxville

Title: Projecting 3D Protein Manifolds into Biophysical and Topological State Vectors.

Abstract: Predicting protein thermostability (T_m) is a critical bioengineering challenge. We present a multimodal machine learning architecture integrating 3D biophysical structures with deep 1D sequence semantics (ESM-2).

Our pipeline fuses deterministic geometric and topological state vectors with PCA-reduced language embeddings. To navigate the highly non-linear thermal landscape, we engineered a Trimodal Mixture-of-Experts (MoE).

A gradient-boosting router dynamically assigns proteins to specialized stacking regressors. Crucially, while standard experts operate in normalized Gaussian space, a dedicated high-temperature expert uses unconstrained quantile loss to accurately capture the extreme stability tail, enabling precision thermodynamic forecasting directly from raw structural manifolds.

Thomas A. Scott, University of Texas, Austin

Title: Uncertainty-Aware Model-Constrained Neural Digital Twins for Real-Time Forecast, Calibration, and Control

Abstract: Current structural health monitoring in aerospace systems struggles with recovering hidden parameters from limited sensor data, lacks quantified prediction confidence, and exhibits brittleness under off-nominal conditions. To address these operational gaps, we present a physics-aware neural digital twin (DT) designed for real-time, adaptive monitoring. The proposed DT framework combines three small neural networks for state inversion, stabilizing control, and forward prediction with Bayesian particle filtering for uncertainty quantification. We present applications on aerospace systems featuring incomplete measurements of nonlinear models. The DT is able to recover the full system state rapidly and when subject to unmodeled conditions correctly signals reduced confidence rather than producing overconfident erroneous predictions.

Roxana Barrios, University of Tennessee, Knoxville

Title: Scalable Filtering Algorithms for Applications in Single Molecule Screening

Abstract: Experiments probing \emph{single-molecule Förster resonance energy transfer (smFRET)} are used in molecular biology and biochemistry to study the interactions and conformational dynamics of individual biomolecules. Measurements take the form of time series data that are challenging to analyze because of noise and photophysical artifacts such as fluorophore blinking, background, and cross-talk. For this reason, the analysis of smFRET data requires advanced statistical techniques such as \emph{factorial hidden Markov models (fHMM).}

In particular, a fHMM allows for noise and stochastic transitions over time and, to isolate artifacts, also allows for independent representation of the conformational and photophysical states of the biomolecules and their fluorophores. Nevertheless, existing algorithms for the evaluation of fHMM rely on successive matrix-vector operations with high computational complexity that render them impractical for the analysis of large datasets such as those obtained in a typical smFRET experiment. In this work, we introduce tensor-based operations to reduce the computational complexity of fHMM and obtain efficient algorithms for smFRET data analysis.

Pedro Pessoa, Arizona State University

Title: Inference in Non-Markovian and Multiscale Biological Dynamics

Abstract: Biological systems are fundamentally dynamical. Cells grow and divide, respond to stress, and integrate information over time. Yet the mathematical tools commonly used in dynamical systems theory often fall short when applied to living systems, which are intrinsically stochastic, history-dependent (non-Markovian), and observed only through noisy, indirect measurements. To study such systems, we often turn to Bayesian inference.

However, traditional Bayesian approaches typically require analytical likelihoods, which are rarely available for realistic biological processes, especially when memory effects such as cell-division history and molecular inheritance play a central role. Here, I will discuss neural network assisted Bayesian inference for biological dynamics where the likelihood is difficult or impossible to write down explicitly. As a central case study, I will focus on our recent PNAS work on protein production across dividing cells. In this system, standard inference procedures fail to account for the timing of cell divisions and the inheritance of molecules across generations. By explicitly accounting for cell-division history, our approach reveals that the activation of stress regulating genes (glc3) are rarer and more transient than naïve analyses suggest.

Ngoc Hien Tran, Auburn University

Title: A reduce fracture model for reactive transport

Abstract: Reactive transport refers to the study of modelling underground flow, which plays a vital role in computational geochemistry and has various applications. The mathematical model couples the transport process, described by advection-diffusion PDEs, with the chemical model, which is either ODEs or algebraic equations, depending on whether the reactions involved are of kinetic or equilibrium type. The real-world subsurface, in many cases, has fractures and faults that can speed up or slow down the geochemical process, resulting in more complex flow modelling. We study the reduced fracture model, in which the fractures are treated as interfaces between different subdomains. The well-posedness analysis of the model is carried out, and preliminary numerical results for multiple test cases are shown.

Xiaoqi Wei, North Carolina State University

Title: Synchronization of (Un)balanced Dynamical Optimal Transport across Multiple Spaces

Abstract: Many biological systems are observed through heterogeneous modalities, requiring transport models that couple dynamics across spaces while allowing mass variation. To address this challenge, we introduce (Un)balanced Synchronized Optimal Transport ((Un)SyncOT), a novel dynamical framework that synchronizes transport-reaction flows between spaces via either geometric embeddings (Monge type) or Markov kernels (Kantorovich type). For both cases we prove that (Un)SyncOT can be reduced to a single-space problem: the Monge model becomes a Benamou-Brenier problem with a metric-modified kinetic energy, and the Kantorovich model yields a nonlocal action induced by the synchronization operator, both of which fit within a dissipation-distance formulation. Our experiments validate the convergence, stability, and efficiency, and demonstrate coherent dynamics reconstructions across spaces.

Cao-Kha Doan, Auburn University

Title: Dynamically Regularized Lagrange Multiplier Method for the Cahn-Hilliard-Navier-Stokes System

Abstract: We present efficient and accurate numerical schemes for the Cahn-Hilliard-Navier-Stokes phase field model of binary immiscible fluids. By introducing two Lagrange multipliers and their dynamic equations, we reformulate the original model problem into an equivalent system that incorporates the energy evolution process. First- and second-order dynamically regularized Lagrange multiplier (DRLM) schemes are derived based on backward differentiation formulas, in which all nonlinear terms are treated explicitly and no stabilization term is imposed. These methods are mass conserving, unconditionally

energy stable with respect to the original variables, and fully decoupled (requiring the solution of two biharmonic-type equations and two generalized Stokes systems, together with two nonlinear scalar equations at each time step). Both theoretical results and numerical performance of the DRLM schemes will be presented.

Avery Paulsen, North Carolina State University

Title: Spatially Aware Trajectory Inference with Graph Optimal Transport

Abstract: Single-cell RNA sequencing and spatial transcriptomics provide complementary insights into cellular dynamics. By integrating these datasets, we create a robust framework that captures both expression profiles and spatial organization of a cellular system. In this work, we infer a distance metric for cells by computing the optimal transport between probabilistic mappings of cells to a spatial dataset. This metric is then combined with an expression-based graph to integrate the two data spaces into a unified graph. Using optimal transport on this graph, we infer progeny dynamics and examine cell-cell communication to validate relations between progeny and spatial signaling.

Idowu Esther Ijaodoro, University of Alabama

Title: An Ensemble-Averaged Poisson-Boltzmann Model for Modeling Solute Conformational Flexibility

Abstract: TBA

Abdulmalik Oyedeji, University of Tennessee, Knoxville

Title: Optimal Control of Nutrient Supply in a Free Boundary Avascular Tumor Growth Model

Abstract: We study an optimal control problem for a free boundary model of spherical tumor growth under nutrient supply control. The control is implemented by modifying the boundary condition of the nutrient concentration, reducing the supply available to the tumor from the surrounding healthy tissue. The biological goal is to determine an optimal drug dosing schedule that minimizes tumor size while limiting side effects of treatment.

Md Borhan Uddin, University of Alabama

Title: Size-Modified Poisson_Boltzmann Models: Ion size Effects

Abstract: The classical Poisson–Boltzmann (PB) model treats each ion in the solvent surrounding a solute biomolecule to be a volumeless point and assumes the solute-solvent boundary to be a sharp interface. This theory could yield excessive ion crowding near the molecular surface. To prevent that, various size-modified Poisson–Boltzmann (SMPB) models have been developed, in which each ion will occupy a nonzero volume. However, the difference in potential and energy between the PB and SMPB models is quite small in the sharp interface setting. This work explores the finite ionic size effects in a diffuse interface

setting. A numerical comparative study is conducted by considering Kirkwood spheres and various proteins. Our studies reveal that a notable discrepancy between the PB and SMPB models only happens in the diffuse interface setting. A Stern layer-like ion concentration has been observed in the SMPB model with diffuse interface, while this phenomenon is absent in the standard PB model and in the sharp interface setting. The present study underscores the importance of incorporating diffuse interface setting in the SMPB model for representing finite sized ions in the solvent.

Soumya Chauhan, University of Arkansas

Title: Temporal Variational Graph Autoencoder for Influenza Evolution

Abstract: Frequent mutations in influenza virus surface proteins can increase infectivity while evading host and vaccine-induced immunity, driving recurrent seasonal epidemics. Each year, public health agencies such as the CDC assess thousands of circulating strains to forecast dominant variants for vaccine design, underscoring the need for models that capture viral mutation evolution beyond pairwise similarity. In this study, we propose a temporally informed variational graph autoencoder (VGAE) to model the evolutionary dynamics of influenza hemagglutinin (HA) sequences. We represent HA sequence data as a graph in which nodes correspond to viral sequences and edges encode sequence similarity and temporal proximity. The VGAE learns a probabilistic latent representation by mapping sequences to a continuous distribution whose geometry reflects mutation-driven evolutionary structure. This framework enables quantitative evaluation of how well held-out future sequences align with the learned latent distribution of influenza evolution. When evaluated on H3N2 data with an expanding window training scheme, the model achieves a test AUC of 0.76 for classifying positive pairwise relationships involving future sequences. Our results demonstrate that temporally structured graph embeddings can capture meaningful evolutionary patterns relevant for mutation prediction.

Minghua Wang, University of Tennessee, Knoxville

Title: Sheaf Laplacian Sparsification on Graphs

Abstract: Sheaf Laplacians associated with cellular sheaves generalize graph Laplacians to vector-valued signals, but can become prohibitively large in practical settings. We study sparsification of the zero-dimensional sheaf Laplacian via edge-local decompositions and leverage-score sampling. We present Bernoulli and resampling schemes with unbiased reweighting, and prove a high-probability spectral approximation guarantee on the nullspace-orthogonal subspace. Experiments on synthetic and downstream tasks show that leverage-guided sampling consistently outperforms uniform baselines in spectral and task-level fidelity.