MS1.1: Friday 8/21 at 10:45am – 12:30pm

Numerical Linear Algebra and Randomized Methods for Scalable Scientific Computation

(Organized by Maksim Melnichenko & Piotr Luszczek)

Numerical linear algebra serves as the computational backbone of modern science and engineering, providing core routines for solving differential equations, eigenvalue problems, and least-squares systems that arise across physics, data science, and machine learning. Classical methods have proven foundations, but the demands of modern large-scale problems have driven the rapid rise of randomized numerical linear algebra as a prominent and expanding extension of the field, combining probabilistic sketching and sampling with classical structure to achieve substantial gains in algorithmic performance. Success stories include randomized low-rank approximation, sketch-and-solve least-squares, trace estimation, and matrix function evaluation, with applications spanning scientific simulation, network analysis, and artificial intelligence. Recent advances in theory and software have demonstrated the practicality of randomized methods, yet significant work remains to bring them into the mainstream of high-performance scientific computing. This minisymposium brings together researchers working across numerical linear algebra and its randomized extensions to present recent algorithmic and theoretical advances and discuss open challenges at the frontier of scalable computation.

10:45am–11:05am Maksim Melnichenko (University of California, Berkeley) mmelnich@berkeley.edu

Matrix-Free Cholesky QR with Randomized Preconditioning

Orthogonalization is a basic building block of numerical linear algebra, but the standard tools are a poor fit for the large, implicitly defined operators that show up in least squares, PDE discretizations, and inverse problems. Householder QR needs direct access to the matrix entries, which such an operator cannot give you. Cholesky QR needs only matrix products and parallelizes well, but it squares the condition number and breaks down on ill-conditioned inputs. This talk presents our latest work on a randomized preconditioned Cholesky QR that fixes the stability problem while working directly with linear operators. A single random sketch yields a cheap preconditioner that makes one Cholesky QR pass safe, so randomization buys accuracy rather than speed. Because the orthonormal factor is never formed, the method also uses about a third of the operator applications of shifted Cholesky QR3 at much lower memory. I will focus on the RandLAPACK implementation and on experiments comparing the method against other matrix-free QR approaches.

11:10am –11:30am Piotr Luszczek (MIT Lincoln Lab) luszczek@icl.utk.edu

Mixed Precision Solvers for Accelerated Computing

Modern GPU hardware continues to deliver increasing levels of performance that are the computational foundation of Generative AI and large language models (LLMs). A key driver of this performance has been mixed-precision arithmetic that enables higher performance at lower precision. The availability of high-performance mixed-precision hardware has triggered a revolution in new mixed-precision algorithms. In this talk, we will discuss the underlying forces driving these new capabilities. We will also show ways to harness the recent hardware advances to enable accurate computations while leveraging the power of mixed-precision computational hardware.

11:35am–11:55am Vasileios Georgiou (Purdue University) vgeorgio@purdue.edu

RandNLA Primitives for HPC: The RandBLAS and RandLAPACK Ecosystem.

Randomization is playing an increasingly important role in modern numerical computing, enabling high-performance algorithms with controlled approximation error. This makes RandNLA primitives a key building block for performance modeling, numerical accuracy analysis, and optimized kernel design in scientific computing and machine learning workloads. This talk presents GPU implementations of RandNLA methods and discusses data-management and interface-design challenges in the RandBLAS and RandLAPACK software ecosystem.

12:00pm–12:20pm Mitchell Scott (Emory University) mitchell.scott@emory.edu

Block Subset Selection based on Randomized QR with Column Pivoting

The column subset selection problem seeks to find a collection of the matrix columns that have similar spectral properties to the original matrix. Recently with the large amount of data available, many have turned to using randomization to reduce the problem's computation. While there have been many methods that motivate how to select these columns, they are just that–individual columns. However, by blocking these columns, there is less computational communication needed, which makes the process faster. In this talk we will discuss optimality conditions for selecting these blocks of columns using randomization. We relate the worst case of this randomized method to the deterministic block QR with column pivoting (QRCP). We then corroborate this analysis with numerical experiments to showcase the method's speed and accuracy compared to standard QRCP algorithms.

MS1.2: Friday 8/21 at 10:45am – 12:30pm

Optimal Transport & Related Topics (Organized by Yonah Moise)

Optimal transport provides a rich mathematical framework for studying probability distributions and the geometry of how they relate to one another. This minisymposium brings together a range of perspectives on the theory, computation, and applications of optimal transport. Together, the talks will illustrate the flexibility of optimal transport as both a mathematical language and a computational tool for modern problems.

10:45am–11:05am Prof. Yanlai Chen (UMass Dartmouth) yanlai.chen@umassd.edu
Over collocation based model order reduction for optimal mass transport.

11:10am –11:30am Prof. Bjorn Sandstede (Brown University) bjorn_sandstede@brown.edu
Inference from single-cell data using optimal transport

11:35am–11:55am Prof. James Murphy (Tufts University) JM.Murphy@tufts.edu
Static and Dynamic Optimal Transport for Analysis and Synthesis on Graphs.

12:00am–12:20pm Yonah Moise (Tufts University) Yonah.Moise@tufts.edu
A Dynamical Wasserstein Barycenter framework for Gaussian Mixture Models

MS1.3: Friday 8/21 at 10:45am – 12:30pm
Emerging Mathematical and Computational Approaches to Genomic and Cellular Data Analysis
(Organized by Pengyu Liu and Nic Fisk)

The past decade has seen an explosion in the scale and resolution of biological data. Single-cell sequencing, spatial transcriptomics, immune repertoire profiling, and high-throughput RNA structure probing now routinely produce datasets encompassing millions of cells, sequences, or structural measurements. These technologies are transforming our understanding of cellular heterogeneity, immune response, gene regulation, and disease mechanisms. However, the complexity, high dimensionality, and inherent noise of these data pose mathematical and computational challenges that are only beginning to be addressed.

Extracting meaningful biological signal demands rigorous quantitative methods — from probabilistic models and phylogenetic inference to statistical learning and scalable algorithms — problems that sit naturally at the intersection of applied mathematics, statistics, and computational science. As New England continues to grow as a hub for computational biology, a regional meeting focused on mathematical and computational methods for genomic and cellular data analysis would be valuable for fostering collaboration and exchange of ideas. The SIAM Northeast Section Annual Meeting offers a timely venue for such interdisciplinary gathering.

This minisymposium features four early-career researchers from New England institutions who are developing novel mathematical and computational frameworks for analyzing genomic and cellular data. The session aims to foster new connections and strengthen the region's growing mathematical/computational biology and biodata analysis community.

10:45am–11:05am Kenneth B. Hoehn (Dartmouth College) kenneth.b.hoehn@dartmouth.edu

TyCHE enables time-resolved lineage tracing of B cells, tumors, and other heterogeneously evolving cell populations Phylogenetic methods for cellular lineage tracing have driven significant insights into cell development, immune responses, and tumor evolution. While most methods estimate mutation trees, in which branches represent mutation, time-resolved lineage trees have branches that represent calendar time, meaning they could relate events like cellular migration and differentiation to perturbations like vaccines and drug treatments. However, somatic mutation rates can vary dramatically by cell type, biasing existing methods. For example, B cells undergo rapid somatic hypermutation during immune responses before becoming quiescent memory cells, while tumors, bacteria, and viruses can develop rapidly evolving “hypermutator” variants. To build accurate cellular time trees, we introduce TyCHE (Type-linked Clocks for Heterogenous Evolution), a Bayesian phylogenetics package that infers time-resolved lineage trees even if sub-populations evolve at dramatically different rates. We show through simulations of B cell germinal center reactions that TyCHE estimates more accurate trees, dates, and ancestral cell types than existing methods. We applied TyCHE to single cell and bulk B cell receptor sequences to reconstruct memory cell differentiation during chronic HIV infection, as well as the timing of recall germinal center reactions following repeated influenza vaccination. We further use TyCHE to infer clinically useful lineage trees of a hypermutating glioma tumor lineage and progression of an acute bacterial lung infection, applications where existing methods fail. TyCHE opens new avenues for testing how cell proliferation, differentiation, and migration shape responses to vaccines, drug treatments, and other stimuli. TyCHE and SimBLE are available as open-source software compatible with the BEAST2 and Immcantation ecosystems.

11:10am –11:30am Meng Liu (Yale University) meng.liu.ml3223@yale.edu

From Frequency to Fitness: A Likelihood-Based Framework for Quantifying Selection on Copy Number Alterations
Copy number alterations (CNAs) are among the most prevalent genomic changes in cancer, yet distinguishing selectively advantageous alterations from passenger events remains challenging. Recurrence alone is insufficient because observed CNA frequencies reflect both mutation processes and selection, while chromosomal instability generates extensive spatial correlation among neighboring genomic regions. We developed a likelihood-based evolutionary framework to quantify selection on copy number alterations while explicitly modeling heterogeneous background mutation processes. The approach combines ploidy-aware CNA classification, copy-number signature–based estimation of neutral mutation rates, and interval-level likelihood modeling to infer selection on copy-number increases and decreases. To enable genome-scale analyses despite strong correlations among neighboring loci, we further implemented an iterative multi-locus selection procedure that identifies a parsimonious set of genomic intervals providing independent evidence of selection. Applying this framework to 554 ovarian cancer genomes, we generated genome-wide maps of selection on copy-number alterations. We found substantial discordance between recurrence and selection: several highly recurrent alterations showed limited evidence of positive selection, whereas multiple moderately recurrent loci exhibited strong selective advantage. Established oncogenic amplifications including MECOM, MYC, and CCNE1 emerged as highly selected events, while additional candidate driver loci were identified that would not be prioritized using conventional frequency-based approaches. More broadly, this work demonstrates how explicit modeling of mutation and selection can transform descriptive copy-number data into quantitative estimates of evolutionary fitness effects. The framework is applicable across cancer types and provides a general strategy for identifying selectively important genomic alterations in large-scale genomic datasets.

11:35am–11:55am Adam Sychla (Harvard Medical School) adam_sychla@hms.harvard.edu

An RNA Language Model trained on sequence alone reveals the structural logic of Internal Ribosome Entry Sites

RNA is a dynamic, yet structured molecule bridging high information density with complex higher-order assemblies and interactions. Far from being an inert translator, RNA uses both sequence and structure to enable function. Despite its importance, computational and experimental evaluation of RNA structure remains a core challenge. RNA's dynamic nature means that there are limited "ground truth" structures available by traditional methods. Given the lack of high-quality training data, machine learning models have been relatively ineffective when evaluating RNAs outside a subset of well-resolved structures. For this work, we were interested in Internal Ribosome Entry Sites (IRESes), large and complex structures used by viruses to recruit the ribosome. Although IRESes are well studied, they typically fall far outside the predictive capabilities of other computational methods. In trying to find a method to study IRESes as a broad class, we found that, paradoxically, our best structure predictions were derived without any a priori data on structure. We achieved this by fine-tuning an RNA Language Model on 50,000 IRES sequences on the task of masked-token prediction. Although this model was provided no external knowledge of secondary structure or base pairing rules, an encoding of structure nonetheless emerges. Evaluating structure with this model, we outperformed covariance in F1 and precision. This pipeline enabled us to seek new family-wide patterns of IRES structures and provides a path towards more accurate functional prediction. Together, we demonstrate that emergent properties of RNA can be derived from their sequence alone by carefully probing RNA Language Models.

12:00pm–12:20pm Ying Ma (Brown University) ying_ma@brown.edu

Resolving Tissue Maps: Statistical and Deep Learning Methods for Integrative Spatial Omics Across Samples, Sections, and Modalities.

MS1.4: Friday 8/21 at 10:45am – 12:30pm

Applied Abstract Mathematics (organized by Hayden Jananthan)

Traditional abstract mathematics is being increasingly used in more applied contexts. This mini-symposium focuses on examining some instances of 'applied abstract mathematics' work covering: information diffusion, matrix-based graph theory, associative array algebra, and manifold learning.

10:45am–11:05am Megan Bryson (Queen's University) meganbryson1999@gmail.com
Information Diffusion on Complex Networks: A Proportion Based Approach

11:10am –11:30am Dr. Hayden Jananthan (MIT) hayden.jananthan@ll.mit.edu
Mathematical Foundations of the GraphBLAS

11:35am–11:55am Dr. Jeremy Kepner (MIT) kepner@ll.mit.edu
Accelerating Everything via Associative Array Algebra

12:00pm–12:20pm Dr. Ryan Robinett (University of Chicago) robinett@uchicago.edu
Manifold Learning and Riemannian Optimization

MS2.1a: Friday 8/21 at 2:00pm – 3:45pm

Recent Advances in Numerical Methods for Time-Dependent Problems I

(Organized by Z. Grant and Z. Sun)

This minisymposium highlights recent advancements and emerging frontiers in numerical methods for time-dependent problems—a key domain underpinning the simulation of dynamic processes in science and engineering. As we seek more robust, accurate, and computationally efficient discretization schemes, both the refinement of mathematical models and the evolution of computational tools continue to drive algorithmic innovation. This session brings together active scholars to present a diverse range of cutting-edge methodologies and foundational developments. Topics will include high-order time-stepping strategies, advanced spatial discretizations, mixed-precision algorithms, structure-preserving methods, and novel numerical formulations for evolutionary partial differential equations.

2:00pm – 2:20pm Sigal Gottlieb (UMassD) sgottlieb@umassd.edu

Mixed Precision Two Derivative Runge–Kutta Methods

2:25pm – 2:45pm Joseph Nakao (Swarthmore) jnakao1@swarthmore.edu

An Eulerian-Lagrangian finite volume method with CUR adaptive rank (EL-CUR) for nonlinear convection-diffusion equations

Eulerian-Lagrangian (EL) and semi-Lagrangian methods are popular for solving transport equations due to the large allowable time-step sizes from tracing the characteristics alleviating the CFL condition. For 2D solutions, either a splitting or non-splitting approach can be used. Dimensional splitting is attractive since it can leverage simpler 1D algorithms, but iterating over the entire grid at each stage of the splitting method poses a computational bottleneck. To alleviate this issue and reduce the storage complexity of the 2D solution, we combine the EL framework with matrix cross approximations via CUR decomposition. Hence, the solution is adaptively compressed, large time-step sizes can be taken, and 1D methods can be utilized for easier implementation, such as standard WENO-type methods for spatial reconstruction. Preliminary results are shown to demonstrate the accuracy, robustness, and efficiency of the proposed scheme.

2:50pm – 3:10pm David Shirokoff (NJIT) david.shirokoff@njit.edu

Preconditioning and Linearly Implicit Time Integration for the Serre-Green-Naghdi Equations

The Serre-Green-Naghdi (SGN) equations are fluid models that incorporate dispersion (through higher order asymptotic expansions) into the traditional shallow water equation (SWE). While the presence of dispersion results in the modeling of important physical effects, the SGN equations contain a differential PDE constraint which poses a key numerical challenge. This talk will focus on developing time integration and preconditioning strategies for handling the differential PDE constraint. First, we establish a constant coefficient preconditioner and rigorous bounds on the preconditioned conditioning number. The conditioning bounds incorporate the effects of bathymetry in two dimensions, are quasi-optimal within a class of constant coefficient operators, highlight fundamental scalings for a loss of conditioning, and ensure mesh independent performance for iterative Krylov methods. Utilizing the conditioning bounds, we devise and test two time integration strategies for solving the full SGN equations. The first class combines classical explicit time integration schemes (4th order Runge-Kutta and 2nd--4th order Adams-Bashforth) with the new preconditioner. The second is a linearly implicit scheme where the differential constraint is split into a constant coefficient implicit part and remaining (stiff) explicit part. The linearly implicit methods require a single linear solve of a constant coefficient operator at each time step. We provide a host of computational experiments that validate the robustness of the preconditioners, as well as full solutions of the SGN equations including solitary waves traveling over an underwater shelf (in 1d) and a circular bump (in 2d).

3:15pm – 3:35pm Zachary J. Grant (UMassD) zgrant@umassd.edu

Mixed Accuracy Runge–Kutta Methods for smooth perturbations

MS2.2: Friday 8/21 at 2:00pm – 3:45pm

Designing Well-Behaved Optimization Problems for Learning and Control in Robotics

(Organized by Gabriel Bravo)

A fundamental challenge in robotics is that learning and control rely on solving complex, often high-dimensional non-convex optimization problems, and performance hinges on how reliably we can solve these difficult problems in practice. This mini-symposium explores a unifying perspective: how can we design systems, models, and algorithms so that the resulting optimization problems become easier to solve?

We begin at the level of system design, where morphology, reduced-order models, and hierarchical abstractions reshape the structure of control problems. We argue that co-designing physical systems and control architectures, and embedding control-theoretic structure into learning models, reduces complexity and enables faster, more robust decision making.

We then examine how global optimization tools provide a principled lens for improving problem geometry. We discuss how techniques such as moment hierarchies and sums-of-squares relaxations enable globally-informed policy learning, leading to more optimal and robust solutions, while also informing feature construction and cost design; producing optimization landscapes that are easier to navigate.

At the algorithmic level, we turn to advances in numerical optimization that make problems tractable at scale. For instance, new primal-dual interior-point formulations eliminate classical ill-conditioning by enforcing complementarity by construction, enabling stable, factorization-free solvers and efficient differentiation through optimization layers.

Finally, these ideas come together in scalable and distributed frameworks, including differentiable model predictive control and approaches leveraging decentralized structure and mechanical intelligence for enhanced robustness.

Throughout, the mini-symposium emphasizes a shift from solving hard optimization problems to designing them to be more tractable, through structure, global insight, and scalable algorithms.

2:00pm – 2:20pm Steve Heim (Cornell University) heim.steve@cornell.edu

Locally quadratic value function approximations for fast reactive control

2:25pm – 2:45pm Roland Schwan (Dartmouth College) roland.schwan@dartmouth.edu

Exploiting Structure in Multistage Optimization on CPU and GPU

2:50pm – 3:10pm Jon Arrizabalaga (MIT) jonarri@mit.edu

Implicit Interior-Point Methods for Reliable and Scalable Robotics Optimization

3:15pm – 3:35pm Gabriel Bravo (Dartmouth College) Gabriel.F.Bravo.Palacios@dartmouth.edu

Scalable optimization to leverage learning and decentralized control in robotic systems

MS2.3: Friday 8/21 at 2:00pm – 3:45pm
Mathematical Methods in Network Science (Organized by P. Chodrow, D. DeFord, M. Jones, S. Tymochko)

Many systems are characterized by complex, structured interactions between their constituent parts. Networks and their generalizations offer a powerful modeling framework with which to study these systems. This minisymposium will highlight mathematical methods for studying structure, function, and dynamics in networked systems. Speakers will address higher-order network data analysis, network methods for spatial demographic data, consensus dynamics on social networks, and topological methods for describing dynamics on network substrates.

2:00pm – 2:20pm Atticus McWhorter atticus.w.mcwhorter.gr@dartmouth.edu
Applications of Metropolized Sampling in Computational Redistricting

2:25pm – 2:45pm Tobias Timofeyev (UVM/Dartmouth) Tobias.Timofeyev@uvm.edu
Asymmetric Network Persistence of State Space Attractors
Recent work explores Topological Data Analysis (TDA) as a framework for qualitatively characterizing dynamical data, but standard methods ignore temporal directionality, failing to distinguish between the kinds of dynamical behavior that appear as homological cycles. In this talk, I will present a persistence framework for dynamical data that incorporates sequential information through directed networks constructed from time-series data. I will describe the construction of both the directed network and the Dowker-based persistence framework, then illustrate how this asymmetric framework behaves on a variety of example networks and dynamical systems.

2:50pm – 3:10pm Daryl DeFord (Vassar) ddeford@vassar.edu
Network Science of Census and Precinct Dual Graphs

3:15pm – 3:35pm Matt Jones (Colby) mijones@colby.edu
Colorings and Consensus on Graphs
For hundreds of years, graphs have been used by mathematicians to study the connections between things. I will show how graph colorings can also be used to study group behavior by introducing a new kind of graph coloring: gridlocked colorings. These "locally-optimal'' colorings are relevant when a group tries to reach consensus, and I will describe an algorithm to count them. Finally, I'll talk about how to think of consensus as a stochastic process and how to apply these ideas to real-world scenarios.

MS2.4: Friday 8/21 at 2:00pm – 3:45pm
Recent Advances in Quantum Computing and Quantum Machine Learning
(Organized by D. Shi, L. Lu, P. Xiao, X. Yang)

Quantum computing offers new possibilities for solving problems that are challenging or intractable for classical methods, with potential applications in optimization, simulation, scientific computing, and machine learning. However, realizing these potential advantages requires advances in both quantum algorithms and their practical implementation on near-term quantum devices, where noise, limited scalability, and hardware constraints remain major challenges. This minisymposium presents recent studies in quantum computing from both theoretical and algorithmic perspectives. The topics cover a broad range of emerging directions, including hybrid quantum-classical frameworks, quantum algorithms for optimization and scientific computing, quantum machine learning methods, hardware-efficient circuit designs, and variational quantum models under noise. The goal of this minisymposium is to highlight recent progress, open challenges, and future opportunities in quantum computing and its applications.

2:00pm – 2:20pm Pengpeng Xiao (Yale University) p.xiao@yale.edu
Quantum DeepONet: Neural operators accelerated by quantum computing

2:25pm – 2:45pm Dongwei Shi (Lehigh University) dos222@lehigh.edu
Beyond LXEB: On Test Statistics for Random Circuit Sampling and Certified Randomness

2:50pm – 3:10pm Weiqi Chu (University of Massachusetts Amherst) weiqichu@umass.edu
A Quantum Model of Opinion Dynamics
Classical models of opinion dynamics represent individuals' opinions as scalar values or random variables. However, classical models cannot explain cognitive phenomena such as order effects — where answers to questions depend on the order in which they are asked — or the disjunction effect — where people prefer a given action under every known condition yet refuse to take it when the condition is unknown, violating the law of total probability. As it turns out, some mechanisms in quantum mechanics, such as superposition, non-commuting observables, and interference, are natural tools for modeling cognitive states that are genuinely indefinite until resolved by a question or context. In this talk, I will show the connection between these two fields and introduce a quantum model of opinion dynamics in which each agent in a social network is associated with a density matrix, encoding both an expressed opinion and quantum coherences representing cognitive ambivalence. The governing Lindblad master equation yields the classical Friedkin-Johnsen opinion model when projecting to the opinion observable, while also producing the dynamics of cognitive coherence, which help explain social phenomena such as echo chamber effects and cognitive polarization that are absent from classical models.

3:15pm – 3:35pm Brenda Rubenstein (Brown University) brenda_rubenstein@brown.edu
Quantum Computing Biology
The ability to model biochemical reaction dynamics on quantum hardware would open the door to the virtually exact description of enzymatic catalysis, accelerating the discovery of novel therapeutics. However, noisy hardware, the costs of computing gradients, and the quantum volumes required to simulate large systems present major challenges to realizing the potential of dynamical simulations using quantum hardware. In this talk, I will discuss our recent efforts to model biochemical reactions, including ATP hydrolysis and covalent kinase inhibitor binding, paradigmatic and clinically-important biochemical reactions, on quantum hardware. Key to our modeling is employing transfer learning to learn approximate force fields based on abundant data and then correcting those force fields using data from quantum hardware. To model such molecular systems on modern NISQ quantum hardware, we also reduce our Hamiltonians using downfolding methods and embedding methods and perform state-of-the-art Coupled Exchange Operator ADAPT-VQE calculations. We moreover explore the use of a variety of postprocessing and quantum-boosted algorithms to enhance the accuracy of our results. Using this combination of techniques, I will show how we can gain novel mechanistic insights into a variety of biochemical reactions, opening the door to quantum-informed biomolecular simulation.

MS2.1b: Saturday 8/22 at 10:30am – 12:15pm

Recent Advances in Numerical Methods for Time-Dependent Problems II (Organized by Z. Grant and Z. Sun)

This minisymposium highlights recent advancements and emerging frontiers in numerical methods for time-dependent problems—a key domain underpinning the simulation of dynamic processes in science and engineering. As we seek more robust, accurate, and computationally efficient discretization schemes, both the refinement of mathematical models and the evolution of computational tools continue to drive algorithmic innovation. This session brings together active scholars to present a diverse range of cutting-edge methodologies and foundational developments. Topics will include high-order time-stepping strategies, advanced spatial discretizations, mixed-precision algorithms, structure-preserving methods, and novel numerical formulations for evolutionary partial differential equations.

10:30am – 10:50am Cesar Herrera (Purdue University) herre125@purdue.edu

Mixed-Precision Additive Runge-Kutta Methods

Performing computations in low precision can yield speedups of 4x or greater, though this often comes at the cost of reduced accuracy. To address this tradeoff, we analyze mixed precision additive Runge-Kutta (MP-ARK) methods. These methods reduce the computational burden of the expensive implicit stages by utilizing cheaper, low-precision arithmetic. The explicit stages are then executed using high precision, which provides a necessary correction to the implicit stages and helps recover overall accuracy.

10:55am – 11:15am Chloe Griffin (Brown University) danielle_griffin@brown.edu

Positivity Preservation via Conservative Sweeping for High-Order Discretizations of Hyperbolic Conservation Laws

High-order numerical methods for hyperbolic conservation laws often lack inherent mechanisms to preserve positivity, leading to computational failure near strong shocks or in near-vacuum states. In this talk, we present a novel conservative sweeping procedure for density and the nonlinear pressure function in fifth-order finite-difference WENO discretizations of the compressible Euler equations. Formulated as a global mass-redistribution technique, the method generalizes the Zhang-Shu scaling limiter within a sweeping framework while remaining conservative and high-order accurate. A key advantage of the proposed approach is its modularity. As a standalone post-processing procedure, it applies directly to finite-difference, finite-volume, and discontinuous Galerkin discretizations without modifying the underlying spatial discretization. The framework naturally extends beyond pressure in the Euler equations to any concave function of the conserved variables in hyperbolic systems. Numerical results demonstrate robust performance for challenging compressible flow problems, including strong blast waves and high-Mach flows. We conclude with a discussion of ongoing work extending the framework to implicit time integration and continuous Galerkin discretizations.

11:20am – 11:40am Zheng Sun (The University of Alabama) zsun30@ua.edu

Runge–Kutta discontinuous Galerkin methods with generalized method of lines

11:45am – 12:05pm Zhongqiang Zhang (Worcester Polytechnic Institute) zzhang7@wpi.edu

Large-Step Space-Time PINNs versus Small-Step Time Marching for Fokker-Planck Equations Time discretization plays a central role in the effectiveness of physics-informed neural networks (PINNs) for evolutionary PDEs. Using Fokker-Planck equations as a case study, this talk examines two contrasting strategies: a space-time PINN formulation over large time windows and a sequential time-stepping approach based on small time increments. The discussion highlights the trade-offs between global and local approximations, computational cost, error propagation, and long-time accuracy. Numerical examples demonstrate how these approaches perform in challenging regimes and provide insights into the design of efficient PINN algorithms for time-dependent PDEs.

MS3.1: Saturday 8/22 at 10:30am – 12:15pm

Generative Scientific Machine Learning for PDEs and Complex Physical Systems

(Organized by Lu Lu)

Recent advances in generative AI are creating new opportunities for scientific machine learning. Compared with traditional deterministic models, generative methods provide probabilistic representations of complex systems, enabling uncertainty-aware prediction, inverse inference, sparse-data reconstruction, and data generation for scientific applications. These capabilities are particularly important for nonlinear and stochastic systems arising in fluid dynamics, porous media, climate science, combustion, materials modeling, and other complex physical processes. This mini-symposium focuses on emerging generative AI methods for PDE-governed systems and scientific computing. Topics of interest include but are not limited to diffusion and flow-based models, generative neural operators, probabilistic operator learning, physics-informed generative modeling, uncertainty quantification, inverse problems, and hybrid AI-numerical frameworks. We welcome contributions on theoretical analysis, scalable algorithms, and application demonstrations. A central goal of this mini-symposium is to explore how generative AI can improve the reliability, scalability, and generalizability of PDE modeling under uncertainty, especially in settings involving sparse observations, irregular geometries, and multi-modal dynamics. By bringing together researchers from applied mathematics, machine learning, and computational science, this symposium aims to foster discussion on next-generation AI methodologies for scientific discovery and large-scale physical simulation.

10:30am – 10:50am Yajie Ji (Yale University) yajie.ji@yale.edu

GeoFAE Inverse problems governed by partial differential equations (PDEs) arise widely in science and engineering, but are often ill-posed and limited by sparse, noisy observations. While learning-based methods have greatly accelerated inference, most assume fixed, regular domains and focus primarily on field reconstruction rather than recovery of the underlying geometry. Here we introduce {\em GeoFunFlow}, a geometry-aware diffusion framework that unifies two core tasks: (i) reconstructing multiphysics fields from sparse data on regular and irregular domains, and (ii) inferring unknown geometry directly from partial field observations. GeoFunFlow combines a geometric function autoencoder (GeoFAE) with a latent diffusion model trained using rectified flow, enabling efficient sampling from the posterior distribution. As a unified encoder–decoder architecture, GeoFAE can handle unstructured meshes of varying sizes. When mesh information is not available, it infers the domain geometry directly from the physical fields by representing the geometry as a signed distance function (SDF). In this way, GeoFAE learns the coupling between the physical fields and the underlying geometry directly from data. In the latent space produced by the GeoFAE encoder, the diffusion model samples from the joint posterior over fields and geometry, and the decoder reconstructs both quantities together with calibrated uncertainty estimates. Across multiple benchmarks spanning multiphysics regimes and complex domains, GeoFunFlow achieves competitive reconstruction accuracy and strong geometry recovery performance, while additionally providing posterior uncertainty estimates.

10:55am – 11:15am Siming Shan (Yale University) siming.shan@yale.edu

Regularization by denoising diffusion models for solving inverse PDE problems with application to full waveform inversion

11:20am – 11:40am Guannan Zhang (Oak Ridge National Laboratory) ZHANGG@ORNL.GOV

Dynamic Generative AI for High-Dimensional Nonlinear Data Assimilation We propose an ensemble score filter (EnSF) for solving high-dimensional nonlinear filtering problems with superior accuracy. A major drawback of existing filtering methods, e.g., particle filters or ensemble Kalman filters, is the low accuracy in handling high-dimensional and highly nonlinear problems. EnSF addresses this challenge by exploiting the score-based diffusion model, defined in a pseudo-temporal domain, to characterize the evolution of the filtering density. EnSF stores the information of the recursively updated filtering density function in the score function, instead of storing the information in a set of finite Monte Carlo samples (used in particle filters and ensemble Kalman filters). Unlike existing diffusion models that train neural networks to approximate the score function, we develop a training-free score estimation method that uses a mini-batch-based Monte Carlo estimator to directly approximate the score function at any pseudo-spatial–temporal location, which provides sufficient accuracy in solving high-dimensional nonlinear problems while also saving a tremendous amount of time spent on training neural networks. High-dimensional Lorenz-96 systems are used to demonstrate the performance of our method. EnSF provides superior performance, compared with the state-of-the-art Local Ensemble Transform Kalman Filter, in reliably and efficiently tracking extremely high-dimensional Lorenz systems (up to 1,000,000 dimensions) with highly nonlinear observation processes.

11:45am – 12:05pm Daniel Waxman (Basis Research Institute) dan@basis.ai

A Bayesian Recipe for Learning Hybrid Models from Noisy Data

Learning in complex dynamical systems is traditionally computationally expensive, and often inflexible, catalyzing the development and proliferation of modern machine learning (ML)-based solutions. ML-based solutions, however, pose a variety of troubles related to accuracy, uncertainty quantification (UQ), and extrapolation. Moreover, ML-based methods often struggle with noisy or partial information, where the strong prior knowledge of a mechanistic model may be necessary for identifiability of solutions. We propose a Bayesian recipe for learning "hybrid models," i.e., models that combine the principled extrapolation and UQ of traditional mechanistic models with the flexibility of ML-based solutions. We also present dynestyx, a probabilistic programming language designed to aid in such analyses, and conclude with a case study in nonlinear, stochastic systems with partial, noisy observations.

MS3.2: Saturday 8/22 at 10:30am – 12:15pm

Squeezing into Tight Spaces: Flow in Confined Domains (Organized by A.R. Drumm)

The motion of particles in confined, low Reynolds number flows garners interest in a variety of industrial and scientific applications. Subjects include bacteria, biological vesicles, droplets, polymer solutions, and red blood cells; and problems include clogging of microfluidic channels, measurement of physical properties, identification of threshold values for surface stability, orientation within the flow, and influence of confining geometry on migration and shape. This mini-symposium highlights mathematical efforts using modeling, experimental observation, numerical simulation, or a combination of these to study the motion and behavior of different particle subjects flowing through confined domains.

10:30am – 10:50am Abigail Rose Drumm ardrumm@wpi.edu

Modeling the Transposition of Deformable Bacteria Through Membrane Pores

From research to clinical development and production, *Mycoplasma* are well-recognized and widespread contaminants in biopharmaceutical manufacturing. Their successful proliferation despite the ultrafiltration performed to eliminate them has been attributed in part to the flexibility of their cell walls. How does this bacterium manage to squeeze through pores that are, in some cases, one-third of its size? We build on a force-balance approach to quantify a threshold transmembrane pressure that determines retention versus passage, then use semi-analytical modeling based on elasticity relations, Stokes equations, and the method of reflections to explore the deformation and motion of a bacterium once it has trespassed into a pore. This research aims to identify the maximum flow conditions at which membrane filtration remains a viable strategy for the filtering out of *Mycoplasma* from permeate to effectively inform the processes and materials employed to eradicate it. It is funded by NSF CBET-2211001.

10:55am – 11:15am Thomas Fai tfai@brandeis.edu

Multiscale model of red blood cell clogging in microfluidic devices

11:20am – 11:40am Dana Ferranti dferranti@wpi.edu

Hydrodynamics of Rigid Asters Confined in a Sphere

11:45am – 12:05pm Sara Hashmi s.hashmi@northeastern.edu

Soft materials flowing through small spaces