SIAM Great Lakes 2023 Program

Michigan State University

East Lansing, MI

October 14, 2023

Overview

8:00-8:45am	Registration and Coffee	Wells Hall B wing
8:45-9:00am	Welcome Remarks	Wells Hall B119
9:00-9:50am	Plenary 1: Selim Esedoglou	Wells Hall B119
10:00-Noon	Parallel Session 1	Wells Hall A wing
Noon-1:30pm	Lunch	
1:30-2:20pm	Plenary 2: Elizabeth Munch	Wells Hall B119
2:30-3:20pm	Plenary 3: Takis Souganidis	Wells Hall B119
3:30- 3:50pm	Coffee and Treats	Wells Hall B Wing
4:00-6:00pm	Parallel Session 2	Wells Hall A Wing

Plenary Talks

Plenary 1

Title: *On median filters for motion by mean curvature*
Speaker: Selim Esedoglou, University of Michigan
Location: Wells Hall B119
Time: 9:00-9:50am

Abstract: The median filter scheme is an elegant, monotone discretization of the level set formulation of motion by mean curvature (an evolution that arises in many applications, including materials science and image processing). It turns out to be connected, in a completely precise way, to another class of numerical methods for the same evolution: threshold dynamics. In particular, median filters evolve every upper level set of their initial condition by threshold dynamics. In other words, they are the natural level set versions of threshold dynamics algorithms. Exploiting this connection, we revisit median filters in light of recent progress on the threshold dynamics method. We give a variational formulation of, and exhibit a Lyapunov function for, median filters, resulting in energy based unconditional stability properties. The connection also yields analogues of median filters in the multiphase setting of mean curvature flow of networks. These new multiphase level set methods do not require frequent redistancing, and can accommodate a wide range of surface tensions.

Plenary 2

Title: *Comparing Embedded Shapes using Topological Summaries*
Speaker: Elizabeth Munch, Michigan State University
Location: Wells Hall B119
Time: 1:30-2:20pm

Abstract: The goal of the field of topological data analysis (TDA) is to quantitatively encode and measure shape using Algebraic Topology. The available tools encompass both algebraic constructions (such as persistence diagrams and Euler characteristics) as well as graph based representations (such as Reeb graphs, mapper graphs, and merge trees). Applications of TDA have exploded in recent years, finding use in a diverse array of domains including plant biology, neuroscience, mechanical engineering, and many more. This increased interest is due to its now extensive theoretical foundation, and more recently due to the increased availability of more efficient algorithms and software making TDA pipelines more readily accessible to domain scientists. In this talk, we will review some of the tools available with a particular focus on encoding embedded shapes in $\mathbf{R}^d$ (with most of our applications living in the setting of d=2,3), and for creating metrics between these representations to allow for access to tools such as statistics and machine learning.

Plenary 3

Title: *Regularity and rates of convergence for mean field games of control*
Speaker: Takis Souganidis, University of Chicago
Location: Wells Hall, B119
Time: 2:30-3:20pm

Abstract: We discuss global rates of convergence of the value function and trajectories of N-player controlled games to the value and trajectory of a McKean-Vlasov equation. I will also present some regularity results for the value function of a McKean-Vlasov equation and use them to obtain optimal local convergence rates.

Parallel Session 1
Wells Hall A Wing-- 10:00am-Noon

MS 1 Modeling and analysis of single cell omic data	MS 2 Exploring Nonlinear Phenomena in Applied PDEs	MS 3 Optimization Methods for Large-Scale Data Analysis	MS 4 Nonlinear partial differential equations and optimal transport with applications	MS 5 Graph-based Techniques in Machine Learning	MS 6 Multiscale modeling and numerical methods for material science and biological systems – Part 1
Wells A108	Wells A116	Wells A118	Wells A120	Wells A122	Wells A124

MS 7 Wild behavior in fluid dynamics	MS 8 Collective behavior in physical and social network models	MS 9 AI, PDE, and Graph Theory for Biological Systems	CP 1 Data Driven Analysis	CP 2 Analysis of PDEs
Wells A126	Wells A128	Wells A130	Wells A132	Wells A134

Parallel Session 2
Wells Hall A Wing-- 4:00-6:00pm

MS 10 Mathematical Modeling and Machine Learning for Analyzing Molecular Structure	MS 11 Spectral theory and asymptotic analysis in quantum mechanics	MS 12 Recent Advances in the Analysis of PDEs	MS 13 Modern themes in calculus of variations	MS 14 Mathematical Enhancement of AI for Data Analysis in Biosciences and Molecular Sciences	MS 15 Multiscale modeling and numerical methods for material science and biological systems – Part 2
Wells A108	Wells A116	Wells A118	Wells A120	Wells A122	Wells A124

MS 16 PDE models in Mathematical Biology	MS 17 Topological Data Analysis	MS 18 Analysis and applications of nonlinear PDEs	CP 3 Data Driven Analysis	CP 4 Numerical Analysis
Wells A126	Wells A128	Wells A130	Wells A132	Wells A134

Parallel Session 1

MS 1
Title: Modeling and analysis of single cell omic data
Organizer: Yuta Hozumi, Michigan State University
Location: Wells Hall A108

Abstract: Single cell RNA sequencing (scRNA-seq) is a relatively new method that profiles transcriptomes of individual cells, revealing vast information in the heterogenity within cell population, which has lead to further understanding of gene expression, gene regulation, cell-cell communication, cell differentiation, spatial transcrtiptomics, signal transduction pathways, and more. Analyzing the data is quite challenging due to dropout event-induced zero expression counts, low sequencing depth leading to low reading counts, general noise, and the high dimensionality of the original data. In this mini-symposium, we gathered speakers that will showcase new mathematical models to analyze such complex data. We hope that this will offer new perspective in the field and encourage collaboration to further the understanding of the relation between scRNA-seq data and many complex biological pathways.

10:00-10:30am	Sean Cottrell, Michigan State University	Topological PCA for Single Cell RNA-Sequence Data Analysis
10:30-11:00am	Hongzhi Wen, Michigan State University	Single Cells Are Biological Tokens: Towards Cell Language Models
11:00-11:30am	Zheng Li, University of Michigan	Multi-scale and multi-sample analysis enable accurate cell type clustering and spatial domain detection in spatial transcriptomic studies
11:30-Noon	Ruo-Qiao Chen, Michigan State University	Large-scale surface protein abundance prediction from single-cell transcriptomes with zero-shot learning

MS 2
Title: Exploring Nonlinear Phenomena in Applied PDEs
Organizers: Fernando Charro, Wayne State University and Catherine Lebiedzik, Wayne State University
Location: Wells Hall A116

Abstract: We will explore the impact of nonlinear phenomena in science and engineering. The session covers a wide range of topics in applied partial differential equations (PDEs), including reaction-diffusion systems, free-boundary problems, fluid dynamics, nonlinear waves, stability of geometric flows, and minimal energy configurations. This session aims to offer a platform for exchanging ideas and gaining insights into the challenges and opportunities of nonlinearities in applied PDEs.

10:00-10:30am	Nung-Kwan Yip, Purdue University	Homogenization of Fokker-Planck Equation in Wasserstein Space
10:30-11:00am	Tao Huang, Wayne State University	Poiseuille flow of full Ericksen-Leslie system modeling nematic liquid crystal flows
11:00-11:30am	Fernando Charro, Wayne State University	Asymptotic Mean-Value Formulas for Nonlinear Equations
11:30-Noon	Zaher Hani, University of Michigan	The mathematical theory of wave turbulence

MS 3
Title: Optimization Methods for Large-Scale Data Analysis
Organizers: Longxiu Huang, Michigan State University and Rongrong Wang, Michigan State University
Location: Wells Hall A118

Abstract: In today's data-driven world, an immense volume and diversity of data are generated and collected at an unprecedented rate. Extracting valuable insights and knowledge from such complex and high-dimensional datasets has become a fundamental challenge in data science. Optimization methods, with their mathematical rigor and computational efficiency, have emerged as indispensable tools in addressing these challenges. These methods not only empower researchers and practitioners to process and analyze large datasets but also enable them to make data-driven decisions that are both effective and efficient. As the world becomes more interconnected, and as the volume of data continues to grow, the role of optimization in shaping the future of data science becomes even more important.
This special session seeks to bring together a diverse group of researchers whose work is closely related to the field of optimization methods for large-scale data analysis. The session will provide a platform to discuss and exchange innovative ideas, cutting-edge techniques, and recent advancements in the realm of optimization for large-scale data analysis.

10:00-10:30am	Ilya Krishtal, Northern Illinois University	Low Rank Convex-Convex Quadratic Fractional Programming
10:30-11:00am	Dogyoon Song, University of Michigan	Higher-order Geometry of Losses, Regularizing Norms and Structured M-Estimation
11:00-11:30am	Dustin Mixon, Ohio State University	Bilipschitz invariants
11:30-Noon	Seonho Kim, Ohio State University	Max-affine regression via first-order methods

MS 4
Title: Nonlinear partial differential equations and optimal transport with applications
Organizer: Jun Kitagawa, Michigan State University
Location: Wells Hall A120

Abstract: This mini-symposium will outline recent developments in nonlinear partial differential equations. There will be an emphasis on Hamilton-Jacobi equations, optimal transport, and other variational problems.

10:00-10:30am	Son Tu, Michigan State University	Generalized convergence of solutions for nonlinear Hamilton-Jacobi equations
10:30-11:00am	Nicolò Forcillo, Michigan State University	Lipschitz regularity for almost minimizers of a degenerate Bernoulli-type functional
11:00-11:30am	Florian Gunsilius, University of Michigan	Tangential Projections in Monge-Kantorovich-Wasserstein spaces
11:30-Noon		

MS 5
Title: Graph-based Techniques in Machine Learning
Organizer: Ekaterina Rapinchuk, Michigan State University
Location: Wells Hall A122

Abstract: Graph-based techniques for machine learning tasks involve graph structures which typically contain vertices as complex data and edges as the similarity relationship between the connecting pair of vertices. Such algorithms have demonstrated advantages across many domains due to reasons such as universality of applications and the valuable information they provide about the overall structure of the data. They can also be used to reduce the dimensionality of the problem. Therefore, graph-based methods have emerged as valuable techniques in machine learning. The goal of this mini-symposium is to bring together researchers from different communities to discuss and highlight novel approaches to graph-based learning.

10:00-10:30am	Zach Boyd, Brigham Young University	High-order community detection using multiscale relaxations
10:30-11:00am	Chenghui Li, University of Wisconsin	Spectral neural network: from approximation and optimization perspectives
11:00-11:30am	Kevin Miller, University of Texas	Ensuring Exploration and Exploitation in Graph-Based Active Learning
11:30-Noon	Shih-Hsin Wang, University of Utah	Leveraging Geometric Symmetries with Graph Neural Networks

MS 6
Title: Multiscale modeling and numerical methods for material science and biological systems
Organizer: Huan Lei, Michigan State University
Location: Wells Hall A124

Abstract: Computational modeling of complex systems relevant to materials science and biological systems is a long-standing challenging problem. Numerical methods based on model reduction and scientific computing provide an essential tool to understand the influence of heterogeneous interactions beyond equilibrium and predict collective behaviors across multiple scales. The synergy of model reduction and numerical solutions techniques often leads to novel ideas and promotes the method development in dimension reduction, stochastic models, and fast solvers. In this mini-symposium, we focus on the interaction of the state-of-art computational techniques on dimension reduction, numerical PDE, and machine-learning-based modeling arising from various biological and material science problems, including from micro-scale molecular dynamics, meso-scale kinetic descriptions to macro-scale PDE models. The speakers are expected to have fruitful discussions with special emphasis on the predictive modeling of these systems with physical interpretation, reliability, numerical robustness, and efficiency.

10:00-10:30am	Siyao Yang, University of Chicago	Diagrammatic Monte Carlo methods for open quantum systems
10:30-11:00am	Liyao Lyu, Michigan State University	Consensus-based construction of high-dimensional free energy surface
11:00-11:30am	Shuwang Li, Illinois Institute of Technology	A simple model for simulating vesicle growth and shrinkage
11:30-Noon	Di Liu, Michigan State University	Multiscale Modeling and Computation of Optically Manipulated Nano Devices

MS 7
Title: Wild behavior in fluid dynamics
Organizer: Mimi Dai, University of Illinois, Chicago
Location: Wells Hall A126

Abstract: In the past few decades, mathematical fluid dynamics has been highlighted by numerous constructions of solutions to fluid equations that exhibit what one might call "pathological" or "wild" behavior. These include non-uniqueness, singularity formation, and the loss of energy balance. While these constructions are interesting from the mathematical point of view, as they provide counterexamples to various well-posedness (uniqueness, regularity, stability) results, they are becoming more and more relevant from the physical point of view as well. In this mini-symposium we will discuss progresses in this direction.

10:00-10:30am	Razvan-Octavian Radu, Princeton University	An Onsager theorem in 2D
10:30-11:00am	Alexey Cheskidov, Westlake University	Dissipation anomaly in fluid flows
11:00-11:30am	Mimi Dai, University of Illinois, Chicago	Non-uniqueness constructions for forced systems
11:30-Noon	Xiaoming Zheng, Central Michigan University	Iterative projection method for unsteady Navier-Stokes equations with high Reynolds numbers

MS 8
Title: Collective behavior in physical and social network models
Organizer: Todd Kapitula, Calvin College, and Keith Promislow, Michigan State University
Location: Wells Hall A128

Abstract: Collective behavior arises from groups of identical agents when their behavior under a common set of dynamical rules drives them arrive at distinct equilibrium. These divergent outcomes are a reflection of hidden structure in the dynamics that inhibit consensus. These issues arise in physical systems, such as packing of soft spheres, in social networks, and in opinion dynamics. It is of particular interest to consider the inverse problem of learning the common interaction rules from the divergent outcomes, and here the multiplicity of observed equilibrium enhances the stability of the learning process.

10:00-10:30am	Vinh Nguyen, University of Illinois, Chicago	The kinetic Cucker-Smale model with Rayleigh-type friction and self-propulsion force and its application to opinion dynamic
10:30-11:00am	Ming Zhong, Illinois Institute of Technology	Learning collective behaviors from observation
11:00-11:30am	Keith Promislow, Michigan State University	Frustration in the packing of soft balls
11:30-Noon	Trevor Leslie, Illinois Institute of Technology	Limiting configurations for solutions to the 1D Euler-alignment model.

MS 9
Title: AI, PDE, and Graph Theory for Biological Systems
Organizer: Hongsong Feng, Michigan State University
Location: Wells Hall A130

Abstract: The mini-symposium is concerned with some recent advance of mathematical methods and theories with applications in a series of biological problems. PDEs play important modeling roles in measuring electrostatic potential and testing structural mechanism of fibrin clots' mechanical response to external tensile loads. Novel and robust numerical algorithms are proposed to solve these PDE-related problems. In addition, in recent years, the integration of artificial intelligence (AI) with drug design has led to significant advancements in drug discovery. Some mathematical graph-assisted AI models that offer deep insights into atomic interactions within biomolecules are reported in this mini-symposium.

10:00-10:30am	Robert Krasny, University of Michigan	Integral Equation Calculations for Electrostatics of Solvated Biomolecules
10:30-11:00am	Zhiliang Xu, University of Notre Dame	Discrete and Continuous models of fibrin fibers and blood cells
11:00-11:30am	Duc Nguyen, University of Kentucky	Revolutionizing Drug Discovery by Mathematical Graph-Assisted AI Models
11:30-Noon		

CP1
Title: Data Driven Analysis
Location: A132 Wells Hall

10:00-10:20	Hiruni Pallage, Central Michigan University	Recovery of initial conditions through later time samples
10:20-10:40	Natalia Kravtsova, Ohio State University	Scalable Gromov-Wasserstein based comparison of biological time series
10:40-11:00	Hitesh Gakhar, Michigan State University	Toroidal Coordinates: Decorrelating Circular Coordinates with Lattice Reduction
11:00-11:20	Zongyu Li, University of Michigan	Poisson-Gaussian Holographic Phase Retrieval with Score-based Image Prior
11:20-11:40	Lee Minki, University of Michigan	Wearable data assimilation to estimate the circadian phase
11:40-Noon		

Session: CP1.1
Title: Recovery of initial conditions through later time samples
Speaker: Hiruni Pallage, Central Michigan University
Joint work with: Prof. Yeaon Hyang Kim and Prof. Roza Aceska
Abstract: Full knowledge of the initial conditions of an initial value problem (IVP) is necessary to solve said IVP but is often impossible in real-life applications due to the unavailability or inaccessibility of a sufficiently large sensor network. One way to overcome this impairing is to exploit the evolutionary nature of the sampling environment while working with a reduced number of sensors, i.e., to employ the concept of dynamical sampling. A typical dynamical sampling problem is to find sparse locations that allow one to recover an unknown function from various times samples at these locations. The classical problem of inverse heat conduction has been recently revisited by Devore and Zuazua (2014). We study conditions on an evolving system and spatial samples in a more general setup using bases. Specifically, we study when

$$u(x, t)=\sum_{n>0} a_n f_n(x) g_n(t) \text{ where } a_n \in R,\ x \in [0,1],\ t \in [0,\infty)$$

can be reasonably approximated through later-time samples at a single sampling location. The results of our research are relevant in applications, and we present examples of solving the Laplace equation and variable coefficient wave equation using our general method. Kim and Aceska (2021) retrieved the unknown initial condition function of the above systems via exponentially growing samples. However, in the approximation process, they observed exponential growth in error terms of the coefficients. Our recent research demonstrates that we can incorporate a linear growth pattern of errors in the recovered coefficients in these systems.

Session: CP1.2
Title: Scalable Gromov-Wasserstein based comparison of biological time series

Speaker: Natalia Kravtsova, Ohio State University
Joint work with: Reginald L. McGee II, Adriana T. Dawes
Abstract:
A time series is an extremely abundant data type arising in many areas of scientific research, including the biological sciences. Any method that compares time series data relies on a pairwise distance between trajectories, and the choice of distance measure determines the accuracy and speed of the time series comparison. This paper introduces an optimal transport type distance for comparing time series trajectories that are allowed to lie in spaces of different dimensions and/or with differing numbers of points possibly unequally spaced along each trajectory. The construction is based on a modified Gromov-Wasserstein distance optimization program, reducing the problem to a Wasserstein distance on the real line. The resulting program has a closed-form solution and can be computed quickly due to the scalability of the one-dimensional Wasserstein distance. We discuss theoretical properties of this distance measure, and empirically demonstrate the performance of the proposed distance on several datasets with a range of characteristics commonly found in biologically relevant data. We also use our proposed distance to demonstrate that averaging oscillatory time series trajectories using the recently proposed Fused Gromov-Wasserstein barycenter retains more characteristics in the averaged trajectory when compared to traditional averaging, which demonstrates the applicability of Fused Gromov-Wasserstein barycenters for biological time series. Fast and user friendly software for computing the proposed distance and related applications is provided. The proposed distance allows fast and meaningful comparison of biological time series and can be efficiently used in a wide range of applications. This is a joint work with Reginald L. McGee II and Adriana T. Dawes.
Paper link:
https://link.springer.com/article/10.1007/s11538-023-01175-y

Session: CP1.3
Title: Toroidal Coordinates: Decorrelating Circular Coordinates with Lattice Reduction
Speaker: Hitesh Gakhar, Michigan State University
Joint work with: Luis Scoccola, Johnathan Bush, Nikolas Schonsheck, Tatum Rask, Ling Zhou, Jose A Perea
Abstract: In Topological Data Analysis, the circular coordinates algorithm of de Silva, Morozov, and Vejdemo-Johansson takes as input a dataset together with a cohomology class representing a 1-dimensional hole in the data; the output is a map from the data into the circle that captures this hole, and that is of minimum energy in a suitable sense. However, when applied to several cohomology classes, the output circle-valued maps can be "geometrically correlated" even if the chosen cohomology classes are linearly independent. It is shown in the original work that less correlated maps can be obtained with suitable integer linear combinations of the cohomology classes, with the linear combinations being chosen by inspection. In this talk, we describe a formal notion of geometric correlation between circle-valued maps which, in the Riemannian manifold case, corresponds to the Dirichlet form, a bilinear form derived from the Dirichlet energy. We then describe a systematic procedure for constructing low energy torus-valued maps on data, starting from a set of linearly independent cohomology classes. We showcase our procedure with computational examples.

Paper link: drops.dagstuhl.de/opus/volltexte/2023/17907/pdf/LIPIcs-SoCG-2023-57.pdf

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Session: CP1.4
Title: Poisson-Gaussian Holographic Phase Retrieval with Score-based Image Prior
Speaker: Zongyu Li, University of Michigan
Joint work with: Jason Hu, Xiaojian Xu, Liyue Shen and Jeffrey A. Fessler.
Abstract: Phase retrieval (PR) is a crucial problem in many imaging applications. This study focuses on resolving the holographic phase retrieval problem in situations where the measurements are affected by a combination of Poisson and Gaussian noise, which commonly occurs in optical imaging systems. To address this problem, we propose a new algorithm called "AWFS" that uses the accelerated Wirtinger flow (AWF) with a score function as a generative prior. Specifically, we formulate the PR problem as an optimization problem that incorporates both data fidelity and regularization terms. We calculate the gradient of the log-likelihood function for PR and determine its corresponding Lipschitz constant. Additionally, we introduce a generative prior in our regularization framework by using score matching to capture information about the gradient of image prior distributions. We provide theoretical analysis that establishes a critical-point convergence guarantee for the proposed algorithm. The results of our simulation experiments on three different datasets show the following: 1) By using the PG likelihood model, the proposed algorithm improves reconstruction compared to algorithms based solely on Gaussian or Poisson likelihood. 2) The proposed score-based image prior method, performs better than the method based on denoising diffusion probabilistic model (DDPM), as well as plug-and-play alternating direction method of multipliers (PnP-ADMM) and regularization by denoising (RED).

Session: CP1.5
Title: Lee Minki, University of Michigan
Speaker: Wearable data assimilation to estimate the circadian phase
Abstract: TBD

CP2

Title: Analysis of PDEs and Continuum Models
Location: A134 Wells Hall

10:00-10:20	Michael McNulty, Michigan State University	Singularity Formation for the Higher-Dimensional Skyrme Model in the Strong-Field Limit
10:20-10:40	Koksal Karakus, Central Michigan Univeristy	Modeling the density profile of a supported thin film using nonlinear partial differential equations
10:40-11:00	Yuchuan Yang, University of Michigan	Generalized curvature for the optimal transport problem induced by a Tonelli Lagrangian
11:00-11:20	Evgeniy Khain, Oakland University	Spread of epidemics in a spatial system of weakly connected networks
11:20-11:40		
11:40-Noon		

Session: **CP2.1**
Title: Singularity Formation for the Higher-Dimensional Skyrme Model in the Strong-Field Limit
Speaker: Michael McNulty, Michigan State University
Joint work with: Po-Ning Chen and Birgit Schörkhuber
Abstract: The Skyrme model is a geometric field theory and quasilinear modification of the nonlinear sigma model from nuclear physics (wave maps into a sphere). Tony Skyrme introduced his namesake model in the 1960s as a means to prevent the formation of singularities in the nonlinear sigma model. However, the same heuristics which led Skyrme to this modification suggest that, in his model, singularities may form via self-similar shrinkage of a soliton in five spatial dimensions. In this talk, we will discuss recent work which proves that this model, in the so-called strong-field limit, admits an explicit self-similar solution which is stable within backwards lightcones. In particular, we will emphasize crucial spectral properties of this model linearized around the self-similar solution as well as special structural properties present in the Skyrme model which play a vital role in our stability analysis. Moreover, we will use this work as supporting evidence for singularity formation for the Skyrme model beyond the strong-field limit.

Session: CP2.2
Title: Modeling the density profile of a supported thin film using nonlinear partial differential equations
Presenter: Koksal Karakus, Central Michigan University
Joint work with: Leela Rakesh, Valeriy Ginzburg, Keith Promislow
Abstract: In this study we model the density profile of a supported liquid thin film. The density profile (glycerol on silica) was simulated by Cheng et al. (Journal of Chemical Physics 143,

194704 (2015)) using classical Molecular Dynamics. We attempt to represent this profile as a stationary solution of a nonlinear partial differential equation (PDE). The density profile at the free (air) surface and the middle region of the film is well-described by a kink solution of the sine-Gordon equation (SGE). To describe the density oscillations near the silica surface, we added a term proportional to the fourth-order spatial derivative to the original SGE. This term is needed to capture the strong influence of the crystalline structure of the silica substrate on the ordering of the adjacent glycerol layers. Knowing the functional form and coefficients of our PDE, we can then construct an appropriate density functional theory (DFT) for which the density profile emerges as giving rise to the local or global free energy minimum. Next steps include completing the formulation of our DFT, investigating the stability of its one-dimensional solutions against various perturbations, and exploring non-stationary, time-dependent solutions.

Session: **CP2.3**
Title: Generalized curvature for the optimal transport problem induced by a Tonelli Lagrangian
Speaker: Yuchuan Yang, University of Michigan
Abstract: I will present a new notion of curvature associated with a Tonelli Lagrangian L. This curvature naturally arises in the context of the optimal transport problem with a cost function induced by L. In particular, non-negativity of this curvature implies displacement convexity of the generalized entropy functional on the L-Wasserstein space.
Paper link: https://arxiv.org/abs/2308.04999

Session: **CP2.4**
Title: Spread of epidemics in a spatial system of weakly connected networks
Speaker: Evgeniy Khain, Oakland University
Abstract: A metapopulation consists of a group of spatially distanced subpopulations, each occupying a separate patch. It is usually assumed that each localized patch is well-mixed. In this talk, we will discuss a model for the spread of an epidemic in a system of weakly connected patches, where the disease dynamics of each patch occurs on a network. The SIR dynamics in a single patch is governed by the rate of disease transmission, the disease duration, and the node degree distribution of a network. Monte-Carlo simulations of the model reveal the phenomenon of spatial disease propagation. The speed of front propagation and its dependence on the single patch parameters and on the strength of interaction between the patches was determined analytically, and a good agreement with simulation results was observed.
Paper link: https://journals.aps.org/pre/abstract/10.1103/PhysRevE.107.034309

Parallel Sessions 2

MS 10
Title: Mathematical Modeling and Machine Learning for Analyzing Molecular Structure
Organizer: Yuta Hozumi, Michigan State University
Location: Wells Hall A108

Abstract: Combining advanced mathematics with machine learning has resulted in not only achieving higher accuracy, but also in understanding the intrinsic structure of the data. As a result, it is now possible to do classification tasks with limited labeled data, and it is also possible to generate new data by understanding the underlying data structure. In this symposium, we will have a wide range of topics, including methods for classifying scarcely labeled data, generating new molecules, and modeling protein-protein interactions. Furthermore, topics such as transformers, spectral graph theory, persistent Laplacian and geometric algebra will be highlighted by the speakers.

4:00-4:30pm	Gokul Bhusal, Michigan State University	Persistent Laplacian-enhanced Algorithm for Scarcely Labeled Data Classification
4:30-5:00pm	Nichole Hayes, Michigan State University	Transformer-Assisted Spectral Graph Algorithms for Predicting Scarcely Labeled and Imbalanced Molecular Data
5:00-5:30pm	Azzam Alfarraj, Michigan State University	Geometric Algebra Approaches to Protein-Protein Docking
5:30-6:00pm	Hongyan Du, Michigan State University	A Flexible Data-Free Framework for Structure-Based De Novo Drug Design with Reinforcement Learning

MS 11
Title: Spectral theory and asymptotic analysis in quantum mechanics
Organizer: Jonathan Stanfill, Ohio State University
Location: Wells Hall A116

Abstract: Spectral theory and asymptotic analysis both play an integral role in investigating a variety of operators, systems, and processes in quantum mechanics. This minisymposium will highlight recent results in a variety of directions including zeta regularized functional determinants and ergodic quantum processes. In particular, the zeta regularized functional determinant for singular Sturm--Liouville operators (under sufficient conditions on the coefficients) as well as conical singularities in two dimensions will be discussed. The spectral parameter asymptotics of underlying solutions to the associated eigenvalue problems will play a crucial role in the analysis. In addition, recent results on the evolution of open quantum systems will be presented. This will include results about and applications of the long-time behavior of ergodic quantum processes, composed of random channels sampled along the trajectory of an ergodic map.

4:00-4:30pm	Klaus Kirsten, Baylor University	Polyakov formulas for conical singularities in two dimensions
4:30-5:00pm	Jonathan Stanfill, Ohio State University	Zeta regularized functional determinants for Sturm-Liouville operators
5:00-5:30pm	Jeff Schenker, Michigan State University	Theory of Ergodic Quantum Processes
5:30-6:00pm	Ovidiu Costin, Ohio State University	TBD

MS 12
Title: Recent Advances in the Analysis of PDEs
Organizer: Prerona Dutta, Ohio State University
Location: Wells Hall A118

Abstract: Partial differential equations (PDEs) play a crucial role in several branches of study and their numerical solutions have a wide range of applications. However, computational accuracy is challenging to attain when the solutions to several nonlinear PDEs do not have sufficient regularity. Many fundamental questions need to be answered for the advancement of regularity theory for such PDEs, which should eventually yield more accurate numerical schemes of practical value for these equations. The goal of this mini symposium is to bring together researchers working on different aspects of PDEs and discuss recent results in this area, such as well-posedness and regularity, control theory, inverse problems and numerical methods for PDEs. This will promote an exchange of ideas as well as potential future collaborations, leading to further developments in this field.

4:00-4:30pm	Kriti Sehgal, Ohio State University	Mathematics behind the dynamics of the Henon-Heiles system
4:30-5:00pm	Mathew George, Ohio State University	Fully non-linear PDEs in complex geometry
5:00-5:30pm	Prerona Dutta, Ohio State University	Metric entropy and nonlinear partial differential equations
5:30-6:00pm		

MS 13
Title: Modern themes in calculus of variations
Organizer: Emanuel Indrei, Sam Houston State University
Location: Wells Hall A120

Abstract: The calculus of variations is concerned with some properties of solution(s) to various minimization problems modeling physical phenomena, e.g. in the formation of a soap bubble, the molecules in the soap film align themselves to form a least-energy structure, and the result is a sphere. Mathematically, this phenomenon is encoded in the isoperimetric inequality. A modern theme is to analyze how minimizers in fundamental geometric and functional inequalities are affected by slight perturbations. The underlying mechanism in this theory gives rise to partial differential equations.

4:00-4:30pm	Daesung Kim, Georgia Institute of Technology	The stability of log sobolev inequality and counterexamples
4:30-5:00pm	Timothy Rolling, Marquette University	On Steiner Symmetrizations of First Exit Time Distributions
5:00-5:30pm	Raghavendra Venkatraman, NYU, Courant Institute	Mathematical analysis of some devices made using epsilon-near-zero materials
5:30-6:00pm	Dan Mikulincer, Massachusetts Institute of Technology	Beyond optimal transport

MS 14
Title: Mathematical enhancement of AI for data analysis in biosciences and molecular sciences
Organizer: Cheng Dong, Michigan State University
Location: Wells Hall A122

Abstract: The fusion of advanced mathematical tools and artificial intelligence (AI) methods has been a recent trend in biosciences and molecular sciences. These cutting-edge techniques have profoundly impacted fields such as biology, chemistry, and drug discovery. In this mini-symposium, we explore the latest advancements in combining mathematics and AI to unravel complex biological systems and molecular structures. A wide-ranging outlook will be provided on pioneering mathematical theories like Persistent Ricci Curvature, and Persistent Hyperdigraph and its Laplacian. Furthermore, the symposium will also spotlight the Sequence-based Virtual Screening of Biomolecular Interactions (SVSBI)—a robust AI-driven tool that has revolutionized the analysis of vast bio-molecular datasets from a sequential perspective.

4:00-4:30pm	Li Shen, Michigan State University	SVSBI: Sequence-based virtual screening of biomolecular interactions
4:30-5:00pm	Junjie Wee, Nanyang Technological University	Persistent Ricci Curvature for Biomolecular Data Analysis
5:00-5:30pm	Jian Liu, Nankai University	Persistent hyperdigraph homology and persistent hyperdigraph Laplacians
5:30-6:00pm		

MS 15
Title: Multiscale modeling and numerical methods for material science and biological systems
Organizer: Huan Lei, Michigan State University
Location: Wells Hall A124

Abstract: Computational modeling of complex systems relevant to materials science and biological systems is a long-standing challenging problem. Numerical methods based on model reduction and scientific computing provide an essential tool to understand the influence of heterogeneous interactions beyond equilibrium and predict collective behaviors across multiple scales. The synergy of model reduction and numerical solutions techniques often leads to novel ideas and promotes the method development in dimension reduction, stochastic models, and fast solvers. In this mini-symposium, we focus on the interaction of the state-of-art computational techniques on dimension reduction, numerical PDE, and machine-learning-based modeling arising from various biological and material science problems, including from micro-scale molecular dynamics, meso-scale kinetic descriptions to macro-scale PDE models. The speakers are expected to have fruitful discussions with special emphasis on the predictive modeling of these systems with physical interpretation, reliability, numerical robustness, and efficiency.

4:00-4:30pm	Huan Lei, Michigan State University	A machine-learning based non-Newtonian hydrodynamic model with molecular fidelity
4:30-5:00pm	Yiwei Wang, University of California, Riverside	Energetic variational discretizations for complex fluids models
5:00-5:30pm	Guosheng Fu, University of Notre Dame	High-order variational Lagrangian schemes for compressible fluids
5:30-6:00pm	Sarah Beetham, Oakland University	Discovery of viscoelastic constitutive models with complexity-penalized sparse regression

MS 16
Title: PDE models in Mathematical Biology
Organizer: Alan Lindsay, University of Notre Dame
Location: Wells Hall A126

Abstract: This mini-symposium explores a range of mathematical problems where PDE models are central to deciphering biological phenomena. The topics range from epidemiology, to cancer modeling and cellular dynamics.

4:00-4:30pm	Maria D'Orsogna, California State University, Northridge	Forecasting age-specific drug overdose mortality in the United States
4:30-5:00pm	Thomas Hillen, University of Alberta	How the Tulips get their Stripes
5:00-5:30pm	Wanda Strychalski, Case Western Reserve	Computational modeling of adhesion-independent confined cell migration
5:30-6:00pm	Daniel Cooney, University of Illinois, Champagne-Urban	Long-Time Behavior of a PDE Replicator Equation for Multilevel Selection in Group-Structured Populations.

Mini Symposium 17
Title: Topological Data Analysis
Organizers: Elizabeth Munch, Michigan State University, and Firas Khasawneh, Michigan State University
Location: Wells Hall A128

Abstract: Topological data analysis encompasses a suite of tools which are built to encode shape and structure in data. In this session, we highlight several of the tools which are increasingly popular for applications, including persistent homology, Euler characteristic transforms, and mapper graphs.

4:00-4:30pm	Max Chumley, Michigan State University	Persistent Homology of Coarse-Grained State Space Networks
4:30-5:00pm	Sunia Tanweer, Michigan State University	A Topological Approach to Quantify Phenomenological Bifurcations in Stochastic Dynamical Systems
5:00-5:30pm	Sarah McGuire, Michigan State University	Neural Networks for 2D Euler Characteristic Transforms
5:30-6:00pm	Sarah Percival, Michigan State University	Bounding the Interleaving Distance for Geometric Graphs with a Loss Function

Mini Symposium 18
Title: Analysis and applications of nonlinear PDEs
Organizer: Olga Turanova, Michigan State University
Location: Wells Hall A130

Abstract: This mini-symposium will feature talks on a range nonlinear PDEs and their applications, including to biology and machine learning, as well as on novel numerical methods.

4:00-4:30pm	Anthony Sulak, Michigan State University	Approximating Aggregation-Diffusion via Gradient Flows Methods
4:30-5:00pm	Minh Le, Michigan State University	Global existence of solutions to the chemotaxis system with logistic source under nonlinear Neumann boundary conditions
5:00-5:30pm	Rafael Chiclana Vega, Michigan State University	A local Central Limit Theorem for random walks on expander graphs
5:30-6:00pm	Albert Chua, Michigan State University	Nonwindowed Scattering Transforms and Invariant Representations

CP3

Title: Data Driven Analysis
Location: A132 Wells Hall

4:00-4:20	Santhosh Kartnik, Michigan State University	Tensor Completion for Low CP-Rank Tensors via Random Sampling
4:20-4:40	Sonia Kim, University of Michigan	Patch-based Diffusion Model for Under-sampled MRI
4:40-5:00	Nkechi Nnadi, Wayne State University	Modified Hausdorff Distance for Topological Data Analysis
5:00-5:20	Baoli Hao	Mixed sign interactions in the 1D swarmalator model
5:20-5:40		
5:40-6:00		

Session: CP3.1
Title: Tensor Completion for Low CP-Rank Tensors via Random Sampling
Speaker: Santhosh Kartnik, Michigan State University
Joint work with: Mark Iwen, Cullen Haselby, and Rongrong Wang
Abstract: We propose a provably accurate tensor completion approach based on combining matrix completion techniques for a small number of slices of the tensor with a modified noise robust version of Jennrich's algorithm. In the simplest case, this leads to a sampling strategy that densely samples two slices and sparsely samples the remaining slices. Under mild assumptions on the factor matrices, the proposed algorithm completes an n x n x n tensor with CP-rank r with high probability while using at most O(n*r*log(r)) samples in the adaptive sampling case and O(n*r*log^2(n) + n*r^2*log(n)) samples in the non-adaptive sampling case. Empirical experiments further verify that the proposed approach works well in practice, including as a low-rank approximation method in the presence of additive noise.
Paper link: https://openreview.net/forum?id=UFO5MDZFWs0

Session: CP3.2
Title: Patch-based Diffusion Model for Under-sampled MRI
Speaker: Sonia Kim, University of Michigan
Abstract: Undersampled MRI is a critical technique to speed up MRI scans by capturing only a portion of the necessary k-space data for image reconstruction. This approach enables shorter scan times while still generating diagnostically useful images. By reducing patient discomfort and motion-related artifacts caused by lengthy scans, undersampled MRI holds great potential to improve the overall patient experience. However, the undersampling can result in loss of image detail and introduce unwanted distortions, making accurate reconstruction quite

challenging. Recently, machine learning methods, especially diffusion models, have gained significant attention in the field of MRI reconstruction and have shown promising outcomes across various imaging tasks. Nevertheless, the regular diffusion models typically require substantial training data that may not always be readily available in medical imaging contexts. To overcome this limitation, we introduce the patch-based diffusion model that trains a diffusion model in a patch-by-patch manner by learning the score function of the whole image from representative image patches. We demonstrate the effectiveness of our method on a FastMRI dataset with over 3000 images. This talk will mainly focus on the following key aspects: a brief introduction to diffusion probabilistic models (forward (i.e. training) and reverse (i.e. sampling) process), patch-based score modeling for training image patches (estimating score functions with denoising score matching), and application of patch-based diffusion model to undersampled MRI images.

Session: CP3.3
Title: Modified Hausdorff Distance for Topological Data Analysis
Speaker: Nkechi Nnadi, Wayne State University
Abstract: TBD

CP3.4
Title: Mixed sign interactions in the 1D swarmalator model
Speaker: Baoli Hao
Joint with: Ming Zhong
Abstract: We study a population of swarmalators, mobile variants of phase oscillators, which run on a ring and have mixed sign interactions. This 1D swarmalator model produces several of collective states: the standard sync and async states as well as a novel splay-like “polarized” state and several unsteady states such as active bands or swirling. The model’s simplicity allows us to describe some of the states analytically. The model can be considered as a toy model for real-world swarmalators such as vinegar eels and sperm which swarm in quasi-1D geometries.

CP4
Title: Numerical Analysis
Location: A134 Wells Hall

4:00-4:20	Fatih Celiker, Wayne State University	Flow Problems Discretized with the Peridynamic Differential Operator
4:20-4:40	Tao Hong, University of Michigan	Temporal Second-order methods for image reconstruction
4:40-5:00	Fangyao Zhu, Michigan Technological University	Well-balanced positivity-preserving high-order discontinuous Galerkin methods for Euler equations with gravitation
5:00-5:20		
5:20-5:40		
5:40-6:00		

Session: CP4.1
Title: Flow Problems Discretized with the Peridynamic Differential Operator
Speaker: Fatih Celiker, Wayne State University
Joint work with Burak Aksoylu.
Abstract: We study the incompressible Navier-Stokes equations using the Projection Method. The applications of interest are the classical channel flow problems such as Couette, shear, and Poiseuille. In addition, we consider the Taylor-Green vortex and lid-driven cavity applications. For discretization, we use the Peridynamic Differential Operator (PDDO). The main emphasis of the paper is the performance of the PDDO as a discretization method under these flow problems. We present a careful numerical study with quantifications and report convergence tables with convergence rates and the error of pressure. We also study the approximation properties of the PDDO and prove that the N-th order PDDO approximates polynomials of degree at most N exactly. As a result, we prove that the PDDO discretization guarantees the zero row sum property of the arising system matrix.
Paper Link: https://link.springer.com/article/10.1007/s42102-023-00103-x

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Session: CP4.2
Title: Temporal Second-order methods for image reconstruction
Speaker: Tao Hong, University of Michigan,
Abstract: Over the years, computational imaging with accurate nonlinear physical models has drawn considerable interest due to its ability to achieve high-quality reconstructions. However, such nonlinear models are computationally demanding. A popular choice for solving the corresponding inverse problems is accelerated stochastic proximal methods (ASPMs), with the caveat that each iteration is expensive. To overcome this issue, we propose a mini-batch quasi-Newton proximal method (BQNPM) tailored to image-reconstruction problems with total-variation regularization. It involves an efficient approach that computes a weighted proximal

mapping at a cost similar to that of the proximal mapping in ASPMs. However, BQNPM requires fewer iterations than ASPMs to converge. We assess the performance of BQNPM on three-dimensional inverse-scattering problems with linear and nonlinear physical models. Our results on simulated and real data show the effectiveness and efficiency of BQNPM.
Paper Link: https://arxiv.org/abs/2307.02043.

Session: CP4.3
Title: Well-balanced positivity-preserving high-order discontinuous Galerkin methods for Euler equations with gravitation
Speaker: Fangyao Zhu, Michigan Technological University
Abstract: TBD