Nonlocality: Challenges in Modeling and Simulation
Poster Session Abstracts
Tuesday, April 16, 2024

SAV Ensemble Algorithms for MHD Equations
John Carter, RPI

MHD flows occur in applications that involve plasmas, astrophysics, planetary science and metallized industry. In applications, viscosity and magnetic resistivity, external body forcing and initial conditions, are invariably subject to uncertainty. To quantify the impact of uncertainty and develop high-fidelity numerical simulations, one usually computes the flow ensembles in which the MHD equations are solved repeatedly with different inputs. We develop efficient second-order accurate ensemble algorithms that are suitable for long-time simulations. The coefficient matrix of the resulting linear systems is identical for all realizations, saving both storage and computational cost. We combine this with the Scalar Auxiliary Variable (SAV) approach for gradient flows resulting in unconditionally stable, fully decoupled numerical schemes with constant coefficients.

Nonlocal Properties of the Fractional Schrodinger Equation
Brian Choi, Uniited States Military Academy

The poster surveys some nonlocal properties of the fractional nonlinear Schrodinger equation including the well-posedness theory, modulational instability, and Peierls-Nabarro potential. We emphasize how nonlocal effects perturb the well-known local phenomena. Both regular and singular perturbations are highlighted.

Binary Phase-Separation with Four Critical Mechanisms
Melissa De Jesus, Florida International University

The classical Cahn-Hilliard equation characterizes phase-separation phenomena in a binary system within a bounded measurable domain. We introduce four new mechanisms into this model to add more flexibility. Specifically, we added mechanisms which offer control over both time and space scales of the phase separation process, and a choice of a smooth or singular entropy density potentials. We establish well-posedness results and examine regularity of the solution. Then to complement our theoretical findings we use numerical simulations to check the physical consistency of our model, while also observing the interplay of the scaling parameters.

Compactness results for a Dirichlet energy of nonlocal gradient with applications
Zhaolong Han, University of California San Diego

We prove two compactness results for function spaces with finite Dirichlet energy of half-space nonlocal gradients. Namely, by properly scaling or cutting-off the kernel function defining the nonlocal operator, we show that the sequence of corresponding nonlocal function spaces is asymptotically compactly embedded in the limiting function space. Uniform Poincar\'e inequalities for half-ball gradient operators are derived based on the compactness results. As an application, convergence of nonlocal heterogeneous anisotropic diffusion problems are shown and asymptotically compatible schemes are constructed. Another application concerns the convergence and robust discretization of a nonlocal optimal control problem.

Fractional centralities on networks: Consolidating the local and the global
Kang-Ju Lee, Seoul National University

We propose a new centrality incorporating two classical node-level centralities, the degree centrality and the information centrality, which are considered as local and global centralities, respectively. These two centralities have expressions in terms of the graph Laplacian L, which motivates us to exploit its fractional analogue L^{γ} with a fractional parameter γ. As γ varies from 0 to 1, the proposed fractional version of the information centrality makes intriguing changes in the node centrality rankings. These changes could not be generated by the fractional degree centrality since it is mostly influenced by the local aspect. We prove that these two fractional centralities behave similarly when γ is close to 0. This result provides its complete understanding of the boundary of the interval in which γ lies since the fractional information centrality with $\gamma=1$ is the usual information centrality. Moreover, our computation for the correlation coefficients between the fractional information centrality and the degree centrality reveals that the fractional information centrality is transformed from a local centrality into being a global one as γ changes from 0 to 1.

Peridynamic Neural Operators: data-driven constitutive modeling and microstructure discovery
Siavash Jafarzadeh, Lehigh University

Neural operators, which can act as implicit solution operators of hidden governing equations, have recently become popular tools for learning the responses of complex real-world physical systems. Nevertheless, most neural operator applications have thus far been data-driven and neglect the intrinsic preservation of fundamental physical laws in data. In this work, we introduce a novel integral neural operator architecture called the Peridynamic Neural Operator (PNO) that learns a nonlocal constitutive law from spatial data. This neural operator provides a forward model in the form of state-based peridynamics, with objectivity and momentum balance laws automatically guaranteed. Moreover, the effects from heterogeneity and nonlinear constitutive relationship are captured by the kernel function and the bond force respectively, enabling physical interpretability. As a result, PNO architecture can learn a constitutive model for biological tissues with anisotropic heterogeneous response undergoing large deformation regime. As an example, we use PNO to learn a constitutive model for a particular biotissue from digital image correlation (DIC)-tracked displacement field in a biaxial test. Our PNO is more accurate than the state-of-the-art expert constructed constitutive models. Interestingly, if the microstructure is unknow, the heterogeneous PNO is able to learn microstructure (here the fiber orientation field) from DIC displacements.

Finite element methods for Maxwell's equations in Cole-Cole medium (time-fractional Maxwell's equations)
Jichun Li, University of Nevada Las Vegas

In this poster, I'll present two finite element methods developed for solving the time-dependent Maxwell's equations in the Cole-Cole dispersive medium, whichleads to
time-fractional derivative. Stability and error analysis have been established for both schemes. Numerical results are provided to support our analysis.

Nonlocal Effects on a Generalized Ohta–Kawasaki Model and Its Asymptotically Compatible Scheme
Wangbo Luo, The George Washington University

Joint work with Yanxiang Zhao (The George Washington University)
We propose a generalized Ohta-Kawasaki model to study the nonlocal effect on the pattern formation of some binary systems with general long-range interactions. While in the 1D case, the generalized Ohta- Kawasaki model displays similar bubble patterns as the standard Ohta-Kawasaki model, by performing Fourier analysis, we find that the optimal number of bubbles for the generalized model may have an upper bound no matter how large the repulsive strength is. The existence of such an upper bound is characterized by the eigenvalues of the nonlocal kernels. Additionally, we explore the conditions under which the nonlocal horizon parameter may promote or demote the bubble splitting, and apply the analysis framework to several case studies for various nonlocal operators. Next, we study the asymptotic compatibility of the Fourier spectral method in multidimensional space for the Nonlocal Ohta-Kawasaka (NOK) model. By introducing the Fourier collocation discretization for the spatial variable, we show that the asymptotic compatibility holds in 2D and 3D over a periodic domain. For the temporal discretization, we adopt the second-order backward differentiation formula (BDF) method. We prove that for certain nonlocal kernels, the proposed time discretization schemes inherit the energy dissipation law. In the numerical experiments, we verify the asymptotic compatibility, the second-order temporal convergence rate, and the energy stability of the proposed schemes. More importantly, we discover a novel square lattice pattern when certain nonlocal kernel are applied in the model. In addition, our numerical experiments confirm the existence of an upper bound for the optimal number of bubbles in 2D for some specific nonlocal kernels. Finally, we numerically explore the promotion/demotion effect induced by the nonlocal horizon δ, which is consistent with the theoretical studies presented in 1D case.

Numerical solution of the isotropic Landau–Lifshitz equation using the Hasimoto transform
Georg Maierhofer, University of Oxford

The isotropic Landau–Lifshitz (LL) equation provides a model for a wide range of physical phenomena describing inter alia magnetization dynamics in ferromagnetism and the evolution of vortex filaments in ideal fluids. The fully nonlinear structure of this equation makes computations exceedingly difficult and prior approaches had to resort to comparatively expensive implicit formulations to achieve stable approximations to this equation.

In this work, we introduce a novel numerical approach to computing solutions to the LL equation based on the Hasimoto transform which relates the LL flow to a cubic nonlinear Schr¨odinger (NLS) equation. In exploiting this nonlinear transform we are able to introduce the first fully explicit unconditionally stable symmetric integrators for the LL equation. Our approach consists of two parts: an integration of the NLS equation followed by the numerical evaluation of the Hasimoto transform. Motivated by the desire to study rough solutions to the LL equation, we also introduce a new symmetric low-regularity integrator for the NLS equation. The slow spectral decay of rough solutions leads to nonlocal effects in frequency space whose representation is exceedingly important in the accurate approximation of this type of solution to the LL equation. Based on a tailored analysis of the resonance structures in the Magnus expansion we can represent the dominant contributions to this behaviour in a form which allows for fast computations through block-Toeplitz partitions, to yield an efficient low-regularity integrator for the LL equation – the fast low-regularity Hasimoto (FLowRH) transform.

In this poster we will present an overview of the methodology of this novel approach whose favourable properties are exhibited both in theoretical convergence analysis and in numerical experiments."

Optimal Design and Asymptotic Compatibility of Nonlocal Problems
Joshua Siktar, University of Tennessee-Knoxville

This project gives an analytical and numerical treatment of nonlocal optimal design problems where the underlying physical behavior is governed by either nonlocal diffusion or the bond-based model of peridynamics. One objective of this work is to showcase how to recast classical homogenization theory into the nonlocal setting, with an isotropic class of designs. Beyond that, convergence in the vanishing nonlocal limit and a finite element error analysis are provided. The compliance structure of the cost functional plays an important role in proving these convergence results since it allows us to algebraically relate the state equation to the cost functional.

A Model-Based Approach for Continuous-Time Policy Evaluation with Unknown Lévy Process Dynamics
Qihao Ye, University of California, San Diego

This research presents a framework for evaluating policies in a continuous-time setting, where the dynamics are unknown and represented by Lévy processes. Initially, we estimate the model using available trajectory data, followed by solving the associated PDE to conduct the policy evaluation. Our approach encompasses not only the conventional Brownian motion but also the non-Gaussian and heavy-tailed Lévy processes. We have developed an algorithm that demonstrates enhanced performance compared to existing techniques tailored for Brownian motion. Furthermore, we provide a theoretical guarantee regarding the error in policy evaluation given the model error. Experimental results involving both light-tailed and heavy-tailed data will be presented. This research provides a first step to continuous-time model-based reinforcement learning, particularly in scenarios characterized by irregular, heavy-tailed dynamics.