Workshop on Scientific Computing and Data Science
July 11-12, 2024

Organizing Committee

- **Long Chen**, University of California, Irvine
- **Bangti Jin**, The Chinese University of Hong Kong
- **Liu Liu**, The Chinese University of Hong Kong
- **Ruchi Guo**, The Chinese University of Hong Kong
- **Kuang Huang**, The Chinese University of Hong Kong

Location and Schedule

The workshop will take place at the Yasumoto International Academic Park (YIA), LT4. Here is the instruction from the University Station to YIA:

The detailed location of the dinner on July 11 is: 3 Floor, Pak Shing Building, 31-37 Jordan Road, Jordan, Hong Kong.

Thursday, July 11		
9:20-9:30	Opening remarks	
9:30-10:05	Haizhao Yang	Discretization-Invariant Operator Learning: Algorithms and Theory
10:05-10:40	Jiang Yang	Simulations and analysis of nonlocal phase-field crystal models
10:40-11:05	Coffee break	
11:05-11:40	Mattia Zanella	Condensation effects in kinetic consensus dynamics
11:40-12:15	Xiaoning Zheng	TGM-Nets: A Deep Learning Framework for Enhanced Forecasting of Tumor Growth by Integrating Imaging and Modeling
12:15-14:00	Lunch	
14:00-14:35	Haifeng Ji	Nonconforming immersed finite element methods for interface problems
14:35-15:10	Wei Liu	Second-order flows for non-convex variational problems
15:10-15:45	Bowen Li	Interpolation between modified logarithmic Sobolev and Poincare inequalities for quantum Markovian dynamics
15:45-17:30	Discussion	
18:30-evening	Dinner at Wagyu Yakiniku Ichiro	

Friday, July 12		
9:30-10:05	Ling Guo	Uncertainty Quantification in Scientific Machine Learning
10:05-10:40	Jiaqi Zhang	A Fluid Mechanical Study of Rotation-induced Traumatic Brain Injury
10:40-11:05	Coffee break	
11:05-11:40	Giulia Bertaglia	Gradient-based Monte Carlo methods for hyperbolic equations
11:40-12:15	Andrea Medaglia	Kinetic models in mathematical epidemiology: optimal control in the presence of behavioural uncertainties
12:15-14:00	Lunch	
14:00-14:35	Qiuqi Li	An Adaptive model reduction Method Based on Local Dynamic Mode Decomposition
14:35-15:10	Jianfang Lu	A discontinuous Galerkin method for nonlocal diffusion problems
15:10-15:35	Coffee break	
15:35-16:10	Hao Luo	A family of ODE-solver based fast alternating direction methods of multipliers: with applications to sparse regression
16:10-16:45	Yongke Wu	Energy-stable mixed finite element methods for Rosensweig's ferrofluid flow model
16:45-17:30	Discussion and closing remarks	

Invited Speakers and Talk Information

1. Haizhao Yang, University of Maryland

   Title: Discretization-Invariant Operator Learning: Algorithms and Theory

   Abstract: Learning operators between infinitely dimensional spaces is an important learning task arising in wide applications in machine learning, data science, mathematical modeling and simulations, etc. This talk introduces a new discretization-invariant operator learning approach based on data-driven kernels via deep learning. Compared to existing methods, our approach achieves attractive accuracy in solving forward and inverse problems, prediction problems, and signal processing problems with discretization invariant, i.e., networks trained with a fixed data structure can be applied to heterogeneous data structures without expensive re-training. Under mild conditions, quantitative generalization error will be provided to understand operator learning in the sense of non-parametric estimation.

2. Jiang Yang, Southern University of Science and Technology

   Title: Simulations and analysis of nonlocal phase-field crystal models

   Abstract: We present a nonlocal phase-field crystal (NPFC) model as a nonlocal counterpart of the local phase-field crystal (LPFC) model. The NPFC is a special case of the structural PFC (XPFC) that is derived from classical field theory for crystal growth and phase transition. It incorporates a finite range of spatial nonlocal interactions, whose forms are obtained by fitting the materials structure factor. We compare the fitting results of the NPFC with those of the LPFC and its fractional variant found in the literature. While the fractional variants are designed to match the experimental data of the structure factor up to the first peak, our new approach successfully achieves good agreement up to the second peak. Moreover, we rigorously show that both LPFC and fractional PFC can be distinct scaling limits of the NPFC, which reflects the generality and the potential advantage of NPFC in retaining material properties and suggests that NPFC models may perform better in characterizing liquid-solid transition systems. We present numerical experiments in the two-dimensional space to demonstrate the effectiveness of NPFC models in simulating crystal structures and grain boundaries. The simulations are performed using Fourier spectral methods, and we demonstrate that such methods are asymptotically compatible schemes, thus are able to offer robust numerical discretizations. Furthermore, we observe that while the NPFC model can predict grain boundary simulations similarly to the LPFC model, they can also produce sharp interfaces with integrable kernels instead of the diffusive interfaces generated by the LPFC models.

3. Mattia Zanella, University of Pavia

   Title: Condensation effects in kinetic consensus dynamics

   Abstract: In this talk, we discuss a new class of models to understand the impact of the initial mass on consensus formation dynamics. We will introduce a new kinetic model in which the interaction frequency is weighted by the kinetic density which reduces to a Kaniadakis-Quarati-type equation with quadratic drift, originally introduced for the dynamics of bosons in a spatially homogeneous setting. From the obtained PDE for the evolution of the agents' density, we determine the regime for which a critical mass exists and triggers blow-up of the solution in finite time. Therefore, the model is capable of describing strong conformity phenomena in cases where the total density of individuals holding a given state exceeds a fixed critical size.

4. Xiaoning Zheng, Jinan University

   Title: TGM-Nets: A Deep Learning Framework for Enhanced Forecasting of Tumor Growth by Integrating Imaging and Modeling

   Abstract: Prediction and uncertainty quantification of tumor progression are vital in clinical practice, i.e., disease prognosis and decision-making on treatment strategies. In this work, we propose TGM-Nets, a deep learning framework that combines bioimaging and tumor growth modeling (TGM) for enhanced prediction of tumor growth. This proposed framework, developed based on physics-informed neural networks (PINNs), is capable of integrating the TGM and sequential observations of tumor morphology for patient-specific prediction of tumor growth. The novelties of the design of TGM-Nets include the employment of Fourier layers to extract the features of the input images as well as the utilization of sequential learning and fine-tuning with physics for extrapolation to improve the prediction accuracy. The validity of TGM-Nets for tumor growth forecasting is verified by testing the model performance on synthetic and in-vitro datasets, respectively. Our results show that the TGM-Nets not only can track the growth rates of the mild and aggressive tumors but also capture their detailed morphological features within and outside the training domain. In particular, TGM-Nets can be used to predict the long time dynamics of tumor growth in mild and aggressive cases. Our results show that the parameters inferred from the TGM-Nets can be used for long-time prediction for up to 4 months with a maximum error 4%. We also systematically study the effects of the number of training points and noisy data on the performance of TGM-Nets as well as quantify the uncertainty of the model predictions. We show that TGM-Nets can integrate the biomedical images to predict the growth of the in-vitro cultured pancreatic cancer cells and identify the associated growth rates, demonstrating the possibilities of using TGM-Nets in clinical practice. In summary, we propose a new deep learning model that combines imaging and TGM to improve the current approaches for predicting tumor growth and thus provide an advanced computational tool for patient-specific tumor prognosis.

5. Haifeng Ji, Nanjing University of Posts and Telecommunications

   Title: Nonconforming immersed finite element methods for interface problems

   Abstract: Interface problems arise in many applications. Conventional finite element methods require the mesh to fit the interface, which can be inconvenient for problems involving moving interfaces or complex 3D interfaces. To address these challenges, immersed finite element (IFE) methods have been developed to solve interface problems on unfitted meshes. In this talk, we will discuss 2D/3D nonconforming IFEs, whose degrees of freedom are based on integral values on edges/faces. The nonconforming IFEs possess a very nice property that the IFE basis functions are unisolvent on arbitrary triangles/tetrahedrons without any angle restrictions. The optimal approximation capabilities of the IFE space, along with the inf-sup stability and the optimal a priori error estimate of the IFE method, have been rigorously derived with constants that are independent of the mesh size and the interface location relative to the mesh.

6. Wei Liu, The City University of Hong Kong

   Title: Second-order flows for non-convex variational problems

Abstract: In this talk, we introduce a novel computational framework based on the second-order flows (i.e., a class of dissipative second-order hyperbolic PDEs) for solutions of non-convex variational problems with possible constraint. We explore both the theoretical and numerical aspects of second-order flows and highlight several challenges in analysis and applications. Specifically, efficient second-order flow approaches are developed to address the minimization of the Gross-Pitaevskii energy functional with rotation term under the normalization constraint to compute ground states of rotating Bose-Einstein condensates. Extensive numerical results demonstrate the superiority of second-order flow methods over the commonly used gradient flow methods. Furthermore, the convergence of second-order flows to stationary points is established for a wide class of unconstrained non-convex variational problems through convex-splitting schemes, and typical applications such as the minimization of Ginzburg-Landau energy in phase-field modelings and Landau-de Gennes energy in the Q-tensor model for liquid crystals are explored.

7. Bowen Li, Duke University

   Title: Interpolation between modified logarithmic Sobolev and Poincare inequalities for quantum Markovian dynamics

   Abstract: In this talk, we define the quantum p-divergences and introduce the Beckner's inequalities for the quantum Markov semigroups with detailed balance condition. Such inequalities quantify the convergence rate of the quantum dynamics in the noncommutative p-norm. We obtain a number of implications between Beckner's inequalities and other quantum functional inequalities, as well as the hypercontractivity. In particular, we show that the quantum Beckner's inequalities interpolate between the Sobolev-type inequalities and the Poincare inequality in a sharp way. We also provide a uniform lower bound for the Beckner constants in terms of the spectral gap, and establish its stability with respect to the invariant state. We further introduce a new class of quantum transport distances W 2,p such that QMS with detailed balance is the gradient flow of the quantum p-divergence. We prove that the set of quantum states equipped with such a metric is a complete geodesic space, which allows us to connect the geodesic convexity of p-divergence with quantum Beckner's inequality.

8. Ling Guo, Shanghai Normal University

   Title: Uncertainty Quantification in Scientific Machine Learning

   Abstract: Neural networks (NNs) are currently changing the computational paradigm on how to combine data with mathematical laws in physics and engineering in a profound way, tackling challenging inverse and ill-posed problems not solvable with traditional methods. However, quantifying errors and uncertainties in NN-based inference is more complicated than in traditional methods. In this talk, we will present a comprehensive framework that includes uncertainty modeling, new and existing solution methods, as well as Information bottleneck based uncertainty quantification for neural function regression and neural operator learning.

9. Jiaqi Zhang, Beijing Normal University (Zhuhai)

   Title: A Fluid Mechanical Study of Rotation-induced Traumatic Brain Injury

   Abstract: Traumatic brain injury (TBI) is a serious health issue. Studies have highlighted the severity of rotation induced TBI. However, the role of cerebrospinal fluid (CSF) in transmitting the impact from the skull to the soft brain matter remains unclear. Herein, we use experiments and computations to define and probe this role in a simplified setup. A spherical hydrogel ball, serving as a soft brain model, was subjected to controlled rotation within a water bath, emulating the CSF, filling a transparent cylinder. The cylinder and ball velocities, as well as the ball's deformation over time, were measured. We found that the soft hydrogel ball is very sensitive to decelerating rotational impacts, experiencing significant deformation during the process. A finite-element code is written to simulate the process. The hydrogel ball is modelled as a poroelastic material infused with fluid and its coupling with the suspending fluid is handled by an arbitrary Lagrangian-Eulerian method. The results indicate that the density contrast, as well as the rotational velocity difference, between the hydrogel ball and the suspending fluid play a central role in the ball's deformation due to centrifugal forces. This approach contributes a deeper understanding of brain injuries and may portend the development of preventive measures and improved treatment strategies.

10. Giulia Bertaglia, University of Ferrara

    Title: Gradient-based Monte Carlo methods for hyperbolic equations

    Abstract: Particle methods based on the evolution of the spatial derivatives of the system solution, known as Gradient Random Walk methods, were first presented to model reaction-diffusion processes, inspired mainly by vortex methods for the Navier-Stokes equations. The 1990s saw a great deal of research conducted on these techniques, which have several interesting features, including not requiring a computational grid, automatically fitting the solution by concentrating the elements where the gradient is high, and significantly reducing the variance of the conventional Random Walk approach. In this talk, we revisit these ideas by showing how to generalize the Gradient Random Walk approach to a broader class of partial differential equations, in particular to hyperbolic systems of conservation laws.

11. Andrea Medaglia, University of Pavia

    Title: Kinetic models in mathematical epidemiology: optimal control in the presence of behavioural uncertainties

    Abstract: Kinetic equations have been recently employed to mimic the emergence of collective phenomena in life sciences. In this direction, during the COVID-19 pandemic, compartmental models describing the spreading of an infectious disease coupled with a kinetic-type description of the distribution of social contacts among the population have been developed [1]. In fact, it has been widely recognized that social structures can play an important role in the spreading of an epidemic, being a potential cause of pathogen transmission. In more detail, the microscopic model describing the contact evolution is based on a simple transition operator with uncertain parameters [3]. At the kinetic level, this model can produce a range of equilibrium distributions, ranging from slim-tailed Gamma-type distributions to power-law-type distributions, depending on the introduced uncertainties. These equilibrium distributions are crucial for closing the hierarchy of moments that define the macroscopic observable trends of the infection, taking into account the incomplete knowledge of the actual contact distribution. Furthermore, the presence of available data permits to investigate such models quantitatively. However, their statistical description does not possess universal patterns and may vary spatially and temporally. It is therefore essential to design optimal control strategies at the level of the agents [2], mimicking the effects of non-pharmaceutical interventions (NPIs) to limit efficiently the number of infected cases in the presence of uncertainties. The epidemiological parameters are then calibrated on real-world data and, thanks to a retrospective analysis, it is possible to study the effects of a minimal lockdown strategy achieved by reducing the sociality of the agents with a large number of daily contacts. This is a joint work with Mattia Zanella and Jonathan Franceschi.

12. Qiuqi Li, Hunan University

    Title: An Adaptive model reduction Method Based on Local Dynamic Mode Decomposition

    Abstract: Parametric dynamical systems are widely used to model physical systems, but their numerical simulation can be computationally demanding due to nonlinearity, long-time simulation, and multi-query requirements. Model reduction methods aim to reduce computation complexity and improve simulation efficiency. However, traditional model reduction methods are inefficient for parametric dynamical systems with nonlinear structures. To address this challenge, we propose an adaptive method based on local dynamic mode de- composition (DMD) to construct an efficient and reliable surrogate model. We propose an improved greedy algorithm to generate the atoms set based on a sequence of relatively small training sets, which could reduce the effect of large training set. At each enrichment step, we construct a local sub-surrogate model using the Taylor expansion and DMD, resulting in the ability to predict the state at any time without solving the original dynamical system. Moreover, our method provides the best approximation almost everywhere over the parameter domain with certain smoothness assumptions, thanks to the gradient information. At last, three concrete examples are presented to illustrate the effectiveness of the proposed method. This is a joint work with Chang Liu and Mengnan Li.

13. Jianfang Lu, South China University of Technology

    Title: A discontinuous Galerkin method for nonlocal diffusion problems

    Abstract: In this talk, we study a class of discontinuous Galerkin (DG) methods for one-dimensional nonlocal diffusion (ND) problems. The DG method proposed here have its local counterpart, thus the numerical scheme will converge to the existing DG scheme as the horizon vanishes. We also define the discrete energy norm so as to analyze these DG methods. Rigorous proofs are provided to demonstrate the stability, error estimates, and asymptotic compatibility of the proposed DG schemes. To see the nonlocal diffusion effect, we also consider the time-dependent convection-diffusion problems with nonlocal diffusion. Numerical results show the good performance of the proposed algorithm and also validate the theoretical findings.

14. Hao Luo, Chongqing Normal University

    Title: A family of ODE-solver based fast alternating direction methods of multipliers: with applications to sparse regression

    Abstract: In this talk, we provide a self-contained ordinary differential equation solver approach for separable convex optimization problems. A novel primal-dual dynamical system with built-in time rescaling factors is introduced, and the exponential decay of a tailored Lyapunov function is established. Then several time discretizations of the continuous model are considered and analyzed via a unified discrete Lyapunov function. Moreover, a family of accelerated proximal alternating direction methods of multipliers are derived, and nonergodic optimal mixed-type convergence rates shall be proved for the primal objective residual, the feasibility violation and the Lagrangian gap. Finally, numerical experiments are provided to validate the practical performances on sparse regression. This is a joint work with Dr. Zhang Zihang from Peking University.

15. Yongke Wu, University of Electronic Science and Technology of China

    Title: Energy-stable mixed finite element methods for Rosensweig's ferrofluid flow model

    Abstract: In this talk, we will introduce a mixed finite element method for Rosensweig's ferrofluid flow model which is proposed by Rosensweig (1985). We will introduce some regularity results for the solution and construct energy preserving semi- and fully discrete schemes. We show that the energy inequality of the continuous equation is preserved and give the optimal error estimates in both L^∞ (L^2) and L^2 (H^1) norms for the semi- and fully discrete schemes. Numerical experiments confirm the theoretical results.