CityU-SJTU Joint Workshop on Computational Mathematics

City University of Hong Kong

November 23-24, 2024

Objective

This workshop aims to promote collaboration and the exchange of ideas between Shanghai Jiao Tong University and the City University of Hong Kong. We have an engaging agenda planned, featuring a series of talks and discussions that we believe will be highly beneficial for all attendees.

Abstracts

A robust lower order mixed finite element method for a strain gradient elastic model

Jianguo HUANG

Shanghai Jiao Tong University

In this talk, we will discuss a robust nonconforming mixed finite element method for a strain gradient elastic (SGE) model. Concretely speaking, a lower order C^0-continuous H^2 nonconforming finite element in arbitrary dimension is constructed for the displacement field through enriching the quadratic Lagrange element with bubble functions. This together with the linear Lagrange element is exploited to discretize a mixed formulation of the SGE model. The robust discrete inf-sup condition is established. The sharp and uniform error estimates with respect to both the small size parameter and the Lame coefficient are achieved, which is also verified by numerical results. In addition, the uniform regularity of the SGE model is derived under three reasonable assumptions.

A Cartesian grid method for nonhomogeneous elliptic interface problems on unbounded domains

Wenjun YING

Shanghai Jiao Tong University

We will present a Cartesian grid based fast and accurate method for indirectly evaluating boundary and volume integrals in a boundary-volume integral approach for nonhomogeneous elliptic interface problems on unbounded domains. The indirect calculation is done by solving equivalent but simple interface problems. We accelerate the computation by introducing an intermediate, transitional circle or sphere and taking advantages of super-convergent numerical quadrature or series expansion on circles/spheres. We first map the boundary or volume integral on the irregular boundary or domain to the intermediate circle/sphere; then evaluate the boundary integral on the intermediate circle/sphere to get boundary conditions for the simple interface problem. We will also show numerical results of examples in both two and three space dimensions.

An energy-conserving Fourier particle-in-cell method with asymptotic-preserving preconditioner for Vlasov-Ampère system with exact curl-free constraint

Zhuoning LI

Shanghai Jiao Tong University

We present an efficient and accurate energy-conserving implicit particle-in-cell (PIC) algorithm for the electrostatic Vlasov system, with particular emphasis on its high robustness for simulating complex plasma systems with multiple physical scales. This method consists of several indispensable elements: (i) the reformulation of the original Vlasov-Poisson system into an equivalent Vlasov-Ampère system with divergence-/curl-free constraints; (ii) a novel structure-preserving Fourier spatial discretization, which exactly preserves these constraints at the discrete level; (iii) a preconditioned Anderson-acceleration algorithm for the solution of the highly nonlinear system; and (iv) a linearized and uniform approximation of the implicit Crank-Nicolson scheme for various Debye lengths, based on the generalized Ohm's law, which serves as an asymptotic-preserving preconditioner for the proposed method. Numerical experiments are conducted, and comparisons are made among the proposed energy-conserving scheme, the classical leapfrog scheme, and a Strang operator-splitting scheme to demonstrate the superiority.

Kinetic-fluid multi-phase flow system with random inputs in the fine particle regime

Yiwen LIN

Shanghai Jiao Tong University

Consider kinetic-fluid models for a mixture of flows, where the disperse phase is made of particles with distinct sizes. This leads to a system coupling the incompressible Navier–Stokes equations to the Vlasov–Fokker–Planck equations. For the model with random initial data near global equilibrium, we demonstrate exponential decay of energy over time by hypocoercivity arguments. We also prove that the generalized polynomial chaos stochastic Galerkin method has spectral accuracy uniformly in time and the Stokes number, with exponential decay of an error over time, and propose a stochastic asymptotic-preserving scheme to simulate the behavior of multi-phase flow system, efficiently in both kinetic and hydrodynamic regimes. Additionally, we provide uniform error estimates of the bi-fidelity method for this coupled model with random inputs. Numerical examples illustrate the accuracy and efficiency of the method.

The theory of parameter condensation in neural networks

Tao LUO
Shanghai Jiao Tong University

In this talk, we will first introduce the phenomenon of parameter condensation in neural networks, which refers to the tendency of certain parameters to converge towards the same values during training. Then, for certain types of networks, we prove that condensation occurs in the early stages of training. We further analyze which hyperparameters and training strategies influence parameter condensation. In some cases, we even provide a phase diagram that delineates whether parameter condensation occurs. We will also briefly discuss the relationship between parameter condensation and generalization ability. Finally, towards the end of the training, we study the set of global minima and present a detailed analysis of its geometric structure and convergence properties.

ODE-DPS: ODE-based Diffusion Posterior Sampling for Inverse Problems in Partial Differential Equations

Zheng MA
Shanghai Jiao Tong University

In recent years we have witnessed a growth in mathematics for deep learning, which has been used to solve inverse problems of partial differential equations (PDEs). However, most deep learning-based inversion methods either require paired data or necessitate retraining neural networks for modifications in the conditions of the inverse problem, significantly reducing the efficiency of inversion and limiting its applicability. To overcome this challenge, in this talk, leveraging the score-based generative diffusion model, we introduce a novel unsupervised inversion methodology tailored for solving inverse problems arising from PDEs. Our approach operates within the Bayesian inversion framework, treating the task of solving the posterior distribution as a conditional generation process achieved through solving a reversetime stochastic differential equation. Furthermore, to enhance the accuracy of inversion results, we propose an ODE-based Diffusion Posterior Sampling inversion algorithm. The algorithm stems from the marginal probability density functions of two distinct forward generation processes that satisfy the same Fokker-Planck equation. Through a series of experiments involving various PDEs, we showcase the efficiency and robustness of our proposed method.

A sparse grid wavelet Galerkin method for 3-D static piezoelectric equations

Likun QIU

Shanghai Jiao Tong University

Piezoelectric materials are a kind of smart materials, which have applications in a variety of industrial and engineering devices, such as surface acoustic wave (SAW) devices, sonar devices and aerospace equipments. All of these applications involve the so-called positive and reverse piezoelectric effect, which can be described as the piezoelectric equations. In this paper, we are concerned with the sparse grid wavelet Galerkin method (SWGM) for solving the piezoelectric equations and its convergence analysis. Based on some standard assumptions, the proposed method can greatly reduce the number of degrees of freedom (DOFs) while maintaining almost the same convergence rate as the wavelet Galerkin method upto multiplication of a logarithmic factor. Numerical results show that the proposed method performs better than the classical Lagrange FEM in solving the piezoelectric equations.

Newton's method and its hybrid with machine learning for Navier-Stokes Darcy models Discretized by mixed element methods

Haohao WU

Shanghai Jiao Tong University

Navier-Stokes Darcy (NSD) models are frequently encountered in various industrial and engineering applications. In this talk, we are concerned with proposing and analyzing Newton's method and its hybrid with machine learning for solving a non-linear discrete problem arising from mixed element discretization of the NSD model. At the beginning, Newton's method is designed for such a discrete problem. Under some standard conditions, the method is proved to be convergent quadratically, with the convergence rate independent of the finite element mesh size. To further improve the performance of the previous method, we use the interpolant of the PINN solution of the NSD model as the initial guess, so as to produce a hybrid method associated with machine learning for the previous problem. Numerical results show that the hybrid method performs better over Newton's method by choosing a standard initial guess.

Derivative-free methods for nonlinear least squares problems

Jinyan FAN

Shanghai Jiao Tong University

In this talk we consider nonlinear least squares problems for which the exact Jacobians are not available and replaced by probabilistic or random models. Problems of this nature arise in important practical applications, such as the data assimilation in weather prediction and the estimation of the merit function in deep learning. We will present some derivative-free algorithms for such problems and show the almost sure global convergence and complexity of the algorithms.

A unified HDG method for fluid-structure interaction based on Alfeld splits

Lina ZHAO

City University of Hong Kong

In this talk we present a stabilization-free HDG method in stress-velocity formulation for fluid-structure interaction problem on Alfeld splits. A unified mixed formulation is employed for the Stokes equations and the elastodynamic equations. We use the standard polynomial space with strong symmetry to define the stress space, and use the broken H(div)-conforming space of the same degree to define the vector space in a careful way such that the resulting scheme is stable without resorting to any stabilization. The transmission conditions can be incorporated naturally without resorting to additional variables or Nitsche-type stabilization owing to the bespoke construction of the discrete formulation. To show the optimal convergence, we establish a new projection operator for the stress space whose definition accounts for traces of the method. Several numerical experiments are presented to verify the proposed theories.

Euler's elastica-based Cartoon-smooth-texture image decomposition

HE Roy

City University of Hong Kong

We propose a novel variational model for decomposing grayscale images into three distinct components: the structural part, representing sharp boundaries and regions with strong light-to-dark transitions; the smooth part, capturing soft shadows and shades; and the oscillatory part, characterizing textures and noise. Due to the combination of a generalized L0-gradient energy and the Euler's elastica, our problem is non-convex and non-smooth. An efficient algorithm based on operator-splitting will be discussed, and various examples will be demonstrated to validate our model.

Least-Squares versus Partial Least-Squares Finite Element Methods: Robust Error Analysis

Shun ZHANG

City University of Hong Kong

For the generalized Darcy problem (an elliptic equation with discontinuous coefficients), we study a special partial Least-Squares (Galerkin-least-squares) method, known as the augmented mixed finite element method, and its relationship to the standard least-squares finite element method (LSFEM). Augmented mixed finite element methods and the standard LSFEM uses the same a posteriori error estimator: the evaluations of numerical solutions at the corresponding least-squares functionals. As partial least-squares methods, the augmented mixed finite element methods are more flexible than the original LSFEMs. As comparisons, we discuss the mild non-robustness of a priori and a posteriori error estimates of the original LSFEMs. For the stationary Stokes problem with a piecewise constant viscosity coefficient in multiple subdomains, we propose an ultra-weak augmented mixed finite element formulation. By adopting a Galerkin-least-squares method, the augmented mixed formulation can achieve stability without relying on the inf-sup condition in both continuous and discrete settings. The key step to having a robust priori error estimate is to use two norms, one energy norm and one full norm, in robust continuity. The robust coercivity is proved for the energy norm. A robust a priori error estimate in the energy norm is then derived with the best approximation property in the full norm for the case of multiple subdomains.

Multicontinuum Homogenization and its Application

LEUNG Wing Tat

City University of Hong Kong

In this talk, we will discuss an advancement in multiscale simulations for high-contrast problems without scale separation. We will first present the Nonlocal Multicontinua (NLMC) method, which introduces multiple macroscopic variables within each computational grid. We will present a comprehensive derivation of multicontinuum equations and discuss the formulation of cell problems. Specifically, we will address problems characterized by distinct properties in different regions, resulting in unique macroscopic equations for those regions. We will also explain how to connect these macroscopic equations using interface conditions. Additionally, we will introduce constraint cell problem formulations within a representative volume element, employing an oversampling technique to derive the multicontinuum equations and interface conditions.

Scalable Bayesian Inference with Kinetic Langevin Dynamics

CHADA Neil

City University of Hong Kong

Bayesian inference is focused on sampling from distributions, where the gold-standard technique is Markov chain Monte Carlo. In this talk we focus on an alternative set of algorithms based on unadjusted Langevin methods. These methods utilize splitting order methods for stochastic differential equations which acquire better weak and strong rates of convergence. We propose this in the context of unbiased sampling, where we provide new estimators which are more efficient and accurate. We further provide a range of numerical experiments exemplifying this. Recent work will also show how these estimators can be used on Bayesian neural networks for classification problems in machine learning.

Operator Learning for Nonsmooth Optimal Control of PDEs

Yongcun SONG

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Optimal control problems with nonsmooth objectives and partial differential equation (PDE) constraints are challenging, mainly because of the underlying nonsmooth and nonconvex structures and the demanding computational cost for solving multiple high-dimensional and ill-conditioned systems after mesh-based discretization. To mitigate these challenges numerically, we propose an operator learning approach combined with an effective primal-dual optimization idea that can decouple the treatment of the control and state variables so that each resulting iteration only requires solving two PDEs. Our main purpose is to construct neural surrogate models for the involved PDEs by operator learning, allowing the solution of a PDE to be obtained with only a forward pass of the neural network. The resulting algorithmic framework offers a hybrid approach that combines the flexibility and generalization of operator learning with the model-based nature and structure-friendly efficiency of primal-dual-based algorithms. The primal-dual-based operator learning approach offers numerical methods that are mesh-free, easy to implement, and adaptable to various optimal control problems with nonlinear PDEs. Notably, the neural surrogate models can be reused across iterations and parameter settings hence, computational cost can be substantially alleviated. We validate the effectiveness and efficiency of the primal-dual-based operator learning approach across a range of typical optimal control problems with nonlinear PDEs.

Sensitivity analysis of colored-noise-driven interacting particle systems

MERTZ Laurent

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We present an efficient sensitivity analysis method for a wide class of colored-noise-driven interacting particle systems (IPSs). Our method is based on unperturbed simulations and significantly extends the Malliavin weight sampling method proposed by Szamel [Europhys. Lett. 117, 50010 (2017)] for evaluating sensitivities such as linear response functions of IPSs driven by simple Ornstein-Uhlenbeck processes. We show that the sensitivity index depends not only on two effective parameters that characterize the variance and correlation time of the noise, but also on the noise spectrum. In the case of a single particle in a harmonic potential, we obtain exact analytical formulas for two types of linear response functions. By applying our method to a system of many particles interacting via a repulsive screened Coulomb potential, we compute the mobility and effective temperature of the system. Our results show that the system dynamics depend, in a nontrivial way, on the noise spectrum. This is a joint work with Josselin Garnier (École Polytechnique) and Harry Ip (CityUHK).

Efficient quantum Gibbs samplers

Bowen LI

City University of Hong Kong

Lindblad dynamics and other open-system dynamics provide a promising path towards efficient Gibbs sampling on quantum computers. In these proposals, the Lindbladian is obtained via an algorithmic construction akin to designing an artificial thermostat in classical Monte Carlo or molecular dynamics methods, rather than treated as an approximation to weakly coupled system-bath unitary dynamics. In this talk, we build upon the structural characterization of KMS detailed balanced Lindbladians by Fagnola and Umanita, and develop a family of efficient quantum Gibbs samplers using a finite set of jump operators (the number can be as few as one), akin to the classical Markov chain-based sampling algorithm. Compared to the existing works, our quantum Gibbs samplers have a comparable quantum simulation cost but with greater design flexibility and a much simpler implementation and error analysis.

Simultaneously Cloaking Electric and Hydrodynamic Fields via Electro-osmosis

Zhiqiang MIAO

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We develop a general mathematical framework for the design and analysis of a novel coupled-physics invisibility cloaking scheme that can simultaneously cloak microscale electric and hydrodynamic fields via scattering cancellation for the electric potential and electro-osmosis for the pressure in a Hele-Shaw configuration. As a proof of this concept, the perfect electric and hydrodynamic cloaking conditions are derived for the cloaks with the cross-section being annulus or confocal ellipses using the layer potential techniques. Furthermore, we develop an optimization scheme for the design of approximate cloaks within general geometries and prove the well-posedness of the optimization problem. In particular, the conditions that can ensure the simultaneous occurrence of approximate cloaks for general geometries are established. Our theoretical findings are corroborated by several numerical results. Our results are new to the literature.

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