四川大學 SICHUAN UNIVERSITY 数学学院

“2025 科学计算前沿进展”论坛

主办单位：四川大学数学学院

资助单位：国家天元数学西南中心

会议日程安排

2025 年 07 月 25 日至 2025 年 07 月 27 日，四川大学，成都

组委会：包维柱、唐庆粦

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会议地点：四川大学（望江校区）数学学院西 303

住宿地点：世外桃源酒店（科华北路 69 号）

“2025科学计算前沿进展”论坛

26/07/2025 （星期六） 会议室：数学学院西303会议室，数学学院，四川大学		主持人
8:45-9:00	签到、开幕式	包维柱
9:00-9:30	高卫国（复旦大学） Toward theoretical insights into diffusion trajectory distillation via operator merging	包维柱
9:30-10:00	聂玉峰（西北工业大学） Stability and error analysis of reduced-order methods based on POD with finite element solutions for nonlocal diffusion problems	包维柱
10:00-10:30	休息	
10:30-11:00	徐振礼（上海交通大学） Local Gauss's law preserving method for PNP and Vlasov-Poisson equations	谢小平
11:00-11:30	孙志刚（中科院大连化学物理研究所） Accurate and FFT-enabled trigonometric discrete variable representations for the singular Coulomb potential	谢小平
11:30-12:00	蔡勇勇（北京师范大学） Multiscale numerical methods and analysis for the oscillatory dispersive equations	谢小平
12:30-13:40	午餐	
14:30-15:00	黄忠亿（清华大学） An energy stable TFPM-based Petrov-Galerkin scheme for solving Allen-Cahn equation	高卫国
15:00-15:30	李晓丽（山东大学） Physics-preserving schemes for thermodynamically consistent model of two-phase flow in porous media	高卫国
15:30-16:00	赵泉（中国科学技术大学） Stable parametric finite element methods for Willmore flow	高卫国
16:00-16:30	休息	
16:30-17:00	杨将（南方科技大学） ϵ-rank and the staircase phenomenon: new insights into neural network training dynamics	聂玉峰
17:00-17:30	毛志平（宁波东方理工大学） Solving PDEs using deep neural networks with error control	聂玉峰
17:30-18:00	闫亮（东南大学） 基于深度学习的偏微分方程反问题求解及其应用	聂玉峰
18:30-20:00	晚餐	

报告题目和摘要

报告人：蔡勇勇（北京师范大学）

题目： Multiscale numerical methods and analysis for the oscillatory dispersive equations

摘要： Dispersive PDEs, such as Klein-Gordon equation, Dirac equation, Schrodinger equation, arise from many different areas, e.g. computational chemistry, plasma physics, quantum mechanics. Typical computational tasks in dispersive PDEs are finding the ground/stationary states and solving the dynamics. In this talk, we report some recent advances on the numerical methods and analysis for the time-dependent dispersive PDEs, paying particular attention to the highly oscillatory PDEs, which usually exhibit solutions with high frequency waves in time and/or in space, and are generally computational expensive.

报告人：高卫国（复旦大学）

题目： Toward theoretical insights into diffusion trajectory distillation via operator merging

摘要： Diffusion trajectory distillation methods aim to accelerate sampling in diffusion models, which produce high-quality outputs but suffer from slow sampling speeds. These methods train a student model to approximate the multi-step denoising process of a pretrained teacher model in a single step, enabling one-shot generation. However, theoretical insights into the trade-off between different distillation strategies and generative quality remain limited, complicating their optimization and selection. In this work, we take a first step toward addressing this gap. Specifically, we reinterpret trajectory distillation as an operator merging problem in the linear regime, where each step of the teacher model is represented as a linear operator acting on noisy data. These operators admit a clear geometric interpretation as projections and rescalings corresponding to the noise schedule. During merging, signal shrinkage occurs as a convex combination of operators, arising from both discretization and limited optimization time of the student model. We propose a dynamic programming algorithm to compute the optimal merging strategy that maximally preserves signal fidelity. Additionally, we demonstrate the existence of a sharp phase transition in the optimal strategy, governed by data covariance structures. Our findings enhance the theoretical understanding of diffusion trajectory distillation and offer practical insights for improving distillation strategies. This is joint work with Ming Li.

报告人：黄忠亿（清华大学）

题目： An energy stable TFPM-based Petrov-Galerkin scheme for solving Allen-Cahn equation

摘要： In this talk, we propose an energy stable tailored finite point method (TFPM) based Petrov-Galerkin scheme to solve Allen-Cahn equation. In time discretization, we present both first-order and second-order semi-discrete schemes based on stabilized and convex-splitting techniques, which satisfy unconditional energy stability. We prove the maximum bound preserving principle for first-order schemes. As the nature of singularly perturbation in semi-discrete level remains when ϵ is extremely small, we establish a specified Petrov-Galerkin scheme which leads to a unified way for space discretization. Specialized TFPM schemes are incorporated into our Petrov-Galerkin scheme to compute test functions. Numerical experiments validate the accuracy and efficiency of the proposed method and show that our scheme performs well on uniform meshes even when mesh size h is great larger than ϵ.

报告人：李晓丽（山东大学）

题目： Physics-preserving schemes for thermodynamically consistent model of two-phase flow in porous media

摘要： In this talk, In this talk, we present several high-order and physics-preserving numerical schemes for thermodynamically consistent model of incompressible and immiscible two-phase flow in porous media. The constructed schemes only need to solve one linear system and a nonlinear algebraic equation with negligible computational cost at each time step. We also prove that the proposed schemes are energy stable, mass-conservative and bounds-preserving for each phase without any restrictions of time step size. Finally, various interesting numerical examples are presented to verify the accuracy and efficiency of the proposed schemes.

报告人：毛志平（宁波东方理工大学）

题目： Solving PDEs using deep neural networks with error control

摘要： Neural networks have shown significant potential in solving partial differential equations (PDEs). While deep networks are capable of approximating complex functions, direct one-shot training often faces limitations in both accuracy and computational efficiency. To address these challenges, we propose both Galerkin and collocation adaptive methods that uses neural networks to construct basis functions guided by the equation residual. The approximate solution is computed within the space spanned by these basis functions. As the approximation space gradually expands, the solution is iteratively refined; meanwhile, the progressive improvements serve as reliable a posteriori error indicators that guide the termination of the sequential updates. Additionally, we introduce adaptive strategies for collocation point selection and parameter initialization to enhance robustness and improve the expressiveness of the neural networks. We also derive the approximation error estimate and validate the proposed method with several numerical experiments on various challenging PDEs, demonstrating both high accuracy and robustness of the proposed methods.

报告人：聂玉峰（西北工业大学）

题目： Stability and error analysis of reduced-order methods based on POD with finite element solutions for nonlocal diffusion problems

摘要： In this talk, we will introduce the formulation and theoretical analysis of the reduced-order numerical method constructed by proper orthogonal decomposition (POD) for nonlocal diffusion problems with a finite range of interactions. Due to the nonlocality, the corresponding discrete systems of nonlocal models have less sparsity than those for PDEs. Given the challenges of frequently handling large systems of linear equations with much lower sparsity, we establish a reduced-order model (ROM) for nonlocal diffusion problems to expedite the iterative solution process. The ROM is constructed using FE solutions in a very small time interval as snapshot data and has much fewer degrees of freedom than FEMs. In this contribution, we focus on discussing mathematical justifications for the existence, stability, and error estimates of the ROM method, which have not been considered in previous research for nonlocal models. Another important component of our work is that we systematically explore the effect of different parameters on the behavior of the POD algorithms. Numerical examples will be finally presented to validate the theoretical conclusions and to illustrate the efficiency of the proposed method.

报告人：孙志刚（中科院大连化学物理研究所）

题目：Accurate and FFT-enabled trigonometric discrete variable representations for the singular Coulomb potential

摘要： It is important in atomic physics, especially in the currently popular attosecond physics field, to efficiently and accurately solve the Schrodinger equation (SE) with a singular Coulomb potential. Using modern (pseudo-)spectral method to solve it is a long-standing difficulty problem. A brand-new pseudo-spectral method, which is of unprecedented efficiency and accuracy for solving it, was proposed in our work. Especially, this new, nearly perfect pseudo-spectral method, could be directly applied with the fast Fourier transform technique and could boost computing speed significantly. This method could be of extensive applications.

报告人：徐振礼（上海交通大学）

题目： Local Gauss's law preserving method for PNP and Vlasov-Poisson equations

摘要： We introduce structure-preserving numerical methods for models in plasma simulations including Poisson-Nernst-Planck (PNP) equations and Vlasov-Poisson equations. A fast Poisson method is developed by reformulating the Poisson equation into a minimization procedure of electrostatic energy under the constraint of the Gauss law. A local curl-free relaxation is then introduced to obtain the solution. Incorporating this solver into the PNP and VP equations leads to efficient methods for solving these equations together with nice features of structure preserving. Numerical results are present to show the attractive performance of the new methods.

报告人：闫亮（东南大学）

题目：基于深度学习的偏微分方程反问题求解及其应用

摘要：近年来，基于深度学习和微分方程（PDE）结合的科学机器学习（SciML）方法逐渐成为科学计算领域研究的热点，在科学探究和工程应用的诸多领域得到广泛应用。本报告中，我们在回顾深度学习求解偏微分方程反问题的几种常用框架的基础上，介绍我们在该领域所设计的几种方法，包括自适应算子学习、基于失效信息的 PINNs 方法以及针对反障碍散射所设计的深度反演框架等。

报告人：杨将（南方科技大学）

题目： ϵ-rank and the staircase phenomenon: new insights into neural network training dynamics

摘要： Understanding the training dynamics of deep neural networks (DNNs), particularly how they evolve low-dimensional features from high-dimensional data, remains a central challenge in deep learning theory. In this work, we introduce the concept of ϵ-rank, a novel metric quantifying the effective feature of neuron functions in the terminal hidden layer. Through extensive experiments across diverse tasks, we observe a universal *staircase phenomenon*: during training process implemented by the standard stochastic gradient descent methods, the decline of the loss function is accompanied by an increase in the ϵ-rank and exhibits a staircase pattern. Theoretically, we rigorously prove a negative correlation between the loss lower bound and ϵ-rank, demonstrating that a high ϵ-rank is essential for significant loss reduction. Moreover, numerical evidences show that within the same deep neural network, the ϵ-rank of the subsequent hidden layer is higher than that of the previous hidden layer. Based on these observations, to eliminate the staircase phenomenon, we propose a novel pre-training strategy on the initial hidden layer that elevates the ϵ-rank of the terminal hidden layer. Numerical experiments validate its effectiveness in reducing training time and improving accuracy across various tasks. Therefore, the newly introduced concept of ϵ-rank is a computable quantity that serves as an intrinsic effective metric characteristic for deep neural networks, providing a novel perspective for understanding the training dynamics of neural networks and offering a theoretical foundation for designing efficient training strategies in practical applications.

报告人：赵泉（中国科学技术大学）

题目： Stable parametric finite element methods for Willmore flow

摘要： In this talk, I will introduce a new parametric fintie element method for Willmore flow of hypersurfaces in a unified framework. The method is linear and employs a splitting of the normal and tangential velocity of the flow. The normal velocity is approximated via an evolution equation for the curvature, and follows the arbitrary Lagrangian-Eulerian approach. This enables an unconditional energy stability with respect to the discrete energy. We also incorporate the ‘BGN’ tangential velocity through a curvature identity. This helps to preserve the mesh quality. We show various numerical examples to demonstrate the favorite properties of the method.