会议通知

偏微分方程数值解和计算物理是哈尔滨工业大学数学学科的主要研究方向之一。为加强国内外研究机构和高校在偏微分方程数值解领域的学术合作，促进与计算物理专家的深入交流，并推动学科建设，哈尔滨工业大学数学学院举办《偏微分方程数值解及计算物理前沿发展研讨会》的学术活动。会议将邀请著名计算数学家和计算物理学家共同探讨偏微分方程数值解的最新研究进展及其在诸多领域的应用。现将相关事宜通知如下：

一、会议主题

主题为：偏微分方程数值解及计算物理前沿发展研讨会

二、会议安排

1. 报到：2024 年 7 月 10 日 10:00-20:00，地点：哈尔滨馨特商务酒店一楼大厅（南岗区西大直街 108 号）

2. 会议：2024 年 7 月 11 日-12 日

三、会议费用

本次会议免收会务费，会议期间餐费与交通费自理、无补贴，住宿费由会议方支付。

四、会议联系人

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会议日程表

<table>
<tr><td colspan="4">2024 年 7 月 11 日 上午
地点：理学楼 308</td></tr>
<tr><td>时间</td><td>报告人</td><td>题目</td><td>主持人</td></tr>
<tr><td>9:00-9:30</td><td>Rémi Abgrall</td><td>A Novel Kinetic Scheme for the Compressible Navier Stokes Equations</td><td>明平兵</td></tr>
<tr><td>9:30-10:00</td><td>明平兵</td><td>A pre-training Deep Learning Method for Simulating the Large Bending Deformation of Bilayer Plates</td><td rowspan="2">乔中华</td></tr>
<tr><td>10:00-10:30</td><td>戴小英</td><td>Orthogonality Preserving Methods for Electronic Structure Calculation</td></tr>
<tr><td>10:30-10:50</td><td colspan="3">休息</td></tr>
<tr><td>10:50-11:20</td><td>乔中华</td><td>Energy-Dissipative Spectral Renormalization Exponential Integrator Method for Gradient Flow Problems</td><td rowspan="2">Rémi Abgrall</td></tr>
<tr><td>11:20-11:50</td><td>李步扬</td><td>New Artificial Tangential Motion for Computing Surface Evolution under Geometric Flow</td></tr>
</table>

2024 年 7 月 11 日 下午 **地点：理学楼 308**			
时间	**报告人**	**题目**	**主持人**
14:00-14:30	汤华中	Genuinely Multidimensional PCP Finite Volume Schemes for the Special Relativistic Hydrodynamics	成娟
14:30-15:00	吴开亮	A Journey into Bound-Preserving Schemes and Theory	
15:00-15:20	**休息**		
15:20-15:50	成娟	The High Order Positivity-Preserving Conservative Remapping Methods and their Application in the ALE Simulation of Compressible Fluid Flow	汤华中

2024 年 7 月 12 日 **地点：理学楼 308**
自由讨论

报告摘要
（按姓氏首字母排序）

A Novel Kinetic Scheme for the Compressible Navier Stokes Equations

Rémi Abgrall，苏黎世大学

In this talk, I will first review kinetic method of Xi-Jin. After the work of Xi and Jin [1], there has been a considerable interest for nonlinear hyperbolic problem because there was no need of using Riemann Solver, see [2, 3, 4]. Extensions have been provided for some parabolic problems see [5, 6] among others. The problem is that the time step depends on the inverse of a relaxation parameter which is assumed to tend to zero, hence implicit schemes become a must.

Here starting from the work of [7], we show how to construct kinetic schemes written in the spirit of Xi and Jin that are able to approximate parabolic problems with a time step that is independent of the relaxation parameter while staying explicit. This is described in [8] and [9].

The fundamental principles are: (1) rather than aiming for the desired equations in the strict limit of a vanishing relaxation parameter, as is commonly done in the diffusion limit of kinetic methods, diffusion terms are sought as a first-order correction of this limit in a Chapman-Enskog expansion, (2) introducing a coupling between the conserved variables within the relaxation process by a specifically designed collision matrix makes it possible to systematically match a desired diffusion. Extending this strategy to multi-dimensions cannot, however, be achieved through simple directional splitting, as diffusion is likely to couple space directions with each other, such as with shear viscosity in the Navier-Stokes equations. In this work, we show how rewriting the collision matrix in terms of moments can address this issue, regardless of the number of kinetic waves, while ensuring conservation systematically. This rewriting allows for introducing a new class of kinetic models called regularized models, simplifying the numerical methods and establishing connections with Jin-Xin models. Subsequently, new explicit arbitrary high-order kinetic schemes are formulated and validated on standard two-dimensional cases from the literature. Excellent results are obtained in the simulation of a shock-boundary layer interaction, validating their ability to approximate the Navier-Stokes equations with kinetic speeds obeying nothing but a subcharacteristic condition along with a hyperbolic constraint on the time

step.

References

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conservation laws. Journal of Statistical Physics, 95(1/2), 1999.

[5] S. Boscarino, L. Pareschi, and G. Russo. Implicit-explicit Runge-Kutta schemes for hyperbolic systems and kinetic equations in the diffusion limit. SIAM J. Sci. Comput., 35(1):A22 – A51, 2013.

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[7] R. Abgrall and D. Torlo. Some preliminary results on a high order asymptotic preserving computationally explicit kinetic scheme. Communications in Mathematical Sciences, 20(2):297 – 326, 2022.

[8] G. Wissocq and R. Abgrall. A new local and explicit kinetic method for linear and non-linear convection-diffusion problems with finite kinetic speeds: I. one-dimensional case, 2023. arXiv.2310.08356.

[9] Gauthier Wissocq and R. Abgrall. A new local and explicit kinetic method for linear and non-linear convection-diffusion problems with finite kinetic speeds: II. multi-dimensional case, 2023. arXiv.2312.16323.

The High Order Positivity-Preserving Conservative Remapp-ing Methods and their Application in the ALE Simulation of Compressible Fluid Flow

成娟，北京应用物理与计算数学研究所

The arbitrary Lagrangian-Eulerian (ALE) method has a wide range of applications in numerical simulation of multi-material fluid flow. The indirect ALE method consists of three steps: Lagrangian step, rezone step and remapping step. In this talk, we propose two classes of high order positivity-preserving conservative remapping methods in the finite volume and discontinuous Galerkin (DG) frameworks respectively. Combined with the finite volume and DG Lagrangian schemes and the rezoning strategies, we present two types of high order

positivity-preserving conservative ALE methods individually. For the finite volume framework, we adopt the multi-resolution WENO reconstruction which can achieve optimal accuracy in the smooth regions and keep non-oscillatory near discontinuities. Also, we incorporate an efficient local limiting to preserve positivity for the positive physical variables involved in the ALE framework without sacrificing the original high-order accuracy and conservation. For the DG framework, we develop a high-order positivity-preserving polynomial projection remapping method based on the L2 projection for the DG scheme. A series of numerical tests are provided to verify properties of our remapping algorithms, such as high-order accuracy, conservation, essential non-oscillation, positivity-preserving and efficiency. The performance of the ALE methods using the above discussed remapping algorithms is also tested for the Euler system.

Orthogonality Preserving Methods for Electronic Structure Calculation

戴小英，中国科学院数学与系统科学研究院

To obtain convergent numerical approximations without orthogonalization operations is of great importance in electronic structure calculations. In this talk, we will introduce an extended gradient flow based Kohn-Sham DFT model, for which we prove the flow is orthogonality preserving and the solution evolves to the ground state. With the help of the gradient flow based Kohn-Sham DFT model, we propose and analyze a class of iteration schemes for the discretized Kohn-Sham model, which preserves the orthogonality of the Kohn-Sham orbitals automatically. With our schemes, the iterative approximations are guaranteed to converge to the Kohn-Sham orbitals without any orthogonalization operations when the initial orbitals are orthogonal. We prove the convergence and get the local convergence rate of the numerical approximations under some reasonable assumptions. This is a joint work with Qiao Wang, Liwei Zhang and Aihui Zhou.

New Artificial Tangential Motion for Computing Surface Evolution under Geometric Flow

李步扬，香港理工大学

We review the development of parametric finite element approximations to surface evolution under geometric flows, as well as the development of artificial tangential motion for improving the mesh quality of the computed surfaces. Then we report our recent discovery of instability of a widely used artificial tangential motion proposed by Barrett, Garcke, Nurnberg, and introduce our new artificial tangential motion which could improve the stability and accuracy of numerical approximations as well as mesh quality of the computed surfaces.

A Pre-training Deep Learning Method for Simulating the Large Bending Deformation of Bilayer Plates

明平兵，中国科学院数学与系统科学研究院

We propose a deep learning based method for simulating the large bending deformation of bilayer plates. Inspired by the greedy algorithm, we propose a pre- training method on a series of nested domains, which accelerate the convergence of training and find the absolute minimizer more effectively. The proposed method exhibits the capability to converge to an absolute minimizer, overcoming the limitation of gradient flow methods getting trapped in the local minimizer basins. We showcase better performance with fewer numbers of degrees of freedom for the relative energy errors and relative L2-errors of the minimizer through numerical experiments. Furthermore, our method successfully maintains the L2-norm of the isometric constraint, leading to an improvement of accuracy. This is a joint work with Xiang Li and Yulei Liao.

Energy-dissipative spectral renormalization exponential integrator method for gradient flow problems

乔中华，香港理工大学

In this talk, we present a novel spectral renormalization exponential integrator method for solving gradient flow problems. Our method is specifically designed to simultaneously satisfy discrete analogues of the energy dissipation laws and achieve high-order accuracy in time. To accomplish this, our method first incorporates the energy dissipation law into the target gradient flow equation by introducing a time-dependent spectral renormalization (TDSR) factor. Then, the coupled equations are discretized using the spectral approximation in space and the exponential time differencing (ETD) in time. Finally, the resulting fully discrete nonlinear system is decoupled and solved using the Picard iteration at each time step. Furthermore, we introduce an extra enforcing term into the system for updating the TDSR factor, which greatly relaxes the time step size restriction of the proposed method and enhances its computational efficiency. Extensive numerical tests with various gradient flows are also presented to demonstrate the accuracy and effectiveness of our method as well as its high efficiency when combined with an adaptive time-stepping strategy for long-term simulations.

Genuinely Multidimensional PCP Finite Volume Schemes for the Special Relativistic Hydrodynamics

汤华中，北京大学

We develop the genuinely multidimensional HLL Riemann solver for the two-dimensional special relativistic hydrodynamic equations on Cartesian meshes and studies its physical-constraint -preserving (PCP) property. Based on the resulting HLL solver, the first- and high-order accurate PCP finite volume schemes are proposed. In the high-order scheme, the WENO reconstruction, the third-order accurate strong-stability-preserving time discretizations and the PCP flux limiter are used. Several numerical results are given to demonstrate the accuracy, performance and resolution of the shock waves and the genuinely multi-dimensional wave structures etc. of our PCP finite volume schemes.

A Journey into Bound-Preserving Schemes and Theory

吴开亮，南方科技大学

Solutions to many partial differential equations (PDEs) are subject to certain bounds or constraints. For instance, in fluid dynamics, density and pressure must remain positive, while in relativistic cases, fluid velocity must not exceed the speed of light. Developing bound-preserving numerical methods that uphold these intrinsic constraints is crucial. Recently, significant attention has been given to design provably bound-preserving schemes, though challenges remain, particularly for systems with nonlinear constraints.

In this talk, I will present our recent efforts in developing fundamental bound-preserving theories:

1. Geometric Quasilinearization (GQL): Drawing on key insights from geometry, we propose a novel and general framework called geometric quasilinearization. GQL offers an effective approach for addressing bound-preserving problems with nonlinear constraints by transforming these constraints into linear ones through the introduction of auxiliary variables. We establish the fundamental principles and general theory of GQL using the geometric properties of convex regions and present three effective methods for constructing GQL.

2. Optimal Cell Average Decomposition (OCAD): Utilizing convex geometry and symmetric group theory, we develop the optimal cell average decomposition theory, which provides a foundation for constructing more efficient bound-preserving schemes. We demonstrate that the classic Zhang-Shu CAD is optimal in one dimension but generally not in multiple dimensions, thereby addressing their conjecture proposed in 2010.

We apply the GQL and OCAD approaches to various PDEs, showcasing their effectiveness and advantages through diverse and challenging examples and applications, including

magnetohydrodynamics (MHD), relativistic hydrodynamics, and the ten-moment Gaussian closure system.