

复杂流体力学问题建模、算法与分析研讨会

**Workshop on Modelling, Algorithm and
Analysis on Complex Fluid Dynamics**

会议手册

October 27-30, 2019

Beijing, China



北京计算科学研究中心
BEIJING COMPUTATIONAL SCIENCE RESEARCH CENTER



北京大学

复杂流体力学问题建模、算法与分析研讨会

2019年10月27日-30日，北京

随着大型计算机的出现，计算数学和计算力学在国防建设事业中日趋重要。高效计算方法与高性能并行计算能力的结合使得成功模拟多物理，大尺度的极端问题成为可能。但使用计算数学、力学方法解决实际应用问题，需要了解相关背景知识，提炼合适的科学问题。该研讨会旨在促进国防一线工作人员与国内外知名学者的相互交流。我们还将一起探讨如何促进计算数学和计算力学更好地为国家的国防建设服务，同时帮助更多青年学者了解具体国防建设应用问题的背景知识，调动他们参与国防建设的积极性。会议主题包括但不限于：多介质流体力学、动理学方程、辐射输运方程、矩方法、高精度保物理性质算法。本次研讨会由北京计算科学研究中心与北京大学共同举办。

会议学术委员会（按姓名的拼音字母顺序排列）：

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会议相关信息

1. 注册信息:

◇ 时间: 14:00~17:30 (10月27日, 星期日), 08:00~17:00 (10月28日, 星期一)

◇ 地点: 北京计算科学研究中心 一层, 第一会议室门口

2. 会议地点: 北京计算科学研究中心 一层, 第一会议室

3. 用餐地点: 中心地下一层餐厅(参会及就餐时请佩戴会议胸牌)

4. 合影时间地点: 中心一层大厅, 10月28日下午4:00

5. 海报环节:

◇ 海报尺寸: 120cm 高 * 90cm 宽

◇ 海报张贴时间: 星期日下午 (10月27日), 星期一全天 (10月28日)

◇ 海报张贴时间地点: 中心一层大厅, 11:00~14:30 (10月28日)

6. 中心地址:

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会议日程安排

28 Morning	8:40-9:00	<i>Opening</i>	
	Chair: Bao-Lin Tian (IAPCM)		
	9:00-9:40	Jie-Quan Li (IAPCM)	Do you really believe numerical simulations in CFD?
	9:40-10:10	Zhen-Ning Cai (NUS)	Regularized 13-Moment Equations for Inverse-Power-Law Models
	10:10-10:50	<i>Tea break</i>	
	Chair: Jie-Quan Li (IAPCM)		
	10:50-11:20	Hai-Jun Yu (LSEC)	Efficient Numerical Approximations for the Phase-Field Modelling of Multi-Phase Flow with Moving Contact Lines
	11:20-11:50	Wei-Ming Li (IAPCM)	On Levermore's Five-Moment System
	11:50-14:30	<i>Lunch, Poster Session</i>	
28 Afternoon	Chair: Ruo Li (PKU)		
	2:30-3:00	Hao Wu (THU)	非平衡最优输运在机器学习中的应用
	3:30-4:00	Jin Qi (IAPCM)	Primary Applications of Fundamental Processes Theory of Fluid Dynamics in ALE Method and ICF Research
	4:00-4:40	<i>Photo, Tea Break</i>	
	Chair: Juan Cheng (IAPCM)		
	4:40-5:10	Yi Shi (IAPCM)	An Asymptotic Preserving Unified Gas Kinetic Particle Method for Radiative Transfer Equations
	5:10-5:30	Ze-Yu Jin (PKU)	Moment Closure for Kinetic Equations by Machine Learning
	5:30-5:50	Yi-Nuo Ren (PKU)	Numerical Simulation of Plasma Instabilities Using Hermite-Galerkin Spectral Method
		6:00-8:00	<i>Banquet</i>

会议日程安排

29 Morning	Chair: Yi-Qing Shen (IM, CAS)		
	9:00-9:40	Wen-An Yong(THU)	Construction of Boundary Conditions for Hyperbolic Relaxation Approximations
	9:40-10:10	Ying-Zhou Li(Duke)	Distributed-Memory Hierarchical Interpolative Factorization
	10:10-10:50	<i>Tea Break</i>	
	Chair: Wen-An Yong (THU)		
	10:50-11:20	Liang Pan(BNU)	High-Order Gas-Kinetic Scheme for Euler and Navier-Stokes Equations
	11:20-11:50	Gang Li (QU)	基于微分变换的 ADER-DG 方法
	11:50-2:00	<i>Lunch</i>	
29 Afternoon	Chair: Peng Song (IAPCM)		
	2:00-2:30	Ji-Zu Huang (LSEC)	A Lattice Boltzmann Model for 3D Multiphase Flows with Moving Contact Line
	2:30-3:00	Zhi-Yuan Sun (IAPCM)	The Subzonal Predictor-Corrector Algorithm for Hourglass Control
	3:00-4:40	<i>Tea Break</i>	
	Chair: Ji-Zu Huang (LSEC)		
	4:40-5:10	Shu-Jie Li (CSRC)	三维超高精度间断有限元方法若干研究进展
	5:10-5:50	Xiao-Hua Zhang(CTGU)	A Finite Volume Scheme for Savage-Hutter Equations on Unstructured Grids

会议日程安排

30 Morning	Chair: Zhi-Qiang Sheng (IAPCM)		
	9:00-9:40	Wen-Jun Sun (IAPCM)	粒子运输的多尺度动理学数值方法
	9:40-10:10	Lei Li (SJTU)	Direct Simulation Approach for Poisson-Boltzmann Equation Using Random Batch Method
	10:10-10:50	<i>Tea break</i>	
	Chair: Wen-Jun Sun (IAPCM)		
	10:50-11:20	Yi-Xuan Wang (PKU)	Multiscale Edge Basis for Helmholtz Equation with High Contrast
	11:20-11:50	Yan-Li Wang (CSRC)	Numerical Simulation of Microflows Using Hermite Spectral Methods

会议摘要

Do ou really believe numerical simulations in CFD?

Jie-Quan Li (李杰权)

Institute of Applied Physics and Computational Mathematics (IAPCM)

Peter D. Lax ever quoted Ami Harten's observation: "For computational scientists there are two kinds of truth: the truth that you prove, and the truth you see when you compute" [P.Lax Computational Fluid Dynamics, J. Sci. Comput., 31(2007), 185-193]. Do you really believe the "truth" you see when you compute? Due to intricate differences of discrete (computable) models from the corresponding physical models and those of discrete data for computers from the corresponding data for computation, this issue is quite subtle and was ever visited by extending the approaches of discrete Fourier analysis and modified equations for a large range of Fourier modes, particularly highest frequency (Fourier, oscillatory) modes.

In this talk, we will discuss this issue through very simple examples and bring you some new observations.

Numerical Simulation of Plasma Instabilities Using Hermite-Galerkin Spectral Method

Yi-Nuo Ren (任一诺)

Peking University

We developed an Hermite-Galerkin spectral method to numerically solve the spatially homogeneous Fokker-Planck-Landau equation with singular quadratic collision model. An innovative approximation featuring a combination of a simple linear term and a quadratic term which requires high computation cost. Using the Hermite expansion, the quadratic term is evaluated exactly by calculating the spectral coefficients. To deal with singularities, we make use of Burnett polynomials so that even very singular collision model can be handled smoothly. Numerical examples demonstrate that our method can capture low-order moments with satisfactory accuracy and performance. Our method is also utilized to simulate plasma instabilities, numerical results of which are evaluated for comparison with the latest theoretical results.

An Asymptotic Preserving Unified Gas Kinetic Particle Method for Radiative Transfer Equations

Yi Shi (施意)

Institute of Applied Physics and Computational Mathematics (IAPCM)

In this work, we propose a unified gas kinetic particle (UGKP) method for solving the nonlinear thermal radiative transfer equations. The UGKP method is a multiscale method in that the macro and microscopic variables are coupled and updated in a consistent way. It employs a finite volume formulation for the macroscopic variable evolution, and a particle-based Monte Carlo solver for tracking the non-equilibrium transport. The stiff coupling between the radiation and material energy is included and resolved efficiently by the coupled macroscopic equations. Compared with the implicit Monte Carlo (IMC) method, it does not employ the effective scattering events. Moreover, we demonstrate that the UGKP method has the asymptotic preserving property in capturing the diffusion limit in optically thick regions. Numerical simulations show that our method is comparable in computational cost to the IMC method for optically thin problems, and becomes much more efficient for optically thick problems.

Construction of Boundary Conditions for Hyperbolic Relaxation Approximations

Wen-An Yong (雍稳安)

TsingHua University

With the linearized Suliciu model as an example, I intend to present a program aiming at construction of boundary conditions (BCs) for hyperbolic relaxation systems. Physically, such BCs are not always available. The construction is based on the assumption that the relaxation systems and well-posed BCs for the corresponding equilibrium systems are given. We obtain strictly dissipative and compatible BCs for the linearized model with different non-characteristic boundaries. Moreover, the effectiveness of the constructed BCs is shown by resorting to formal asymptotic solutions and energy estimates.

Primary Applications of Fundamental Processes Theory of Fluid Dynamics in ALE Method and ICF Research

Jin QI (齐进)

Institute of Applied Physics and Computational Mathematics (IAPCM)

Arbitrary Lagrangian–Eulerian (ALE) methods for large deformation problems were developed and widely used in engineer research of weapons and ICF. This family of methods often consist of three steps: a Lagrangian step to solve Lagrangian equations, a rezone step to generate the mesh of better geometric qualities for the next time step, and a remapping step to interpolate physical values from the Lagrangian mesh to the rezoned mesh.

In practical applications, it will takes too much computing time if rezone and remap preformed at each step, so it's important to predict. There are many ways to predict, and here we describe the studies of the optimal evaluation index of auto-rezone with theory of fundmental processes of fluid dynamics. According to typical large deformation compressible computational fluid dynamics problems, we studied vorticity, dilatation, Lamb vector, generalized Lamb vector, and their divergence, curl and time derivatives, respectively for Eulerian and Lagrangian meshes. We try to understand the effects of the fundmental processes of fluid dynamics in the studies of large deformation compressible computational fluid dynamics problems, and look for the optimal evaluation index for the starring of rezoning stage of ALE meshes in order to carry out the optimal self-adaption strategy of ALE processes. It has shown effectiveness in ICF applications.

Moment Closure for Kinetic Euations by Machine Learning

Ze-Yu Jin (金则宇)

Peking University

The kinetic equations are difficult to solve due to the high dimensionality of phase space. Hence moment methods are used to reduce the model. We develop several moment closures based on machine learning method. The training data are created by discrete-ordinates method. We also consider the maximum-entropy closure based on machine learning with self-refreshing to ensure hyperbolicity. Several numerical experiments are carried out to indicate accuracy of our model.

A Lattice Boltzmann Model for 3D Multiphase Flows with Moving Contact Line

Ji-Zu Huang (黄记祖)

Institute of Computational Mathematics and Scientific/Engineering, CAS

In this talk, we discuss an efficient lattice Boltzmann model for the two-phase moving contact line problem. The Navier-Stokes and Cahn-Hilliard equations are recovered from the lattice Boltzmann model. In order to describe the behavior of the contact line motion on the boundary, we incorporate the generalized Navier boundary condition by the non-equilibrium extrapolation method. The proposed method is easy to implement and retains the advantage of the standard lattice Boltzmann method. Several three dimensional numerical tests are carried out to verify the proposed method.

Multiscale Edge Basis for Helmholtz Equation with High Contrast

Yi-Xuan Wang (王逸轩)

Peking University

We propose a novel edge basis approach for Helmholtz equations, where traditionally the pollution effect is hard to avoid. Over sampling technique is invoked to provide a theoretical guarantee of exponential accuracy

The Subzonal Predictor-Corrector Algorithm for Hourglass Control

Zhi-Yuan Sun (孙致远)

Institute of Applied Physics and Computational Mathematics (IAPCM)

We proposed a subzonal predictor-corrector algorithm for the hourglass control in Lagrangian hydrodynamics. The algorithm can provide proper hourglass parameter in a wide range which is based on the prediction and the correction of the subzonal density. The parameter varies elementwise that producing high-quality mesh and reducing the spurious mesh motion. Some benchmark problems demonstrate the efficiency of the proposed algorithm.

粒子输运的多尺度动理学数值方法

孙文俊、江松、徐昆、谭爽

北京应用物理与计算数学研究所

中子、光子等粒子输运的计算是核武器、反应堆物理、惯性约束聚变等研究中不可缺少的重要课题。但粒子在不同介质区的传输行为有明显不同。在粒子自由程小的介质区，粒子具有扩散传播性质，而对粒子自由程大的介质区，粒子具有输运传播性质。对于粒子输运方程的计算，为了能够分辨相应的物理尺度，获得合理的计算结果，往往要求计算所用的空间网格步长与介质中粒子的平均自由程相当。因此对自由程小的介质区来说，所要求的空间计算网格步长就非常小，从而大大增加了计算量。因此，如何减少自由程小的介质区中的计算量是近年来粒子输运方程计算中一个重点研究领域。

针对粒子输运方程在自由程小介质区的计算效率低的难题。进一步发展了渐近保持的统一分子动理学 (UGKS) 算法的隐式算法、柱坐标辐射输运问题以及三维中子输运等应用问题的研究中。该计算格式具有多尺度特性，在自由程小介质区，收敛到宏观扩散极限方程的解，因此格式自动满足渐进保持特性；在自由程大介质区，收敛到自由传输解；而在过渡区，能够实现自然过渡。另外，UGKS 方法本身基于 FV 格式建立，容易和流体力学等物理过程耦合，设计辐射流体力学方程的渐近保持格式。

Direct Simulation Approach for Poisson-Boltzmann Equation Using Random Batch Method

Lei Li (李磊)

Shanghai Jiao Tong University

The Poisson-Boltzmann equation is a nonlinear elliptic equation that describes how electronic potential changes in the screening layer when charged particle or cell is immersed in an ion solution. It is the equilibrium state formed by many charged particles interacting with each other through Coulomb potentials. We propose to solve the Poisson Boltzmann equation effectively by simulating the charged (numerical or physical) particles directly using Random Batch Method proposed by Jin et al, which costs $O(N)$ time each iteration. This particle method is preferable in two aspects: in 3D space, directly solving the nonlinear elliptic equations in the unbounded domain may be difficult, especially when the domain is not in the rectangular or circular shapes; meanwhile, direct simulation may be preferred as people may be interested in the physical dynamics, and our approach is simple and effective in higher dimensions.

This is a joint work with Shi Jin, Jian-Guo Liu and Yijia Tang.

A Finite Volume Scheme for Savage-Hutter Equations on Unstructured Grids

Xiao-Hua Zhang (张小华)

China Three Gorges University

Landslides and debris flow are natural disasters that often occur in mountain areas. It is almost impossible to use engineering measures to control them completely, and numerical simulation can provide help for the study of these disasters. Here we focus on the Savage-Hutter model describing particle flow. A Godunov-type finite volume scheme on unstructured grids is proposed to numerically solve the Savage-Hutter equations in curvilinear coordinate. We show the direct observation that the model isn't a Galilean invariant system. At the cell boundary, the modified Harten-Lax-van Leer (HLL) approximate Riemann solver is adopted to calculate the numerical flux. The modified HLL flux is not troubled by the lack of Galilean invariance of the model and it is helpful to handle discontinuities at free interface. Rigidly the system is not always a hyperbolic system due to the dependence of flux on the velocity gradient. Even though, our numerical results still show quite good agreements to reference solutions. The simulations for granular avalanche flows with shock waves indicate that the scheme is applicable.

On Levermore's Five-Moment System

Wei-Ming Li (李蔚明)

Institute of Applied Physics and Computational Mathematics (IAPCM)

The Boltzmann equation describes particle motion and interaction on a scale between the hydrodynamics and the molecular dynamics, and has received widespread attention in recent years in fields such as rarefied gas dynamics, micro-flow and so on. Moment method is a model reduction strategy based on the kinetic equation, and at the same time it could recover the solution of the underlying kinetic equation itself. The moment method has widespread application and plays an important role in gas kinetic theory. This talk focuses on Levermore's maximum entropy-based moment method in gas kinetic theory. We discuss an accurate and efficient implementation of Levermore's five-moment maximum entropy system. Based on this implementation, we give a detailed study of the characteristic structure of the system. We also present analysis of the limiting behaviour of the Lagrange multipliers within the realizability region. These studies give us a deeper understanding of the maximum entropy moment model.

Efficient Numerical Approximations for the Phase-Field Modelling of Multi-Phase Flow with Moving Contact Lines

Hai-Jun Yu (于海军)

Institute of Computational Mathematics and Scientific/Engineering, CAS

Phase-field model is one of the major tools to deal with multi-phase flow and moving contact line problem. In this talk, we discuss some efficient energy stable numerical schemes for a phase-field model of moving contact line problem. The model is proposed by Qian et al in 2013, consists of incompressible Navier-Stokes equations with a generalized Navier boundary condition and Cahn-Hilliard equation with a dynamic contact line condition. We present several energy stable first order and second order time discretization schemes for the coupled nonlinear PDE system. In those schemes, pressure-correction projection methods are used to deal with the Navier-Stokes equations and stabilization skill and an energy quadratization strategy are used for the non-convex Ginzburg-Landau bulk potential and non-convex boundary surface energy. Efficient spectral-Galerkin spatial discretization for both 2d and 3d are implemented to verify the accuracy and efficiency of proposed schemes. Numerical results will be presented to demonstrate the accuracy and efficiency of the proposed schemes.

References:

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2. J. Shen, X. Yang and H. Yu, Efficient Energy Stable Numerical Schemes for a Phase Field Moving Contact Line Model, *Journal of Computational Physics* 284(2015):617--630.
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4. X. Yang and H. Yu, Efficient Second Order Unconditionally Stable Schemes for a Phase Field Moving Contact Line Model Using an Invariant Energy Quadraticization Approach, *SIAM Journal on Scientific Computing* 40(3)(2018):B889--B914.
5. X. Xu, Y. Di and H. Yu, Sharp-Interface Limits of a Phase-Field Model with a Generalized Navier Slip Boundary Condition for Moving Contact Lines, *Journal of Fluid Mechanics* 849(2018):805--833.

Numerical Simulation of Microflows Using Hermite Spectral Methods

Yan-Li Wang (王艳莉)

Beijing Computational Science and Research Center (CSRC)

We propose a Hermite spectral method for the spatially inhomogeneous Boltzmann equation. For the inverse-power-law model, we generalize a class of approximate quadratic collision operators defined in the normalized and dimensionless setting to operators for arbitrary distribution functions. An efficient algorithm with a fast transform is introduced to discretize the new collision operators. The method is tested for one- and two-dimensional benchmark microflow problems.

非平衡最优输运在机器学习中的应用

吴昊
清华大学

我们将首先回顾平衡和非平衡最优输运理论。然后介绍它们在自然语言处理和生成对抗网络等领域的应用。

Regularized 13-Moment Equations for Inverse-Power-Law Models

Zhen-Ning Cai (蔡振宁)

National University of Singapore

For general inverse-power-law models in the gas kinetic theory, we derive the regularized 13-moment equations based on the Boltzmann equation with linearized collision operators. The derivation is based on the order-of-magnitude method, and it includes three steps. First, we write down Grad's moment equations up to 20th order. Second, we examine the magnitude of every moment in the equations, and determine which terms are to be preserved in the final system. Third, by asymptotic analysis, we express all terms with the first 13 moments and their derivatives. The resulting model contains at most second-order derivatives, and it involves all information of the Chapman-Enskog expansion up to third order (super-Burnett accuracy). It is numerically verified that the model has better accuracy than Navier-Stokes equations and Grad's 13-moment equations

High-Order Gas-Kinetic Scheme for Euler and Navier-Stokes Equations

Liang Pan (潘亮)

Beijing Normal University

The high-order gas-kinetic scheme (HGKS) has achieved success in simulating compressible flows. Different from the numerical methods based on the Riemann flux, GKS presents a gas evolution process from kinetic scale to hydrodynamic scale, where both inviscid and viscous fluxes can be recovered from the time-dependent and multi-dimensional gas distribution function at a cell interface. Recently, based on the time-dependent flux function, a two-stage fourth-order method was developed for Lax-Wendroff type flow solvers, particularly applied for the hyperbolic conservation laws. Under the multi-stage multi-derivative framework, a reliable two-stage fourth-order GKS has been developed, and even higher-order of accuracy can be achieved. In comparison with the formal third-order GKS, the current fourth-order method not only improves the accuracy of the scheme, but also reduces the complexity of the gas-kinetic flux solver greatly. More importantly, this scheme is as robust as the second-order scheme and works perfectly from subsonic to hypersonic flows. With the two-stage framework, the HGKS with moving-meshes and HGKS in the curvilinear coordinates are developed as well. Numerical results validate the outstanding reliability and applicability of the scheme for three-dimensional flows, such as the direct numerical simulation for supersonic isotropic turbulence.

基于微分变换的 ADER-DG 方法

李刚

青岛大学数学与统计学院

浅水波方程可以保持定常解。离散状态下，能保持该定常解的方法是非常受欢迎的，因为其可以利用较粗的网格来捕捉较小的摄动，以节约计算成本。这样的方法被称为 well-balanced 方法。这里，针对保持静水定常解的浅水波方程，我们构造了 well-balanced ADER-DG 方法。与 Runge-Kutta DG 方法相比较，该方法是全离散的、单级的，在时间空间上能够达到任意高阶精度，且存储量小。同传统的 ADER 方法相比较，该方法基于微分变换策略将时间导数通过空间导数来表示，来达到时间的高阶精度，从而避免了复杂的 Cauchy-Kowalewski 步骤，程序编写更加高效和紧致。严格的数值分析以及广泛的数值试验均表明该方法能保持定常解、具有高阶精度、保持高分辨率。

关键词 浅水波方程； ADER-DG 方法； 微分变换； 高阶精度

Distributed-Memory Hierarchical Interpolative Factorization

Ying-Zhou Li (李颖洲)

Duke University

The hierarchical interpolative factorization (HIF) offers an efficient way for solving or preconditioning elliptic partial differential equations. By exploiting locality and low-rank properties of the operators, the HIF achieves quasi-linear complexity for factorizing the discrete positive definite elliptic operator and linear complexity for solving the associated linear system. In this paper, the distributed-memory HIF (DHIF) is introduced as a parallel and distributed-memory implementation of the HIF. The DHIF organizes the processes in a hierarchical structure and keep the communication as local as possible. The computation complexity is $O(N \log N / P)$ and $O(N / P)$ for constructing and applying the DHIF, respectively, where N is the size of the problem and P is the number of processes. The communication complexity is $O(P^{1/2} (\log P)^3 \alpha + O(N^{2/3} / P^{1/2})) \beta$ where α is the latency and β is the inverse bandwidth. Extensive numerical examples are performed on the NERSC Edison system with up to 8192 processes. The numerical results agree with the complexity analysis and demonstrate the efficiency and scalability of the DHIF.

三维超高精度间断有限元方法若干研究进展

李书杰

北京计算科学研究中心

传统的高阶精度方法应用到实际三维计算流体力学（CFD）问题中存在计算量大，稳定性弱等一系列问题。其中，高阶间断有限元方法虽然优点突出，但是在三维问题中计算量随空间精度立方增长，配合传统的时间推进格式难以实用化。采用显式方法受 CFL 条件的约束，在大拉伸比的密网格上时间步长严重受限，导致海量的时间推进步。而常用的隐式方法如 Backward Euler, BDF2 等虽不受 CFL 条件限制，但是存在精度效率比较低等若干问题。在本次报告中，我们将在介绍本人在三维并行高精度算法发展及求解器开发上所做到的一整套工作：介绍如何克服三维高阶方法计算精度，效率，鲁棒性实现三维并行自适应计算软件 HA3D；介绍三维超大规模混合曲面网格的生成工作；介绍作者在发展具有高精度效率比特征的指数时间推进格式 PCEXP 上所做的工作。该格式不受 CFL 条件限制，对稳态问题具有很高的收敛率，对非稳态问题比经典的隐式 BDF2 在绝对时间误差，精度效率上均高出了一个量级，并且适用于各种强刚性方程组的求解及三维高阶求解器效率加强。