实际问题驱动的可计算建模与随机模拟

国际研讨会

会议手册

2022 年 12 月 17-18 日

数学科学中心 & 数学与物理学院

中国地质大学

湖北 武汉

为了探讨可计算建模与随机模拟相关领域的最新研究成果和学术发展动态，促进学术交流与合作，中国地质大学（武汉）于 2022 年 12 月 17-18 日通过腾讯会议平台举行“实际问题驱动的可计算建模与随机模拟” 国际研讨会，主题涵盖计算系统生物、计算神经科学、高性能科学计算、可计算建模、随机数值分析等。会议以加强可计算建模与随机模拟及相关领域的学术交流为主旨，展示和介绍理论及应用方面的最新研究成果和进展。

会议方式：腾讯会议(259-298-922)

会议链接：https://meeting.tencent.com/dm/RBbpPTenRb2z

特邀专家名单（以姓氏拼音为序）：

序号	名称	单位	序号	名称	单位
1	柴振华	华中科技大学	13	施保昌	华中科技大学
2	邓伟华	兰州大学	14	孙桂全	中北大学
3	胡耀忠	University of Alberta	15	汤华中	北京大学 南昌航空大学
4	黄乘明	华中科技大学	16	汤　涛	北京师范大学-香港浸会大学联合国际学院
5	黄云清	湘潭大学	17	陶　实	东莞理工学院
6	黄子罡	西安交通大学	18	吴付科	华中科技大学
7	江　松	北京应用物理与计算数学研究所	19	谢资清	湖南师范大学
8	焦　锋	广州大学	20	杨　银	湘潭大学
9	李东方	华中科技大学	21	杨志坚	武汉大学
10	刘　锐	华南理工大学	22	俞连春	兰州大学
11	刘阳晖	City University of New York	23	张诚坚	华中科技大学
12	罗　康	哈尔滨工业大学	24	张　磊	北京大学北京国际数学研究中心

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中国地质大学（武汉）数学与物理学院
2022 年 12 月

中国地质大学（武汉）数学与物理学院

数学与物理学院前身为北京地质学院的数学教研室和物理教研室， 2005 年成立数学与物理学院。1977 年开始招收数学专业本科生，1987 年开始招收物理专业本科生，2001 年开始招收硕士研究生，2011 年开始招收少数民族预科生，2021 年开始招收博士研究生，实现“预-本-硕-博”各层次类型的人才培养体系。2020 年《数学学科特区建设实施方案（2020-2023）》正式实施，并成立了数学科学中心，学院现已发展成为培养数理学科高级复合型人才、从事数理基础理论与应用的教学研究型学院。

学院现有数学与应用数学系、物理系、信息与计算科学系、大学数学教学部、大学物理教学部和物理实验中心 6 个系部。教职员工 125 人，其中教授 24 人、副教授 58 人，博士生导师 19 人；2021 科睿唯安全球高被引科学家 1 人，2021 中国高被引学者 2 人，有湖北省教学名师、湖北省有突出贡献的中青年专家等各类省部级高层次人才 9 人。

学院现有在校本科生 800 余人、硕士研究生 320 人，博士研究生 17 人。数学和物理学 2 个一级学科，数学与应用数学、物理学、信息与计算科学 3 个本科专业，数学、物理学、应用统计学、材料和化工 4 个硕士点，现代数学与控制理论 1 个二级博士点。学院开设“数学与应用数学专业菁英班”，探索拔尖创新人才培养新模式，加强“大学生数学建模创新基地”和“学生科技创新实验基地”建设。5 年以来，我院学生获得国家级大学生创新创业训练项目 22 项，学生以第一作者发表三大检索论文 62 篇，有 18 名硕士毕业生选择在国内外知名高校攻读博士学位。

近年来，我院新增国家自然科学基金 48 项，新增横向项目 39 项，新增科研经费 2445.4 万；我院教师以第一作者/通讯作者发表国际 SCI 期刊论文 587 篇，其中 T1 论文 96 篇，T2 论文 208 篇，高被引论文 18 篇；举办学院“数理论坛”学术交流专题系列讲座 303 期，含数学科学中心系列专题讲座 93 场，举办“名家论坛”18 期。举办了如北京谱仪 III2021 冬季合作组国际会议，2021 年非线性偏微分方程理论学术会议等国际国内学术会议 9 场。

数学与应用数学专业获国家一流专业建设项目；大学物理课程思政案例获教育部大学物理课程教学指导委员会资助；信息与计算科学专业课程组获评湖北高校省级优秀基层教学组织；《高等数学》线上课程获湖北省线上一流课程建设，《大学物理》（力学、电磁学）课程获湖北省线上一流课程建设；《线性代数》课程获湖北省线下一流课程建设。

2019 年，121171 团支部荣获湖北省百生讲坛“活力团支部”特等奖，2020 年 121171 团支部获评湖北省“五四红旗团支部”。

实际问题驱动的可计算建模与随机模拟国际研讨会日程安排

12 月 17 日（上午） 腾讯会议 ID：259-298-922

时间	主持人	开幕式 （一）、中国地质大学（武汉）校长、中国科学院院士王焰新致辞 （二）、中国科学院院士江松致辞
8:10-8:30	郭上江	
主持人：黄云清		
时间	报告人	报告题目
8:30-9:10	谢资清	A review on several monotonely descent local minimax methods for finding saddle points and an application
9:10-9:50	杨志坚	Absorbing boundary and interface conditions for MD
休息（9:50-10:00）		
主持人：易　鸣		
时间	报告人	报告题目
10:00-10:40	胡耀忠	Mean square stability of stochastic theta method for stochastic differential equations driven by fractional Brownian motion
10:40-11:20	刘阳晖	Statistical inference for rough volatility
11:20-12:00	吴付科	Approximation of invariant measures of a class of backward Euler-Maruyama scheme for stochastic functional differential equations

12 月 17 日（下午） 腾讯会议 ID：259-298-922

主持人：朱　媛		
时间	报告人	报告题目
14:00-14:40	张　磊	Network design principle for biological dual functions
14:40-15:20	孙桂全	Pattern dynamics and optimal control of networked reaction-diffusion systems
15:20-16:00	刘　锐	生物分子网络动态差异的量化与分析算法
休息（16:00-16:10）		
主持人：鹿露露		
时间	报告人	报告题目
16:10-16:50	焦　锋	What can we learn when fitting complex gene expression models to a simple telegraph model?
16:50-17:30	黄子罡	神经调质系统的动力学及其对类脑智能的启发
17:30-18:10	俞连春	大尺度脑网络上的功能优化原则及其在脑疾病诊疗中的应用

12 月 18 日（上午） 腾讯会议 ID：259-298-922

主持人：江　松		
时间	报告人	报告题目
8:30-9:10	汤华中	狭义相对论流体力学方程组的高阶结构保持格式
9:10-9:50	汤　涛	偏微分方程深度学习算法的自适应采样
休息（9:50-10:00）		
主持人：胡　鹏		
时间	报告人	报告题目
10:00-10:40	邓伟华	反常与非遍历多尺度模型、分析及算法
10:40-11:20	杨　银	Compatible L^2 norm convergence of the variable-step L1 energy stable scheme for the time-fractional MBE model
11:20-12:00	黄乘明	Nonpolynomial collocation for weakly singular Volterra integro-differential equations

12 月 18 日（下午） 腾讯会议 ID：259-298-922

主持人：李　民		
时间	报告人	报告题目
14:00-14:40	张诚坚	A class of one-parameter ADI methods for 2D wave equations with discrete and distributed time-variable delays
14:40-15:20	柴振华	Some recent progress on the phase-field-based lattice Boltzmann method for multiphase flows
15:20-16:00	李东方	Implicit-explicit relaxation Runge-Kutta methods: construction, analysis and applications
休息（16:00-16:10）		
主持人：汪　垒		
时间	报告人	报告题目
16:10-16:50	施保昌	Mesoscopic numerical methods for partial differential equations: modeling, analysis, and elements
16:50-17:30	罗　康	Computational technology in flow instability and heat transfer enhancement in electroconvection
17:30-18:10	陶　实	Immersed boundary-discrete unified gas kinetic scheme for complex multi-scale fluid-solid flows

报告题目与摘要(以姓氏拼音为序)

实际问题驱动的可计算建模与随机模拟国际研讨会

2022. 12. 17-12. 18

Some recent progress on the phase-field-based lattice Boltzmann method for multiphase flows

柴振华

华中科技大学

Multiphase flow is not only ubiquitous in nature, industry and everyday life, but also a profound problem of interest to a wide range of engineering, geophysical, and environmental applications. In this talk, we will first give a brief introduction to the phase-field theory for the multiphase flows, including the Cahn-Hilliard equation/conservative Allen-Cahn equations for phase field and the Navier-Stokes equations for flow field. Then we present some fundamentals of the mesoscopic lattice Boltzmann method (LBM), and mainly focus on how to develop the phase-field-based lattice Boltzmann method (PF-LBM) for multiphase flows. Finally, some physical problems are adopted to test the robustness of the PF-LBM in the study of the complex multiphase flows.

反常与非遍历多尺度模型、分析及算法

邓伟华

兰州大学

反常与非遍历现象在自然界中无处不在. 随着实验技术的发展，各种新的实验现象仍不断涌现. 为解释现象/揭示机理，我们建立微观模型（随机过程），对微观模型作随机分析和统计分析. 同时，我们导出一些宏观统计量（如，粒子位置、泛函、逃逸概率、首次通过时间等）的概率分布满足的宏观方程，进而研究方程解的正则性及方程的数值计算方法.

Mean square stability of stochastic theta method for stochastic differential equations driven by fractional Brownian motion

胡耀忠
University of Alberta

I will present a result on the mean square stability of the solution and its stochastic theta scheme for the linear stochastic differential equations drive by fractional Brownian motion with Hurst parameter 1/2<H<1.

Nonpolynomial collocation for weakly singular Volterra integro-differential equations

黄乘明
华中科技大学

In this talk, we propose an hp-version fractional collocation method for solving second kind Volterra integro-differential equations with weakly singular kernels. We derive hp-version error estimates in a weighted H1-norm for the method on arbitrary meshes. The results show that for any given mesh partition, exponential rates of convergence can be achieved for certain weakly singular solutions by linearly increasing the degrees of piecewise fractional polynomials. The results also imply that in the case of uniform mesh, the method has no (h-version) order barrier for weakly singular solutions, which is different from classical polynomial collocation methods. This talk is based on the joint work with Dr. Zheng Ma.

神经调质系统的动力学及其对类脑智能的启发

黄子罡
西安交通大学

神经调质系统对生物脑正常功能的维持至关重要，能够促进其灵活应对复杂环境，实现趋利避害。对神经调质系统的动力学建模不仅能够帮助理解其工作机制，还能够有效地支持基于计算的神经功能障碍临床研究，以及基于脉冲神经网络的全新的类脑智能研究。本报告围绕神经调质系统如多巴胺、去甲肾上腺素、乙酰胆碱系统介绍从机制到功能的动力学建模进展，概括神经调质系统在感知、认知、记忆、决策等功能实现中的重要作用，包括去甲肾上腺素系统实现注意力调控、辅助应激决策，多巴胺系统提升信息处理的信噪比，以及乙酰胆碱系统提升感知效能、调节记忆存取切换等功能。并概述神经调质系统的动力学模型在类脑智能领域的重要应用前景。

What can we learn when fitting complex gene expression models to a simple telegraph model?

焦　锋
广州大学

Gene expression is a stochastic process supported by fluctuations of mRNA and protein copy numbers in single cells within an isogenic cell population. One of classical stochastic gene expression models is telegraph model. We reveal three uniform rules when fitting complex gene expression models to the simple telegraph model. These rules provide theoretical basis for using extensive results of telegraph model to analyze complex models on distribution modality, parameter estimation and gene regulation scenarios.

Implicit-explicit relaxation Runge-Kutta methods: construction, analysis and applications

李东方
华中科技大学

Spatial discretizations of time-dependent partial differential equations usually result in a large system of semi-linear and stiff ordinary differential equations. Taking the structures into account, we develop a family of linearly implicit and high order accurate schemes for the time discretization, using the idea of implicit-explicit Runge-Kutta methods and the relaxation techniques. The proposed schemes are monotonicity-preserving/conservative for the original problems, while the previous linearized methods are usually not. We also discuss the linear stability and strong stability preserving (SSP) property of the new relaxation methods. Numerical experiments on several typical models are presented to confirm the effectiveness of the proposed methods.

生物分子网络动态差异的量化与分析算法

刘　锐
华南理工大学

很多生物系统的动态发展过程中都存在状态临界改变现象，例如疾病，在离突变点较远时，病情不明显；而到达临界点时，病情在很短的时间内从稳定期突然恶化而成为重病期。如何基于高维生物医学数据，找到可用于识别生物系统状态改变临界期的标记物，对包括疾病的早期诊断等课题具有重要意义。围绕生物系统临界点预警这一课题，基于动态网络标志物理论，我们针对不同的数据情况

开发了适用的生物分子网络动态差异的量化与分析算法，这些算法在许多实际数据上得到了成功的应用，报告主要就将介绍这些算法及其具体应用。

Statistical inference for rough volatility

Yanghui Liu
City University of New York, Baruch College

In recent years, there has been substantive empirical evidence that volatility is “rough”. In other words, the local behavior of volatility is much more irregular than semi-martingales and resembles that of a fractional Brownian motion with Hurst parameter $H < 0.5$. An intriguing question is then whether we can estimate the roughness "indicator” H, and if so with which accuracy? In this talk, we derive a consistent and asymptotically mixed normal estimator of H based on high-frequency price observations. In contrast to previous works, we work in a nonparametric setting and do not assume a priori relationship between volatility estimators and true volatility. Our estimator attains a rate of convergence $1/(4H+2)$, which is known to be optimal in a minimax sense in parametric rough volatility models. This talk is based on a joint work with Chong, Hoffmann, Rosenbaum and Szymanski.

Computational technology in flow instability and heat transfer enhancement in electroconvection

罗　康
哈尔滨工业大学

The flow motion driven by the Coulomb force exerted by the electric field on free space charges is fundamental problems in Electro-Hydro-Dynamics (EHD). Such flow plays an important role in a wide range of applications in industrial processes, such as EHD pumps, EHD turbulent mixer and electrostatic precipitators. In general, flow control and heat transfer enhancement with electricity-based techniques has some unique advantages, such as no moving mechanical parts, rapid and smart control, and low power consumption and noise. In this talk, I will review our last five years numerical works on EHD of our group, including the theoretical analysis of rich linear and nonlinear instabilities in EHD, lattice Boltzmann simulation of EHD, Cellular flow patterns and their subcritical bifurcation phenomena of EHD, solid-liquid and solid-gas two phase EHD problems, electro-thermo-convection in non-Newtonian dielectric liquid.

Mesoscopic numerical methods for partial differential equations: modeling, analysis, and elements

施保昌
华中科技大学

Transport processes such as flow, heat and mass transfer are common basic problems in many fields including energy, environment and chemical industry. They are widely used in oil and gas exploitation, greenhouse gas storage and utilization, fuel cell design and optimization, microfluidics, and other fields. The basic mathematical models for describing such problems are Navier-Stokes equations (NSEs) and convection-diffusion equation (CDE). However, this kind of problem often has the multi-scale, multi-physics and nonlinear characteristics, and its transport mechanism is very complex. Both the micro molecular simulation method and the macro traditional numerical method are limited in studying this kind of problem. The Mesoscopic Numerical Method (MNM) based on the kinetic theory provides an advanced and feasible solution for the study of these complex problems. MNM is a bottom-up modeling method, which has solid physical basis and computational advantages. It can directly describe the interaction between fluid and fluid (different phases and different components) and between fluid and solid, and is easy to treat various complex boundaries. It is suitable for simulating multiphase/multicomponent flows, fluid flows in porous media, and hemodynamics, etc. Its algorithm is simple, universal, efficient, and has natural parallelism, which makes it suitable for running on GPU and massively parallel computers.

This talk will focus on the lattice Boltzmann method (LBM), a popular MNM for solving NSEs and CDE and their coupled systems, and introduce the modeling principle, basic model, basic theory and key elements of LBM in combination with some works of our group in recent years. The main contents can be summarized as follows: Two objects, one basis, two distributions, two spaces, two paths, two analyses. The partial differential equations involved mainly include: Navier-Stokes Equations, nonlinear Schrödinger equations, complex Ginzburg-Landau equation, nonlinear Dirac equation, generalized Zakharov system, Burgers-Fisher equation, nonlinear heat conduction equation, Cahn-Hilliard equation, reaction-diffusion system, etc.

Pattern dynamics and optimal control of networked reaction-diffusion systems

孙桂全
中北大学

Pattern dynamics is one of the main research contents of nonlinear dynamics, which is widely used in mathematics, physics, chemistry, biology, ecology, computer science and other fields. At present, the research on the pattern of reaction-diffusion systems

focuses on the reaction-diffusion equations based on standard Brownian motion in continuous space. However, the discreteness of population distribution, the heterogeneity of diffusion, and the large scale and long distance do not conform to the standard Brownian motion, so it is not suitable to use reaction diffusion equations to model such reaction diffusion processes. Complex networks usually have the characteristics of small world and heterogeneity. Networked reaction-diffusion system makes it possible to describe the reaction-diffusion process more accurately. This talk first discusses Turing pattern of network reaction diffusion system, and gives the qualitative and quantitative relationship between network average degree and pattern structure. Then, based on the differential equation optimal control theory, the optimal control strategy of pattern structure is discussed.

狭义相对论流体力学方程组的高阶结构保持格式

汤华中
北京大学、南昌航空大学

将简要介绍两种用于狭义相对论流体力学(RHD)的高精度保结构的有限差分格式。第一种是保物理约束(PCP)格式：能保持静止质量密度、压力的正性和流体速度的界；基于局部 Lax-Friedrichs 分裂、WENO 重构、PCP 通量限制器和高阶保强稳定性的时间离散。发展格式的关键是：证明可容许状态集的凸性及其它性质，和发现关于守恒向量的一个凹函数。第二种是熵稳定(ES)格式，其半离散形式满足熵不等式。关键点是从技术上构造满足所选的凸熵对的半离散熵等式的半离散二阶精确 EC 格式的熵守恒(EC)通量。一旦得到 EC 通量，就可以添加耗散项给出满足半离散熵不等式的半离散 ES 格式。对缩放后的熵变量进行 WENO 重构并采用之前的时间离散，则可以获得全离散的高阶“ES”格式。数值实验论证了所提出格式的性能。此外，我们还将简要回顾关于狭义 RHD 的保结构格式的其它相关工作。本报告拟通过上述工作的介绍展示流体力学中的一些数学。

偏微分方程深度学习算法的自适应采样

汤　涛
北京师范大学-香港浸会大学联合国际学院

自适应计算在科学与工程计算中长期扮演着重要角色。本次报告将首先对自适应计算做一个简单的介绍，包括网格自适应，时间自适应，参数空间自适应等。随后我们将着重讨论深度学习求解偏微分方程的自适应采样问题。

Immersed boundary-discrete unified gas kinetic scheme for complex multi-scale fluid-solid flows

陶　实
东莞理工学院

Pulverized coal combustion, nano particle preparation, haze, etc. are fluid-solid two-phase flows that exist widely in nature and energy-chemical fields. In recent years, remarkable scale effects in those fluid-solid systems, for example interfacial velocity slip, temperature jump, thermal creep flow, abnormal Fourier heat transfer and other phenomena of micro/nano particles, as well as complex micro gas-solid interaction, have attracted extensive attention, and also brought great challenges to understanding such problems. Starting from Boltzmann equation, this report introduces the application of a typical mesoscopic method lattice Boltzmann (LBM) in micro scale fluid-solid two-phase flows, and then presents the development of immersed boundary-discrete unified gas kinetic scheme (DUGKS, a new multi-scale mesoscopic numerical method) in handling complex fluid-solid two-phase flow. The results indicate the initially establishment of a direct numerical simulation tool for complex multi-scale fluid-solid flows.

Approximation of invariant measures of a class of backward Euler-Maruyama scheme for stochastic functional differential equations

吴付科
华中科技大学

This paper is concerned with the approximations of invariant probability measures for stochastic functional differential equations (SFDEs) using a backward Euler-Maruyama (BEM) scheme under one-sided Lipschitz condition on the drift coefficient. Firstly, the strong convergence of ``segment process" associated with the BEM scheme is established on finite time interval [0,T] with the help of a Forward-Backward Euler-Maruyama (FBEM) scheme. Then, it is demonstrated that the segment process for BEM scheme is a Markov process and the corresponding discrete-time semigroup admits a unique numerical invariant probability measure. Finally, based on the strong convergence result, we reveal that the numerical invariant probability measure converges in the Wasserstein distance to the underlying one.

A review on several monotonely descent local minimax methods for finding saddle points and an application

谢资清
湖南师范大学

In this talk，we will introduce three monotonely descent local minimax methods for finding saddle points of PDES based on different search rules. The feasibility and gobal convergence wil be verified. Finally as an application, the LMM is used to compute the multiple solutions of a singularly perturbed semi-linear Neumann problems and the so-called critical perturbed value is found and then proved strictly.

Compatible L^2 norm convergence of the variable-step L1 energy stable scheme for the time-fractional MBE model

杨　银
湘潭大学

The convergence of the variable-step L1 schemes are studied for the time-fractional molecular beam epitaxy (MBE) model with or without slope selection. By taking advantage of the convex splitting of nonlinear bulk, a novel asymptotically compatible L^2 norm error estimates of the variable-step L1 schemes are established under a convergence-solvability-stability (CSS)-consistent time-step constraint. Just as the backward Euler scheme can maintain the physical properties of the MBE equation, the variable-step L1 scheme can also preserve the corresponding properties of the time-fractional MBE model, including the volume conservation, variational energy dissipation law and L^2 norm boundedness. Numerical experiments are presented to support our theoretical results.

Absorbing boundary and interface conditions for MD

杨志坚
武汉大学

In this talk, I will illustrate the model reduction techniques through typical examples to address the issues of boundary and interface conditions between different domains or models. I will introduce an efficient and easy to implement boundary condition for molecular dynamics simulations.

大尺度脑网络上的功能优化原则及其在脑疾病诊疗中的应用

俞连春
兰州大学

脑疾病已成为严重影响人类健康的重要疾病，目前亟需针对脑疾病的精准医疗手段。统计物理与复杂系统的大量研究揭示了系统利用临界性和异质性实现功能优化的原则。基于这一原则的脑影像数据分析和数字孪生脑技术在脑疾病精准医疗方面有广阔的应用前景。本次报告我将介绍课题组围绕大尺度脑网络利用临界性和异质性实现脑网络功能和认知能力优化方面的若干工作进展，并结合目前脑疾病病理学、临床诊断以及临床干预的最新进展，讨论脑网络的功能优化理论在未来脑疾病精准医疗中的应用。

A class of one-parameter ADI methods for 2D wave equations with discrete and distributed time-variable delays

张诚坚
华中科技大学

For solving the IBVPs of 2D wave equations with discrete and distributed time-variable delays, in the present talk, we first construct a class of basic one-parameter methods. In order to raise the computational efficiency of this class methods, we remold the methods as one-parameter alternating direction implicit (ADI) methods. Under the suitable conditions, the remolded methods are proved to be stable and convergent of second order in both of time and space. With several numerical experiments, the computational effectiveness and theoretical exactness of the methods are confirmed. Moreover, it is illustrated that the proposed one-parameter ADI method has the better advantage in computational efficiency than the basic one-parameter methods.

Network design principle for biological dual functions

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Biological systems are capable of performing complex functions with a remarkable degree of accuracy, reliability, and robustness. We postulate that behind the celebrated diversity of the biological world lie “universal” principles that emerge at various levels of organization. For example, many signaling systems execute adaptation under noisy circumstances, and transcriptional regulatory networks can robustly achieve accurate oscillation in the presence of biological noise. In this talk, we will explore two dual functions: one is adaptation and noise attenuation, and the other one is oscillation and noise attenuation. By analyzing and computing three-node or four-node networks, we reveal essential network design principles for biological dual functions, which can be utilized in synthetic biology.