北京师范大学珠海校区、上海财经大学联合主办

科学计算系列报告(2)
谱方法及相关应用进展

腾讯会议：白天 681-348-011　晚上 869-777-251　　密　　码：1119

开幕致辞：08:50-09:00		
11 月 19 日 上午报告　　时间：9:00-11:15　　腾讯会议：681-348-011		
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9:45-10:30	王海永	Error localization of spectral approximations
10:30-11:15	侯典明	A linear maximum bound principle-preserving BDF2 scheme for the Allen-Cahn equation with a general mobility
11 月 19 日 下午报告　　时间：14:00-16:15　　腾讯会议：681-348-011		
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11 月 19 日 晚上报告　　时间：19:00-21:15　　腾讯会议：869-777-251		
19:00-19:45	安静	A class of efficient spectral methods and error analysis for nonlinear Hamiltonian systems
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Convergence analysis of the Multi-scale Deep Neural Network (MscaleDNN)

Bo Wang (汪波)

湖南师范大学

In this talk, we will present a numerical analysis for the convergence of the machine learning algorithm with Multi-scale neural network. We prove that the training process for some one layer neural networks with gradient descent optimization algorithm tends to diffusion process in the Fourier spectral domain as the learning rate goes to zero. Consequently, the multi-scale neural network is shown to have diffusion coefficients covering a wider range of frequency compared to fully connected neural network.

报告人简介：汪波，湖南师范大学数学与统计学院教授，国家高层次青年人才计划入选者。2011 年在湖南师范大学获计算数学博士学位。2011 年至 2013 年在新加坡国立大学从事博士后研究工作。主要研究方向包括超材料中电磁场计算的 DG 方法、波散射问题高精度方法、界面问题 HDG 方法、多层媒质中的快速多极法等。在《SIAM J. Sci. Comp.》、《SIAM J. Numer. Anal.》、《Comput. Methods Appl. Mech. Engrg.》、《SIAM J. Appl. Math.》等国内外著名刊物发表论文 20 多篇，主持国家基金 4 项。

Error localization of spectral approximations

Haiyong Wang (王海永)

华中科技大学数学与统计学院

Spectral approximations are widely used in many branches of scientific computing such as Gauss-type quadrature, rootfinding, matrix functions and spectral methods for ODEs and PDEs. For functions with a singularity, it has been observed by Nick Trefethen in 2011 that the pointwise error of Chebyshev interpolants has an error localization phenomenon, that is, the error at each point away from the singularity is much smaller than the error at the singularity. In this talk, I shall present a theoretical justification for this phenomenon and clarify the latent mathematical theory.

报告人简介：王海永，2001-2010 年于中南大学数学与统计学院本硕博连读，2011-2012 年在比利时鲁汶大学（荷语）从事博士后研究，2013 年进入华中科技大学数学与统计学院工作至今。主要从事谱方法、高振荡问题高效数值方法等问题的研究，在 SIAM J. Numer. Anal.、Numer. Math.、Math. Comp.、IMA J. Numer. Anal.等计算数学知名期刊发表论文二十余篇。

A linear maximum bound principle-preserving BDF2 scheme for the Allen-Cahn equation with a general mobility

Dianming Hou (侯典明)

江苏师范大学数学与统计学院

In this talk, we present and analyze a linear second-order numerical method for solving the Allen-Cahn equation with a general mobility. The proposed fully-discrete scheme is carefully constructed based on the combination of first and second-order backward differentiation formulas with variable time steps for temporal approximation and the central finite difference for spatial discretization. The discrete maximum bound principle is proved of the proposed scheme by using the kernel recombination technique under certain mild constraints on the time steps and the ratios of adjacent time step sizes. Furthermore, we rigorously derive the discrete H^{1} error estimate and energy stability for the classic constant mobility case and the L^{∞} error estimate for the general mobility case. Various numerical experiments are also presented to validate the theoretical results and demonstrate the performance of the proposed method with a time adaptive strategy.

报告人简介：侯典明，男，江苏师范大学副教授，硕士生导师。2013 年本科毕业于新疆大学数学与系统科学学院；2019 年博士毕业于厦门大学数学科学学院，计算数学专业，师从许传炬教授；2021 年 8 月至今，香港理工大学应用数学系博士后，师从乔中华教授。主要研究领域为偏微分方程数值解与计算流体力学，在 SIAM J. Sci. Comp., J. Sci. Comp., J.Comp. Phys.等计算数学著名期刊上发表学术论文十余篇。现主持国家和江苏省自然科学青年基金各一项。

A unified fast method for the fractional operators

Fanhai Zeng(曾凡海)

山东大学

Time-dependent fractional partial differential equations typically require huge amounts of memory and computational time, especially for long-time integration, which taxes computational resources heavily for high-dimensional problems. Here, we first analyze existing numerical methods of sum-of-exponentials for approximating the kernel function in constant-order fractional operators, and identify the current pitfalls of such methods. In order to overcome the pitfalls, an improved sum-of-exponentials is developed and verified. We also present several sum-of-exponentials for the approximation of the kernel function in variable-order fractional operators. Subsequently, based on the sum-of-exponentials, we propose a unified framework for fast time-stepping methods for fractional integral and derivative operators of constant and variable orders. We test the fast method based on several benchmark problems, including fractional initial value problems, the time-fractional Allen–Cahn equation in two and three spatial dimensions, and the

Schrodinger equation with nonreflecting boundary conditions, demonstrating the efficiency and robustness of the proposed method. The convergence analysis of the fast method is also displayed. The results show that the present fast method significantly reduces the storage and computational cost especially for longtime integration problems

报告人简介：曾凡海，山东大学数学学院教授、博士生导师。2005 年在西北工业大学数学系获学士学位，2014 年在上海大学数学系获得博士学位。2014 年至 2020 年分别在美国布朗大学、澳大利亚昆士兰科技大学和新加坡国立大学做博士后研究。2020 年获得“山东大学杰出中青年学者”称号。2015 年合作出版专著 1 部、在 SINUM, SISC, JSC, JCP 和 CMAME 等国际期刊上发表论文 30 余篇，SCIE 他引 1000 余次。

Numerical method for some nonlocal phase field models

Jiangxing Wang (王疆兴)
湖南师范大学

In this talk, we first construct an arbitrarily high order energy stable scheme for solving the nonlocal Cahn-Hilliard equation based on IEQ approach and the Runge-Kutta method. We prove that the proposed scheme is unconditional energy stable and can preserve the energy dissipation law. Then, by using the idea of SAV and “zero-energy-contribution” approach, a highly efficient fully-decoupled, linear, second-order and unconditionally energy stable scheme for the nonlocal two-phase incompressible flows is developed. At each time step, we only needs to solve a few poisson-type equations with constant coefficients. The unconditional energy stability of the scheme is proved. Finally, some numerical simulations in 2D and 3D are carried out to demonstrate the accuracy, stability, and effectiveness of the scheme.

报告人简介：

Polynomial approximation of singular functions in new fractional spaces

Wenjie Liu (刘文杰)
哈尔滨工业大学

In this talk, we introduce a new theoretical framework built upon fractional spaces for optimal error estimates of orthogonal polynomial approximations to functions with limited regularity. It naturally arises from exact representations of orthogonal polynomial expansion coefficients. Here, the essential pieces of the puzzle for the error analysis include (i) fractional integration by parts (under the weakest possible conditions); (ii) fractional taylor formula; (iii) generalised Gegenbauer functions of fractional degree (GGF-Fs): a new family of special functions with

notable fractional calculus properties, and (iv) asymptotic formulas or uniform upper bounds of GGF-Fs. Finally we introduce the hypothesis of Babuska and Hakula.

报告人简介：刘文杰，现为哈尔滨工业大学数学学院副教授。曾经为新加坡南洋理工大学的 Research Fellow。主要研究谱方法及其应用、多项式逼近理论、奇异性问题的 hp 有限元法等。获得中国博士后科学基金面上项目（一等资助）、国家自然科学基金青年项目和面上项目的资助。在 Mathematics of Computation、Journal of Approximation Theory、Journal of Computational Physics 等国际著名期刊发表 SCI 论文 19 篇。

A class of efficient spectral methods and error analysis for nonlinear Hamiltonian systems

Jing An(安静)

贵州师范大学

We investigate efficient numerical methods for nonlinear Hamiltonian systems. Three polynomial spectral methods (including spectral Galerkin, Petrov-Galerkin, and collocation methods) coupled with domain decomposition are presented and analyzed. Our main results include the energy and symplectic structure-preserving properties and error estimates. We prove that the spectral Petrov Galerkin method preserves the energy exactly while both the spectral Gauss collocation and spectral Galerkin methods are energy conserving up to spectral accuracy. While it is well known that collocation at Gauss points preserves symplectic structure, we prove that, for both the Petrov-Galerkin method and the spectral Galerkin method, the error in symplecticity decays with spectral accuracy. Finally, we show that all three methods converge exponentially with respect to the polynomial degree. Numerical experiments indicate that our algorithms are efficient.

报告人简介：安静，男，博士，贵州师范大学数学科学学院教授，博导，中国数学会计算数学分会第十届委员。主要从事偏微分方程及其特征值问题的理论和数值计算方面的研究，研究问题包括传输特征值问题，非线性哈密顿系统，电磁场方程等。2013 年 6 月于厦门大学获得计算数学理学博士学位。曾先后赴美国普渡大学、新加坡南洋理工大学、中国科学软件研究所做访问学者。2016 年 1 月-2018 年 12 月先后于北京计算科学研究中心从事博士后研究和天元数学访问学者。截至目前主持完成国家自然科学基金项目 2 项，在研国家自然科学基金项目 1 项，主持完成贵州省科技厅基金项目 2 项，以一作或通讯在《J SCI COMPUT》、《APPL NUMER MATH》、《NUMER ALGORITHMS》、《COMPUT MATH APPL》等期刊发表 SCI 学术论文 20 余篇，并于 2018 年获得贵州省人民政府特殊津贴，2021 获得贵州省自然科学三等奖。

Stokes Eigenmodes on two-dimensional regular polygons

Lizhen Chen (陈丽贞)

北京计算科学研究中心

The Stokes eigenmodes on two-dimensional regular polygons of apexes, , are studied numerically using two different solvers: the lattice Boltzmann equation and the Legendre-Galerkin spectral element method. In particular, the lowest 55 eigenmodes on regular -polygons have been computed and investigated for the following properties including (a) symmetries, (b) the asymptotic behaviour of the Stokes eigenvalues in the limit of the apex number , i.e., in the limit of a regular -polygon becoming its circumcircle, (c) the splitting doublet modes due to boundary geometry of -polygons, and (d) the one-to-one correspondence between the Stokes modes on regular -polygons and on the disc.

报告人简介：陈丽贞博士，北京计算科学研究中心特聘副研究员，2011 年获得厦门大学博士学位，师从许传炬教授和沈捷教授，博士后期间先后与罗礼诗教授、王奇教授、包维柱教授合作。研究兴趣主要为计算流体力学的谱元方法及并行算法设计和程序实现。

Exact structure-preserving spectral method for plasma simulations

Zhiguo Yang (杨志国)

上海交通大学数学科学学院

In this talk, we present H^1-, H(div) and H(curl)-conforming spectral method with exact preservation of the curl/divergence-free constraints for two typical PDEs arising from plasma simulations. One is the incompressible visco-resistive MHD system and the other one is the Vlasov-Ampere system. Two key ingredients, i.e. exact de Rham complexes and their commuting diagram, and the derivative property of the generalized Jacobi polynomials are essential for the derivation of the desired basis functions. Besides, several novel second-order energy-stable or energy-conserving time discretization schemes are proposed. Ample 2D and 3D numerical examples illustrate both the accuracy of the structure-preserving basis functions and the efficiency of the proposed schemes.

报告人简介：杨志国，2017 年博士毕业于新加坡南洋理工大学，2017-2020 年于美国普渡大学任职访问助理教授，2020 年加入上海交通大学数学院任副教授。报告人长期从事谱与谱元方法、保结构数值算法及其在电磁、流体模拟中的应用。研究成果发表于计算数学的高水平期刊如 SIAM 系列、JCP、CMAME、JSC 等。入选 2020 年上海海外高层次人才引进计划，2021 年入选国家青年特聘专家，主持扬帆计划基金、国自然青年科学基金，参与中科院先导专项等研究课题。