上海交通大学 SHANGHAI JIAO TONG UNIVERSITY | 数学科学学院 SCHOOL OF MATHEMATICAL SCIENCES

科学与工程问题的先进算法新进展研讨会

上海交通大学数学科学学院

会议安排

中国上海，上海交通大学

2023 年 5 月 13-14 日

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会议宗旨

现代科技与工程领域的大量理论与实际问题都有赖计算领域的稳健、高效算法进行数值模拟，进而付诸应用，为国民经济和国防建设服务。本次研讨会旨在交流先进算法与分析方面的前沿研究成果，加强国内同行之间的科研合作，为解决科学与工程中的瓶颈问题提供新思路与新方法。期望本研讨会对人才培养和学科建设具有积极的推动作用，对解决国家有关重要需求问题有所裨益。

会议信息

注册时间：2023 年 5 月 12 下午 2:00 起
注册地点：上海市闵行区白金汉爵大酒店一楼
会议时间：2023 年 5 月 13 日-14 日
会议地点：上海交通大学数学科学学院理科楼群 6 号楼 706 室

会议组织者

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会议资助方

- **上海交通大学数学科学学院**
- **国家自然科学基金**
- **国家重点研发计划项目**

日程安排

5 月 13 日

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9:10-9:50	周涛	Deep adaptive density approximation for Fokker -Plank type equations
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10:20-11:00	陈艳萍	An adaptive hdg method for the pointwise tracking optimal control problem of elliptic equations
11:00-11:40	武海军	Dispersion analysis of CIP-FEM for Helmholtz equation
11:40-14:00		**午餐**
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14:40-15:20	张镭	Machine learning based numerical methods for multiscale problems
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11:00-11:40	陈文斌	EnVarA-FEM for the flux-limited porous medium equation
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14:00-14:40	李常品	Numerical approximations to ψ fractional derivative
14:40-15:20	蔡勇勇	Numerical methods for computing ground states of spinor Bose-Einstein condensates
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15:50-16:10	于海军	An energy stable spectral element in time method for nonlinear gradient systems
16:30-17:10	郭玲	IB-UQ: Information bottleneck based uncertainty quantification for neural function regression and neural operator learning
17:10-17:50	程青	Constructing structure-preserving schemes via Lagrange multiplier approach
18:10-19:30		晚餐

摘要

Numerical methods for computing ground states of spinor Bose-Einstein condensates

蔡勇勇
北京师范大学

The remarkable experimental achievement of Bose-Einstein condensation (BEC) in 1995 has drawn significant research interests in understanding the ground states and dynamics of trapped cold atoms. Different from the single component BEC, spinor BEC possesses the spin degree of freedom and exhibits rich phenomenon. In the talk, we will present some recent work for computing ground states of general spin-F BECs.

EnVarA-FEM for the flux-limited porous medium equation

陈文斌
复旦大学

In this work, we will proposed one EnVarA-FEM for solving the flux-limited porous medium equation (PME). Based on two kinds of energy dissipation laws, we construct two structure-preservation numerical schemes, which can be proved to be uniquely solvable and energy dissipative. The optimal convergence analysis for the nonlinear numerical scheme is presented by applying the technique of combining the rough and refined error estimates. Finally, some numerical experiments are carried out to validate the theoretical results. The finite propagation speed and waiting time phenomena can be computed effectively and the convergence order can be given numerically. We simulate the jump fronts case, and give the time where discontinuous interfaces occur with its convergence order numerically.

An adaptive hdg method for the pointwise tracking optimal control problem of elliptic equations

陈艳萍
华南师范大学

In this talk, we study an optimal control problem with point values of the state in the objective functional. The state and adjoint state are approximated by a hybridized discontinuous Galerkin (HDG) method, and the control is discretized by the variational discretization concept. With the help of the error estimates of Green’s function and Oswald interpolation, reliable and efficient a posteriori error estimates for the errors in the control, state and adjoint state variables are obtained. Several numerical examples are provided to show the performance of the obtained a posteriori error estimators.

一类弹性力学中的反接触问题

程晋
复旦大学

在弹性力学中，描述两个接触物体在压力下的局部应力和变形的问题被称为接触问题。接触问题广泛存在于工程的许多领域，如轴承、凸轮机构、齿轮、硬度计、轧辊、桥支承和刚性头等。接触问题曾经是应用数学家和力学的一个非常困难的问题。在实践中，很难或不可能观察到一些量，例如在某些情况下接触表面和接触表面上的应力分布。因此，如何从弹性体的观测数据中构建其他信息在理论和实践意义上都变得重要。在本次报告中，我们将提出一类反问题，即根据弹性体非接触域上的边界位移数据确定应力分布和接触面。证明了观测数据可以唯一地确定未知函数。我们说明了这个问题是一个严重的不适定问题。通过唯一连续性的方法，我们证明了这个问题具有一定的条件稳定性，这为构造稳定的数值算法提供了理论保证。同时，为了获得准确的测量数据，我们提出了一种使用大量数据来换取测量精度的方法。

Constructing structure-preserving schemes via Lagrange multiplier approach

程青
同济大学

In the talk, I will introduce a new Lagrange multiplier approach to construct efficient and accurate structure-preserving schemes for a class of semi-linear and quasi-linear parabolic equations. To be more specific, I will introduce how to construct positivity/bound-preserving, length-preserving, energy-dissipative schemes for a large class of PDEs. I will establish stability results under a general setting, and carry out an error analysis for second-order structure-preserving schemes. Finally, I will apply our approach to several typical PDEs which preserve structures described above. Some numerical results will be presented to validate our approach.

IB-UQ: Information bottleneck based uncertainty quantification for neural function regression and neural operator learning

郭玲
上海师范大学

In this talk, we will present a novel framework for uncertainty quantification via information bottleneck (IB-UQ) in scientific machine learning tasks, including deep neural network (DNN) regression and neural operator learning (DeepONet). IB-UQ can provide both mean and variance in the label prediction by explicitly modeling the representation variables. Compared to most DNN regression methods and the deterministic DeepONet, the proposed model can be trained on noisy data and provide accurate predictions with reliable uncertainty estimates on unseen noisy data. The capability of the proposed IB-UQ framework is demonstrated with some numerical examples.

Numerical approximations to ψ fractional derivative

李常品
上海大学

A generalised fractional derivative (the ψ-Caputo derivative) is studied. Generalisations of standard discretisations are constructed for this derivative: L1, L1-2, L2-1$_{\sigma}$ for derivatives of order $\alpha\in(0,1)$, and L2, H2N2, L2$_1$ for derivatives of order $\alpha\in(1,2)$. These new discretisations extend known results for the standard Caputo derivative, the Caputo-Hadamard derivative, etc. Numerical examples are given to demonstrate their performance.

$curl^2$-conforming spectral elements for quad-curl problem

李会元
中国科学院软件研究所

In this talk, we present first some ideas and tools to explicitly construct $curl^2$-conforming spectral elements, which possess a hierarchical structure and can be categorized into the kernel space and non-kernel space of the curl operator. Then, we propose the $curl^2$-conforming spectral element approximation schemes together with their implementation algorithms to solve the quad-curl problems. Next, we study the $curl^2$-conforming spectral approximation. Notably, the polynomial degree in the kernel space affects the convergence rate in $L^2(\Omega)^2$-norm, but not those measured in $H(curl;\Omega)$- and $H(curl^2;\Omega)$-seminorms. This allows us to obtain eigenvalue approximations from the upper or lower side by choosing different polynomial degrees for the kernel space and non-kernel space of the curl operator. Finally, numerical results demonstrate the effectiveness and efficiency of our method.

Energy stable numerical methods for a fully coupled multiphysics model of ferrofluids

毛士鹏
中国科学院数学与系统科学研究院

The ferrofluids models frequently-used in the computation are usually obtained under the assumption of static magnetic field and non-conductive fluid, which are quite difficult to design energy stable numerical methods and establish the corresponding convergence theory. In this work, we consider a fully coupled multiphysics ferrofluids model composed of the incompressible Navier-Stokes equation, magnetization equation and Maxwell equation, which allows it to cover more kinds of magnetic fluids and possess a higher model accuracy than the ferrofluids equation commonly used in traditional computation. We show the energy law based on the appropriate variational model of the fully coupled ferrofluids and propose a fully discrete finite element scheme with unconditional energy stability. The existence theory and convergence analysis for the numerical solutions are established. Finally, we test the influence of a physical parameter on the fluid flow and simulate that the applied magnetic field can drive the ferrofluid flow in three-dimensional case.

A fourth-order conservative semi-Lagrangian finite volume WENO scheme

without operator splitting for kinetic and fluid simulations

邱建贤
厦门大学

In this presentation, we present a fourth-order conservative semi-Lagrangian (SL) finite volume (FV) weighted essentially non-oscillatory (WENO) scheme without operator splitting for two-dimensional linear transport equations with applications of kinetic models including the nonlinear Vlasov-Poisson system, the guiding center Vlasov model and the incompressible Euler equation in the vorticity-stream function formulation. To achieve fourth-order accuracy in space, two main ingredients are proposed in the SL FV formulation. Firstly, we introduce a so-called cubic-curved quadrilateral upstream cell and applying an efficient clipping method to evaluate integrals on upstream cells. Secondly, we construct a new WENO reconstruction operator, which recovers a P3 polynomial from neighboring cell averages. Mass conservation is accomplished with the mass conservative nature of the reconstruction operator and the SL formulation. A positivity-preserving limiter is applied to maintain the positivity of the numerical solution wherever appropriate. For nonlinear kinetic models, the SL scheme is coupled with a fourth-order Runge-Kutta exponential integrator for high-order temporal accuracy. Extensive bench marks are tested to verify the designed properties.

Space-time spectral methods and eigenvalue analysis of related spectral differentiation matrices for IVPs

王立联
南洋理工大学

Spectral methods typically use global orthogonal polynomials/functions as basis functions which enjoy high-order accuracy and gain increasingly popularity in scientific and engineering computations. In most applications, spectral methods are employed in spatial discretization, but low-order schemes are used in time discretization. This may create a mismatch of accuracy in particular for problems with evolving dynamics that require high-resolution in both space and time, e.g., oscillatory wave propagations. In this talk, we conduct eigenvalue analysis for the spectral discretization matrices for initial value problems based on the Legendre dual-Petrov-Galerkin spectral method (LDPG). While the spectrum of second-order derivative operators for boundary value problems are well understood, the spectrum of spectral approximations of initial value problems are far under explored. Here, we precisely characterize the eigen-pairs of the spectral discretisation matrices through the generalized Bessel polynomials. Such findings have much implication in, e.g., theoretical foundation of time spectral methods, stability of explicit time discretization of spectral methods for hyperbolic problems and parallel-in-time algorithms among others. We also introduce effective matrix decomposition algorithms to alleviate the burden of the extra works for spectral methods in time. This talk is based on joint works with Desong Kong (Central South China University), Jie Shen (Purdue University) and Shuhuang Xiang (CSU).

An efficient spectral-Galerkin method for elliptic equations in 2D complex

geometries

王中庆
上海理工大学

A polar coordinate transformation is considered, which transforms the complex geometries into a unit disc. Some basic properties of the polar coordinate transformation are given. As applications, we consider the elliptic equation in two-dimensional complex geometries. The existence and uniqueness of the weak solution are proved, the Fourier-Legendre spectral Galerkin scheme is constructed and the optimal convergence of numerical solutions under H^1-norm is analyzed. The proposed method is very effective and easy to implement for problems in 2D complex geometries. Numerical results are presented to demonstrate the high accuracy of our spectral-Galerkin method.

Dispersion analysis of CIP-FEM for Helmholtz equation

武海军
南京大学

When solving the Helmholtz equation numerically, the accuracy of numerical solution deteriorates as the wave number k increases, known as `pollution effect' which is directly related to the phase difference between the exact and numerical solutions, caused by the numerical dispersion. In this paper, we propose a dispersion analysis for the continuous interior penalty finite element method (CIP-FEM) and derive an explicit formula of the penalty parameter for the $p^{\rm th}$ order CIP-FEM on tensor product (Cartesian) meshes, with which the phase difference is reduced from $\mathcal{O}\big(k(kh)^{2p}\big)$ to $\mathcal{O}\big(k(kh)^{2p+2}\big)$. Extensive numerical tests show that the pollution error of the CIP-FE solution is also reduced by two orders in kh with the same penalty parameter.

Second-order flows for computing the ground states of rotating Bose-Einstein condensates

谢资清
湖南师范大学

In this talk, two types of second-order damped hyperbolic flows for approaching the ground states of rotating Bose-Einstein condensates (BECs) are proposed. It was inspired by the recent advances in inertial dynamics with damping in convex optimization. The ground state of a rotating BEC can be mathematically modeled as a "minimizer" of the Gross-Pitaevskii energy functional with angular momentum rotational term under the normalization constraint. The proposed two types of second-order dissipative hyperbolic PDEs are served as energy minimization strategies for this constrained non-convex optimization problem. We shall mainly focus on their numerical aspects.

Eigensolvers with domain decomposition

许学军
同济大学

In this talk, we shall present a two-level block preconditioned Jacobi-Davidson (BPJD) method for solving discrete eigenvalue problems resulting from finite element approximations of 2mth (m = 1, 2) order elliptic eigenvalue problems. A new and efficient preconditioner is constructed by an overlapping domain decomposition (DD). This method may compute the first several eigenpairs, including simple, multiple and clustered cases. In each iteration, we only need to solve a couple of parallel subproblems and one small scale eigenvalue problem. This is a joint work with Qigang Liang and Wei Wang.

An energy stable spectral element in time method for nonlinear gradient systems

于海军
中国科学院数学与系统科学研究院

In this talk, we present a spectral element in time spectral method for nonlinear gradient systems with the phase-field Allen-Cahn equation as an example. Different from commonly-used spectral in time methods, which employ spectral Petrov-Galerkin or weighted Galerkin approximations, the presented method use a natural (energetic) variational Galerkin form that can maintain the volume conservation and energy dissipation property of the continuous dynamical system. Another advantage of this method is that superconvergence is achieved at nodal points. To handle the nonlinear term, we use a spectral extrapolation. The explicit method can be improved by a few Picard iterations to obtain superconvergence. Numerical experiments verify that the method using elements of polynomial degree 3 outperforms the 4th-order BDF scheme and the ETD-RK4 method, which are known to have good performances in solving phase-field equations. In addition to the standard Allen-Cahn equation, we also applied the method to a conservative Allen-Cahn equation. We note that the application of this method is not limited to phase-field Allen-Cahn equations. It is suitable for solving general, large-scale nonlinear dynamical systems.

Machine learning based numerical methods for multiscale problems

张镭
上海交通大学

In this talk, I will introduce our work on the machine learning based numerical methods for multiscale problems. We will start with deep neural network based solver for multiscale elliptic equations, then a hierarchical attention based model for multiscale operator learning. If time allowed, I will also introduce a deep learning-based non-Newtonian hydrodynamic model.

Deep adaptive density approximation for Fokker-Plank type equations

周涛

中国科学院数学与系统科学研究院

We propose adaptive deep learning method based on normalizing flow for classic/nonlocal Fokker-Planck equations. The solution of such equation is a probability density function. Traditional mesh-based methods may across difficulties since the dimension of spatial variable can be very high. To this end, we represent the solution by a flow-based generative model (e.g. KRnet) which constructs a mapping from a simple distribution to the target distribution (i.e., the unknow solution). An adaptive procedure for choosing the training set is presented. Meanwhile, either Monte Carlo sampling or an auxiliary density model, Gaussian radial basis functions which have analytical fractional Laplacian, is applied to approximate the fractional Laplacian. Numerical examples are presented to show the effectiveness of the proposed approach. Finally, we design bounded KRnet and show applications for solving Keller-Segel equations and kinetic Fokker-Planck equations.