科学与工程中的计算与优化方法研讨会(II)

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

2021 年 11 月 27-28 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与优化领域的稳健、高效算法进行数值模拟以付诸应用，为国民经济和国防建设服务。本系列研讨会旨在邀请海内外计算与优化领域的高水平专家进行学术研讨，交流所取得的前沿研究成果，加强彼此间的科研合作。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，对解决国家重要需求问题有所裨益。

会议信息

会议地点

腾讯会议 APP
时间: 2021/11/27 8:00-18:00　ID: 427 434 065
链接: https://meeting.tencent.com/dm/ZUPwl1BK8Ygf

时间: 2021/11/28 8:00-13:00　ID: 706 855 481
链接: https://meeting.tencent.com/dm/Qn8WiY5FrEAR

会议组织者

组委会成员(姓氏拼音序):

范金燕　黄建国　王增琦　徐振礼　杨志国　周圣高

会议联系人: 高伟航 (邮箱: gaowh2019@sjtu.edu.cn)

资助方

- ✧ 上海交通大学数学科学学院
- ✧ 国家自然科学基金
- ✧ 科学和工程计算教育部重点实验室
- ✧ 上海科学技术委员会
- ✧ 上海现代分析前沿科学研究基地
- ✧ 上海应用数学中心上海交大分中心

日程安排

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9:10-9:50	**许传炬**
9:50-10:00	休息
分组报告二　　　主持人：　杨志国	
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10:40-11:20	**季霞**
11:20-12:00	**鲁汪涛**
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报告摘要

Theoretical analysis for rising bubble in Hele-Shaw cell

邸亚娜
北京师范大学-香港浸会大学联合国际学院

In this talk, we calculate the shape and the velocity of a bubble rising in an infinitely large and closed Hele-Shaw cell using Park and Homsy's boundary condition which accounts for the change of the three-dimensional structure in the perimeter zone.

Seismic Tomography with frozen Gaussian approximation

黄忠亿
清华大学

Seismic tomography solves high-dimensional optimization problems to image subsurface structures of Earth. In this talk, we propose to use random batch methods to construct the gradient used for iterations in seismic tomography. Specifically, we use the frozen Gaussian approximation to compute seismic wave propagation, and then construct stochastic gradients by random batch methods. We also provide a rigorous convergence analysis for the inverse problems of acoustic wave propagation arising from seismic tomography.

Inverse scattering with multi-frequency sparse data

季霞
北京理工大学

In this talk, we will introduce a direct sampling method for inverse scattering problems, which uses multi-frequency backscattering far field data taken at sparse directions. The underlying object could be point-like scatterers, small scatterers, or extended inhomogeneities and obstacles. Both the theoretical basis and numerical simulations will be presented

A Fast Maxwell Solver Based on Exact Discrete Eigen-Decompositions

李会元
中国科学院软件研究所

In this paper, we propose a fast solver for the Maxwell's equation in two dimensions. We first discretize the simplified Maxwell's eigenvalue problem by employing the lowest-order rectangular Nedelec elements and derive the discrete eigen-solutions explicitly. Based on the exact eigen-decomposition, we further design a fast solver for the Maxwell's source problem by using the fast discrete sine transform, with computational time reduced from $O(n^2)$ by other direct solvers to $O(n^2 \log n)$, where n is the partition size in each direction. It is also utilized to perform an efficient preconditioning for solving Maxwell's source problem with variable coefficients. Finally, numerical experiments are carried out to illustrate the effectiveness of the proposed fast solver.

PML and high-accuracy boundary integral equation solver for wave scattering by a locally defected periodic surface

鲁汪涛
浙江大学

In this talk, we shall study the perfectly-matched-layer (PML) method for wave scattering in a half space of homogeneous medium bounded by a two-dimensional, perfectly conducting, and locally defected periodic surface, and develops a high-accuracy boundary-integral-equation (BIE) solver. Along the vertical direction, we place a PML to truncate the unbounded domain onto a strip and prove that the PML solution converges to the true solution in the physical subregion of the strip with an error bounded by the reciprocal PML thickness. Laterally, we divide the unbounded strip into three regions: a region containing the defect and two semi-waveguide regions, separated by two vertical line segments. In both semi-waveguides, we prove the well-posedness of an associated scattering problem so as to well define a Neumann-to-Dirichlet (NtD) operator on the associated vertical segment. The two NtD operators, serving as exact lateral boundary conditions, reformulate the unbounded strip problem as a boundary value problem over the defected region. Due to the periodicity of the semi-waveguides, both NtD operators turn out to be closely related to a Neumann-marching operator, governed by a nonlinear Riccati equation. It is proved that the Neumann-marching operators are contracting, so that the PML solution decays exponentially fast along both lateral directions. The consequences culminate in two opposite aspects. Negatively, the PML solution cannot converge exponentially to the true solution in the whole physical region of the strip. Positively, from a numerical perspective, the Riccati equations can now be efficiently solved by a recursive doubling procedure and a high-accuracy PML-based BIE method so that the boundary value problem on the defected region can be solved efficiently and accurately. Numerical experiments demonstrate that the PML solution converges exponentially fast to the true solution in any compact subdomain of the strip.

Generalized SAV-exponential integrator schemes for Allen-Cahn type gradient flows

乔中华
香港理工大学

The energy dissipation law and the maximum bound principle (MBP) are two important physical features of the well-known Allen-Cahn equation. While some commonly-used first-order time stepping schemes have turned out to preserve unconditionally both energy dissipation law and MBP for the equation, restrictions on the time step size are still needed for existing second-order or even higher-order schemes in order to have such simultaneous preservation. In this paper, we develop and analyze novel first- and second-order linear numerical schemes for a class of Allen-Cahn type gradient flows. Our schemes combine the generalized scalar auxiliary variable (SAV) approach and the exponential time integrator with a stabilization term, while the standard central difference stencil is used for discretization of the spatial differential operator. We not only prove their unconditional preservation of the energy dissipation law and the MBP in the discrete setting, but also derive their optimal temporal error estimates under fixed spatial mesh. Some experiments are also carried out to numerically illustrate the properties and performance of the proposed schemes.

Positivity/bound preserving schemes for complex nonlinear systems

沈捷
普渡大学

Solutions for a large class of partial differential equations (PDEs) arising from sciences and engineering applications are required to be positive to be positive or within a specified bound. It is of critical importance that their numerical approximations preserve the positivity/bound at the discrete level, as violation of the positivity/bound preserving may render the discrete problems ill posed. I will review existing approaches for constructing positivity/bound preserving schemes, and then present several efficient and accurate approaches which are relative easy to implement and can be combined with most spatial discretization.

Deep Learning for Multiscale Molecular Modelling

王涵
北京应用物理与计算数学研究所

We introduce a series of deep learning-based methods for molecular modeling at different scales. We discuss this topic in two aspects: model construction and data generation. In terms of model construction, we introduce the Deep Kohn-Sham, the Deep Potential, Deep coarse-graining schemes. They are proposed to accurately represent the energy functional, the many-body interatomic potential, and the coarse-grained potential, respectively, and share the common idea of preserving the extensibility and symmetries of the system. In terms of data generation, we present a concurrent learning approach, which automatically generates the most compact training dataset without compromising the accuracy of the model. In the last part of the talk, we present the Reinforced Dynamics (RiD) scheme that efficiently explores the configuration space and high-dimensional free energy landscapes. As a demonstrative example, we present a protein structure refinement protocol based on RiD, which gives rise to an overall improvement of 14.6 units over the initial GDT-HA score.

Numerical Analysis of Some PDEs with Logarithmic Nonlinearity

王立联
新加坡南洋理工大学

The presence of logarithmic nonlinear term of the form f(u)=u log(|u|) in parabolic PDEs or Schrodinger's equations brings out significant challenges in both numerical discretization and analysis. The nonlinear term is non-differentiable but Holder continuous at u=0, and the underlying energy does not have a definite sign. Such PDEs exhibit interesting dynamics that may not possess for general smooth nonlinearity. In this talk, we shall present our recent attempts for such problems and introduce some new tools for the analysis.

扩展子空间算法及其应用

谢和虎
中国科学院数学与系统科学研究院

本报告将介绍我们提出并发展的求解特征值问题和非线性问题的扩展子空间算法。基于有限元离散方法中的粗空间，扩展子空间算法可以将高维空间的特征值或非线性方程的求解转化成高维空间线性方程的求解和低维空间上特征值或非线性问题的求解。由于避免了在高维空间直接求解特征值或非线性问题，扩展子空间算法明显提高了求解效率，尤其是针对一大类问题（多项式类型的非线性特征值问题和非线性问题），扩展子空间算法可以达到绝对渐近最优的程度，即与求解同规模的线性方程的计算量级一致，并且不依赖于非线性迭代的次数。结合扩展子空间算法和多重网格结构，我们可以很自然地构造求解特征值问题和非线性问题的多水平校正算法。本报告将介绍该方法的本质、算法的格式和新的收敛性分析，以及在一些问题中的应用和推广。

Regularization methods for inverse problems of the sub-diffusion equations

许传炬
厦门大学

In this talk I will discuss about inverse problems for the time-fractional diffusion equation, which have been known to be ill-posed problems. Several regularization methods are presented and compared. In particular, a regularized problem with L2 and TV regularization is proposed and analyzed for the inverse source problem. The regularized problem is then approximated by a fully discrete scheme. The convergence rate of the discrete solution with respect to the target source and the convergence of the regularized solution with respect to the noise level will be provided. A series of numerical examples will be given to demonstrate the accuracy of the proposed methods.

Nucleation of Quasicrystals

张磊
北京大学

Despite the fact that tremendous efforts have been made on the study of quasicrystals since their discovery in 1984, nucleation of quasicrystals—the emergence of a quasicrystal from a crystalline phase—still presents an unsolved problem. The difficulties lie in that quasicrystals and crystals are incommensurate structures in general, so there are no obvious epitaxial relations between them. We solved this problem by applying an efficient numerical method to Landau theory of phase transitions and obtained the accurate critical nuclei and transition pathways connecting crystalline and quasicrystalline phases. The proposed computational methodology not only reveals the mechanism of nucleation of quasicrystals, but also paves the way to investigate a wide range of physical problems undergoing the first-order phase transitions.

C1-conforming Petrov-Galerkin methods for 2nd-order elliptic problems and superconvergence

张智民
北京计算科学研究中心

In some applications, due to regularity restriction, 2^{nd}-order elliptic problems have no divergent forms, and therefore we need to discretize the 2^{nd}-order derivatives directly. In this work, we construct a new Petrov-Galerkin method by using C1-conforming finite element for the trial space and L2-discontinuous element for the test space. We prove that the numerical solution by the new method converges to the exact solution with \$2k-1\$-rate (\$k\$ is the polynomial degree) at the nodal points for both function value and gradient under rectangular mesh.

A positivity-preserving stabilized finite element method for quantum drift-diffusion model

郑伟英
中国科学院数学与系统科学研究院

As the size of modern semiconductor devices goes to sub-nanometers, quantum mechanical phenomena become prominent and must be considered in numerical simulations. In 1989, Ancona and Iafrate derived a macroscopic model, called quantum drift-diffusion (QDD) model, which generalizes the classical DD model by incorporating a quantum correction to the electric potential. We derive an equivalent QDD model by expressing carrier densities with potential functions. The finite element method for the new model is positivity-preserving in the sense that discrete carrier densities are always positive. We propose a modified Newton iterative method to solve the nonlinear discrete problem. Numerical experiments for a FinFet device show that the iterative method is convergent for the source-drain bias voltage up to 15V and the source-gate bias voltage up to 5V.

Efficient Sampling of Thermal Averages of Interacting Quantum Particle Systems: simulation with random batches and error analysis

周珍楠
北京大学

An efficient sampling method, the pmmLang+RBM, is proposed to compute the quantum thermal average in the interacting quantum particle system. Benefiting from the random batch method (RBM), the pmmLang+RBM reduces the complexity due to the interaction forces per timestep from O(NP^2) to O(NP), where N is the number of beads and P is the number of particles. We also propose an extension of the pmmLang+RBM, which is based on the splitting Monte Carlo method and is applicable when the interacting potential contains a singular part. Besides, we discuss the long time behavior of the random batch dynamics, and show how the convergence to the equilibrium can be leveraged to quantify the error due to the use of random batches.