**四．报告题目和摘要**

报告人： 贾仲孝 清华大学

题目： The State of the Art of Krylov Iterative Solvers for Large Linear Discrete Ill-posed Problems

摘要： For the large-scale linear discrete ill-posed problem min ∥Ax−b∥ or Ax = b with a noisy b, LSQR, a Krylov iterative solver based on Lanczos bidiagonalization, and its mathematically equivalent Conjugate Gradient method for the normal equation ATAx = AT b (CGLS) are most commonly used. They have intrinsic regularizing effects, where the number of iterations plays the role of regularization parameter. However, there has been no answer to the long-standing fundamental concern: for which kinds of problems LSQR and CGLS can find best possible regularized solutions? The concern was actually raised by Bj¨orck and Eld´en in 1979. Here a best possible regularized solution means that it is at least as accurate as the best regularized solution obtained by the truncated singular value decomposition (TSVD)
method or standard-form Tikhonov regularization. In this talk, we overview the state of the art of many Krylov solvers, including LSQR and GMRES, for the discrete linear ill-posed problems.

报告人： 张振跃 浙江大学

题目：Graph Refinement via Simultaneously Low-rank and Sparse Approximation

摘要：Graphs play an important role in many fields of machine learning such as clustering. A high quality graph could improve the performance for many graph-based machine learning approaches. However, few work have been done for graph denoising or graph refinement, which aims to reduce noises in a graph and clarify its underlying hidden structure. In this work, we propose a novel graph refinement approach to discover the low rank and sparse structure of a noisy graph by simultaneously low-rank and sparse approximation (SLSA). In our SLSA model, we introduce an explicit low-rank constraint to reduce noise in a graph. We propose an iterative algorithm to solve the non-convex optimization problem efficiently and show a global convergence of the algorithm under a weak condition. We compare our SLSA model with other two related methods, which could also be used for graph refinement, and the results on both synthetic and real-world data sets show that the SLSA outperforms the others. We finally experimentally show that the SLSA could significantly improve the performance of graph-based algorithms for three different machine learning applications including subspace learning, nonlinear manifold learning and multi-view learning.

报告人：黄学海 温州大学

题目；Poisson-based approximate block factorization preconditioners for

mixed finite element methods and higher order elliptic problems

摘要： In this talk, Poisson-based approximate block factorization pre-

conditioners with the generalized minimal residual method are presented for mixed finite element methods of linear elasticity, Stokes and Lame systems, and conforming and nonconforming finite element methods of fourth order elliptic problems.

(1) An approximate block factorization preconditioner with the generalized minimal residual method is developed for Hu-Zhang mixed finite element methods of linear elasticity. It's based on a new stability result of the saddle point system in mesh-dependent norms. A fast auxiliary space preconditioner based on the H1 conforming linear element of the linear elasticity problem is then designed for solving the Schur complement. It is proved that the conditioning numbers of the preconditioned systems are bounded above by a constant independent of both the crucial Lame constant and the mesh-size.

(2) According to the discrete Helmholtz decomposition, the conforming and nonconforming finite element methods of Kirchhoff plates are equivalent to two finite element methods of Poisson equation and one mixed method of Stokes equation. Then an approximate block factorization preconditioner is developed for Kirchhoff plates by using the approximate block factorization preconditioner for Stokes equation. The proposed Poisson-based approximate block factorization preconditioners work also well for unstructured shape-regular meshes.

报告人： 王飞 西安交通大学

题目：A Unified Study of Discontinuous Galerkin Methods

摘要：During the past three decades, many different discontinuous finite element methods (FEMs), including discontinuous Galerkin (DG) methods, hybrid DG methods and weak Galerkin methods, have been developed for solving a wide range of partial differential equations. In this talk, taking Poisson problem as an example we present a general framework for understanding these discontinuous finite element methods by the concept of DG-derivatives. In light of this general framework, a new mixed DG method is proposed, and we apply it to solve linear elasticity problem with arbitrary order discontinuous finite element spaces.

报告人： 王涵 北京应用物理与计算数学研究所

题目：Deep Potential Molecular dynamics: a scalable model with the accuracy of quantum mechanics
摘要： We introduce a new scheme for molecular simulations, based on a many-body potential and interatomic forces generated by a deep neural network trained with ab initio data. We show that the proposed scheme, which we call Deep Potential Molecular Dynamics (DeePMD), provides an efficient and accurate protocol in a variety of systems, including bulk materials and molecules. In all these cases, DeePMD gives results that are essentially indistinguishable from the original data, at a cost that scales linearly with system size. Moreover, in a few test cases, DeePMD shows good structural transferability to thermodynamic conditions not included in the original training data.

报告人： 施意 北京应用物理与计算数学研究所

题目：基于泛函展开的辐射输运隐式蒙特卡罗算法

**摘要：**辐射输运方程描述光子在物质中的传输及其与物质的相互作用，其在惯性约束聚变、武器物理、天体物理等过程中具有非常重要的应用。求解辐射输运方程具有维数高（七维）、非线性强耦合、多尺度等计算难点。本报告中，我们将介绍求解辐射输运方程的一种随机模拟算法——隐式蒙特卡罗算法，此方法通过引入“伪散射”代替光子的“吸收-再发射”物理过程，从而将辐射与物质方程解耦。针对光性厚问题，直接使用隐式蒙卡算法的空间离散误差较大，需要很密的网格才能得到正确的结果。为此，我们提出了基于泛函展开的隐式蒙卡抽样算法，其基本思想是利用吸收能量来构造发射能量的分布函数，将每个网格中的吸收能量按Legendre多项式展开到一定阶数，然后通过蒙卡模拟计算相应的展开系数，并由此构造出吸收能量的分布函数。此方法能极大的提高空间分辨率，且不依赖周围网格的信息，易于推广到高阶，数值试验验证了算法的正确性与有效性。

报告人： 黄记祖 中科院数学与系统科学研究院

题目:  A NONLINEARLY PRECONDITIONED INEXACT NEWTON ALGORITHM FOR STEADY STATE LATTICE BOLTZMANN EQUATIONS

摘要: Most existing methods for calculating the steady state solution of the lattice Boltzmann equations are based on pseudo time stepping, which often requires a large number of time steps especially for high Reynolds number problems. To calculate the steady state solution directly without the time integration, in this talk we introduce a nonlinearly preconditioned inexact Newton algorithm with a domain decomposition based linear solver for parallelization. More precisely, the proposed algorithmic framework involves an implicit, second-order discretization, a two-level inexact Newton method, and a nonlinear elimination preconditioner to accelerate the convergenceof Newton iteration. A nonstandard, pollution removing, coarse space is introduced for the two-level method. Numerical experiments are presented to demonstrate the robustness and efficiency of the algorithm, especially for problems at a high Reynolds number. A comparison is also included to show the superiority of the proposed approach over other explicit and implicit methods in terms of the total compute time measured on a parallel computer. This is a joint work with Prof. Xiao-Chuan Cai and Prof. Chao Yang.

报告人： 蔡勇勇 北京计算科学研究中心

题目： A stable scheme for a 2D dynamic Q-tensor model of nematic liquid crystals

摘要: We propose a stable numerical scheme for a $2D$ dynamic $Q$-tensor model of nematic liquid crystals. This dynamic $Q$-tensor model is a $L^2$ gradient flow generated by the liquid crystal free energy that contains a cubic term, which is physically relevant but makes the free energy unbounded from below, and for this reason, has been avoided in other numerical studies. The unboundedness of the energy brings significant difficulty in analyzing the model and designing numerical schemes. By using a stabilizing technique, we construct an unconditionally stable scheme, and establish its unique solvability and convergence. Our convergence analysis also leads to, as a byproduct, the well-posedness of the original PDE system for the 2D Q-tensor model. Several numerical examples are presented to validate and demonstrate the effectiveness of the scheme.

报告人： 王廷春 南京信息工程大学

题目：Unconditional convergence of compact finite difference method for the nonlinear Schrödinger equation

摘要：The purpose of this talk is to establish unconditional and optimal H2 error estimates of two fourth-order compact finite difference schemes for solving the nonlinear Schrödinger equation in two or three dimensions.  The proposed schemes are proved to preserve the total mass and energy in the discrete sense. Besides the standard energy method, the cut-off function technique and a `lifting' technique as well as an induction argument are introduced to establish the error estimates without any constraints on the grid ratios, while the previous works often require certain restriction on the grid ratios. The H2 convergence rate of the proposed schemes is proved to be of fourth order and second order in time and in space, respectively. The analysis method can be directly extended to other finite difference schemes for solving the nonlinear Schrödinger /Gross-pitaevskii equations. Several numerical results are reported to support our theoretical analysis.

报告人：朱小红 暨南大学

题目： Continuum framework for dislocation structure and dynamics of dislocation arrays and low angle grain boundaries

摘要：We present a continuum framework for dislocation structure and dynamics of dislocation arrays and low angle grain boundaries which may be nonplanar and non-equilibrium. We define a dislocation density potential function on the dislocation array surface or grain boundary to describe the orientation dependent continuous distribution of dislocations. The continuum formulations incorporate both the long-range dislocation interaction and the local dislocation line energy, and are derived from the discrete dislocation model.

报告人：薛军工 复旦大学

题目： Accurate computations for M-matrices

摘要：In this talk, we present high-accuracy algorithms for  some problems concerning M-matrices, which include the inverses of M-matrices, M-matrix Sylvester equations, M-matrix algebraic Riccati equations and exponentials of essentially nonnegative matrices. These algorithms can compute the solutions to high entrywise relative accuracy.

报告人：应文俊 上海交通大学

题目：Wetting on rough surfaces by an adaptive multilevel method

摘要：Recently Xianmin Xu et al. developed a threshold dynamics model for wetting on rough surfaces. The model is volume preserving and non-sensitive to the inhomogeneity or roughness of the solid boundary. Data by the model varies significantly only in the regions around the rough surfaces and the boundaries of evolving droplets. This calls for local mesh refinement in numerical simulation. This talk presents an adaptive multilevel method for the threshold dynamics model. This method works with adaptively refined Cartesian grids, where each cell is a square. It places fine grids only in the regions around the rough surfaces and the boundaries of evolving droplets. The method discretizes the PDE of the model by a cell-centered finite volume scheme and solves the resulting discrete equations on the composite grid by a multilevel iteration. Details of the method and some interesting wetting phenomena by the method will be presented. This is joint work with Xianmin Xu.

报告人：戴书洋 武汉大学

题目：Level set simulations of continuum dislocation array dynamics

摘要： We present a simulation method for the dynamics of dislocation arrays. In this numerical method, dislocation arrays are considered as continuous surfaces in three dimensions, and the level set representation is used for these dislocation array surfaces. The driving force of the evolution of the dislocation array surfaces comes from both the long-range interaction of the constituent dislocations and their local curvature effect. The long-range interaction, which is expressed by a complicated integral over the whole dislocation array surface, is calculated efficiently using the fast Fourier transform (FFT) method. Simulations are performed for dislocation arrays bypassing different particles under applied stress and are compared with those of a single dislocation. The long-range nature of the stress fields of nonplanar infinite dislocation arrays is discussed, and is shown to be essentially different from that by a single dislocation.

报告人：彭傲平 中国空气动力研究与发展中心超高速空气动力研究所

题目：求解Boltzmann模型方程的气体动理论统一算法研究进展

摘要：高超声速再入飞行器整个过程需要经历从高真空自由分子流到近地面连续流，属于跨流域多尺度非平衡绕流相互耦合的复杂问题。其中连续流的Navier-Stokes方程快速高效，但对于过渡区和稀薄区流动的适用性问题争议很大；基于仿真分子运动碰撞过程直接模拟的DSMC方法在稀薄流区应用广泛，但由于仿真分子数和网格尺度的限制难以在低Kn数流动中应用，而且对于低速流动可能出现统计波动掩盖有用信息的风险。Boltzmann方程能够描述跨流域气体流动问题，但其速度分布函数的高维属性和极其复杂的碰撞项使得直接求解Boltzmann方程是非常困难的。一种经济有效的方法是数值求解简化了碰撞项的Boltzmann模型方程，气体动理论统一算法就是其中之一。通过离散速度法将速度空间进行离散，宏观流动参数通过相应的数值积分规则得到，再引入传统求解Navier-Stokes方程的位置空间离散、时间迭代方法，得到求解Boltzmann模型方程的气体动理论统一算法。该方法在跨流域复杂外形绕流、微尺度流动、稀薄非定常流动、真空喷流扩散等多个问题中得到应用验证。本文着重介绍气体动理论统一算法的基本原理以及近年来的研究进展，包括基于多块对接网格的隐式气体动理论统一算法、守恒型离散速度数值积分法以及统一算法在高温内能激发气体和多组分混合气体中的应用。

报告人：张振 南方科技大学

题目：Modeling and Simulation of Moving Contact Line Problems for Two-Phase Complex Fluids

摘要：We introduce the sharp interface models for moving contact lines with insoluble surfactants and polymeric fluids. A continuous model with the boundary conditions is derived for the dynamics of two immiscible fluids with moving contact lines and insoluble surfactants based on thermodynamic principles. A finite element numerical method is developed to solve the coupled partial differential equation. We also discuss the model reduction of the slip model to the no-slip limit by the technique of asymptotic analysis.

报告人：高兴誉 北京应用物理与计算数学研究所

题目：The preconditioning methods for self-consistent iteration of Kohn-Sham density functional theory

摘要：It is a usual practice to calculate the occupied orbitals for semiconducting, insulating or isolated systems. It differs significantly in metallic systems and partial occupancies have to be included at the same time. In the language of optimization, this is an ill-conditioning problem with partial occupancies treated as additional variational degrees of freedom. We will find the origin of the conditioning problem related to metallic systems and discuss specific strategies for it. An alternative approach is the self-consistent iteration. One reason why the self-consistent schemes are efficient lies probably in the fact that both subproblems can be preconditioned well with plane wave basis. Combining our recent work, we would like to share our understanding of the preconditioning techniques.

报告人：袁永军 湖南师范大学

题目：Solving Singularly Perturbed Neumann Problems for Multiple

Solutions

摘要：In this talk, based on the analysis of bifurcation points and Morse indices of trivial solutions at any perturbation value, the generating process of nontrivial positive solutions for a general singularly perturbed Neumann boundary value problem is developed. The bifurcation points of each trivial solution and then the exact critical perturbation value $\varepsilon\_c$ which determines the existence or non-existence of nontrivial positive solutions are verified. An efficient local minimax method based on the bifurcation and Morse theory is proposed to compute both M-type and W-type saddle points by introducing an adaptive local refinement strategy, a continuation strategy for initial selection and the Newton method to improve the convergence speed. Extensive numerical results are reported to investigate the critical value $\varepsilon\_c$ and present interesting properties of different types of multiple solutions.

报告人：卢脁 北京大学

题目：Well-posedness of a Kind of Abstract Cauchy Problem in a Banach Space

摘要：The abstract initial value problem for the system of evolution equations for a real-valued function and a function-valued function was considered. The existence and uniqueness of classical solution to the evolution system were proved in a Banach

space under assumptions on the boundedness and smoothness of data. An isomorphism between the solution space of the evolution system and a special subspace of the Schwartz space is established. It is verified that the solution of the evolution system can be mapped to a function which is the solution of the initial value problem of an integral-differential equation. The theoretical finding has a potential application in studying the well-posedness of the stationary Wigner equation with inflow boundary conditions.

报告人：许志国 吉林大学

题目：Quantized vortex dynamics based on the reduced dynamical law of Ginzburg-Landau equation

摘要：We study analytically and numerically stability and interaction patterns of quantized vortex lattices governed by the reduced dynamical law --

a system of ordinary differential equations (ODEs) -- in superconductivity.

By deriving several non-autonomous first integrals of the ODEs, we obtain qualitatively dynamical properties of a cluster of quantized vortices, including global existence, finite time collision, equilibrium solution and invariant solution manifolds. For a vortex lattice with 3 vortices, we establish orbital stability when they have the same winding number and find different collision patterns when they have different winding numbers. In addition, under several special initial setups, we can obtain analytical solutions for the nonlinear ODEs.

报告人：王汉权 云南财经大学

题目：A splitting compact finite difference method for computing the dynamics of dipolar Bose–Einstein condensate

摘要：We numerically study the nonlocal Gross–Pitaevskii equation (NGPE) which describes the dynamics of Bose–Einstein condensates (BEC) with dipole–dipole interaction at extremely low temperature. In preparation for the numerics, first we reformulate the dimensionless NGPE into a Schrödinger–Poisson system. Then, we discretize the three-dimensional Schrödinger–Poisson system in space by a sixth-order compact finite difference method and in time by a splitting technique. By means of three dimensional discrete fast Sine transform, we develop a fast solver for the resulting discretized system. Finally, we present numerical examples in three dimensions to demonstrate the power of the numerical methods and to discuss some physics of dipolar BEC. The merits of the proposed method for the NGPE are that it is fast and unconditionally stable. Moreover, the method is of spectral-like accuracy in space, and conserves the particle number and the energy of the system in the discretized level.

报告人： 张硕 中科院数学与系统科学研究院

题目：An optimal multigrid method for biharmonic eigenvalue problem

摘要：In this talk, I will present an optimal multigrid method for biharmonic eigenvalue problem. Specifically, by transforming the primal problem to an order reduced formulation, a nested discretization scheme is obtained, and an optimal multilevel strategy (with optimal computational cost) can be implemented.  Both theoretical and numerical results will be presented, and particularly, some interesting phenomena can be observed for the scheme.

报告人：方明 中国空气动力研究与发展中心超高速空气动力研究所

题目：热化学非平衡稀薄气体电离效应的DSMC方法

摘要：随着航天器再入速度的不断增大，绕流气体发生较为严重的化学反应和电离现象，传统上发生在连续流区的通信黑障大幅向稀薄区域延伸。基于稀有组分权重因子方法，发展了含电离化学反应的DSMC方法，并以RAM C-II和Stardust为例验证了其有效性。重点考察了类探月返回试验器的稀薄气体电离特性，数值计算结果表明其在85km左右的高度通信将完全中断，与飞行试验的观测结果一致。计算结果表明，对于RAM C-II的接近第一宇宙速度再入，电离的主要来源是N和O的联合电离；而对于类探月返回试验器的接近第二宇宙速度再入，电离的主要来源是N、O与其它粒子的直接碰撞电离。