“科学计算：理论与应用”研讨会

Symposium on ‘Scientific Computing: Theory and Applications’

主办单位：四川大学数学学院

资助单位：国家天元数学西南中心

Hosted by: School of Mathematics, Sichuan University

Supported by: Tianyuan Mathematical Center in Southwest China

会议日程安排

Conference Schedule

2023 年 06 月 25 日至 2023 年 06 月 29 日，四川大学，成都

25th June to 29th June, 2023

Sichuan University, Chengdu, China

一. 住宿安排及交通指引

住宿地点：成都祥宇宾馆
会议地点：四川大学数学学院西 303：　**26 号上午、28 号上午**
成都祥宇宾馆**满庭芳**会议厅：**26 号下午、28 号下午**
成都祥宇宾馆**祥顺厅**会议厅：**27 号上午**
酒店地址：四川省成都市武侯区新南路 103 号
酒店电话：(+028) 8555 1111

交通指引：

1. **双流国际机场**
   地铁：机场 2 号(或 1 号)航站楼站**乘地铁 10 号线**（太平园方向）4 站到**太平园站**下
   太平园站 转乘 **地铁 3 号线**（成都医学院方向）5 站到**磨子桥**站下车
   磨子桥站 B 口出，往南步行 300 米到达成都祥宇宾馆
   滴滴或出租车：约 30 分钟 60 元（21 公里）。
2. **天府国际机场**：　**滴滴或出租车**：约 50 分钟 160 元（60 公里）。
3. **火车东站**
   地铁：成都东客站上车 **乘坐地铁 2 号线**（犀浦方向） 6 站到 **春熙路站** 下车
   春熙路站 转乘 **地铁 3 号线**（双流西站方向） 2 站到 **磨子桥**站 下车
   磨子桥站 B 口出，往南步行 300 米到达成都祥宇宾馆
   滴滴或出租车：约 25 分钟 30 元（10 公里）。

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组织委员会（按姓氏拼音排序）：

陈刚、冯民富、贺巧琳、胡朝浪、李彬杰、马强、孙树瑜
唐庆彝、王皓、谢小平、徐友才、杨凡意、张世全

三. 会议日程

6 月 25 号：14:00—22:00，祥宇宾馆报到。
6 月 26 号—6 月 28 号：会议，日程安排见第三页、第四页彩页。
6 月 29 号：离会。

“科学计算：理论与应用”研讨会
Symposium on ‘Scientific Computing: Theory and Applications’

26/06/2023（星期一） 上午：西303，数学学院，四川大学 下午：满庭芳会议厅， 成都祥宇宾馆		主持人
8:45-9:00	签到、开幕式	王宝富
9:00-9:30	**程晋（复旦大学）** 从数据中学习---微分方程数值解法的创新及其应用	
9:30-10:00	**包维柱（National** University of Singapore) Multiscale methods and analysis for the highly oscillatory nonlinear Klein-Gordon equation	
10:00-10:30	茶歇	
10:30-11:00	林平 (University of Dundee) A thermodynamically consistent phase-field model and an energy-law preserving finite element scheme for vesicles motions and interaction	谢小平
11:00-11:30	许传炬（厦门大学） Certified reduced order method for the parametrized Allen-Cahn equation	
11:30-12:00	陈龙（University of California at Irvine) Transformer meets boundary value inverse problems	
12:30-14:30	午餐	
14:30-15:00	黄忠亿（清华大学） Generalization of deepONets for learning operators arising from a class of singularly perturbed problems	冯民富
15:00-15:30	刘歆（中国科学院数学与系统科学研究院） Optimization models and approaches for strictly correlated electrons	
15:30-16:00	刘海亮（Iowa State University) A dynamic mass-transport method for Poisson-Nernst-Planck systems	
16:00-16:30	茶歇	
16:30-17:00	邱建贤（厦门大学） A robust fifth order finite difference Hermite WENO scheme for compressible Euler equations	包维柱
17:00-17:30	王立联（Nanyang Technological University) Numerical study of logarithmic Schrödinger equation	
17:30-18:00	蔡勇勇（北京师范大学） Numerical methods for computing ground states of spinor Bose-Einstein condensates	
18:30	晚宴	
27/06/2023（星期二），祥顺厅会议厅， 成都祥宇宾馆		
9:00-9:30	沈捷（宁波市东方理工高等研究院） Highly efficient and accurate schemes for Navier-Stokes equations and general dissipative systems	林平
9:30-10:00	袁先旭（中国空气动力研究与发展中心） 智能空气动力学若干研究进展及展望	
10:00-10:30	茶歇、照相	

10:30-11:00	项阳（香港科技大学） Modeling effects of randomness in high entropy alloys	孙树瑜
11:00-11:30	毕林（中国空气动力研究与发展中心） 自适应笛卡尔网格流体仿真方法	
11:30-12:00	苏春梅（清华大学） A convexity-preserving and perimeter-decreasing parametric finite element method for the area-preserving curve shortening flow	
12:00-14:30	午餐	
14:30-17:30	**自由讨论**	
18:00	晚餐	
28/06/2023 （星期三） 上午：西303，数学学院，四川大学 下午：满庭芳会议厅， 成都祥宇宾馆		
9:00-9:30	黄云清（湘潭大学） 二阶椭圆方程的自适应直接间断Galerkin方法	沈捷
9:30-10:00	周爱辉（中国科学院数学与系统科学研究院） 第一原理电子结构模型与计算中的数学发现	
10:00-10:30	照相、茶歇	
10:30-11:00	王筱平（香港中文大学（深圳）/香港科技大学） Topology optimization of flow network and applications	许传炬
11:00-11:30	赵雁翔（George Washington University） Supervised optimal transport	
11:30-12:00	凤小兵（The University of Tennessee） Recent developments in fractional calculus and fractional differential equations and their numerical methods	
12:30-14:30	午餐	
14:30-15:00	明平兵（中国科学院数学与系统科学研究院） Large plate bending with isometry constraint: FEM vs machine learning	凤小兵
15:00-15:30	应文俊（上海交通大学） 一个求解Stefan自由边界问题的基于位势理论的直角网格方法	
15:30-16:00	马敬堂（西南财经大学） A new implicit scheme for American put options	
16:00-16:30	茶歇	
16:30-17:00	李若（北京大学） 北太天元·逆数而行	王筱平
17:00-17:30	徐立伟（电子科技大学） On the coupling schemes of Galerkin finite element and boundary integral equation methods solving the acoustic/elastic scattering problems	
17:30-18:00	钟柳强（华南师范大学） 二阶非线性椭圆问题有限元离散系统的迭代两网格法	
18:00	晚餐	

四．报告题目和摘要

报告人：包维柱（National University of Singapore）

题目： Multiscale methods and analysis for the highly oscillatory nonlinear Klein-Gordon equation

摘要： In this talk, I will review our recent works on numerical methods and analysis for solving the highly oscillatory nonlinear Klein-Gordon equation (NKGE) including the nonrelativistic regime involving a small dimensionless parameter which is inversely proportional to the speed of light. In this regime, the solution is highly oscillating in time and the energy becomes unbounded, which bring significant difficulty in analysis and heavy burden in numerical computation. We begin with four frequently used finite difference time domain (FDTD) methods and obtain their rigorous error estimates in the nonrelativistic regime by paying particularly attention to how error bounds depend explicitly on mesh size and time step as well as the small parameter. Then we consider a numerical method by using spectral method for spatial derivatives combined with an exponential wave integrator (EWI) in the Gautschi-type for temporal derivatives to discretize the NKGE. Rigorous error estimates show that the EWI spectral method show much better temporal resolution than the FDTD methods for the NKGE in the nonrelativistic regime. In order to design a multiscale method for the NKGE, we establish error estimates of FDTD and EWI spectral methods for the nonlinear Schroedinger equation perturbed with a wave operator. Based on a large-small amplitude wave decomposition to the solution of the NKGE, a multiscale time integrator (MTI) is presented for discretizing the NKGE in the nonrelativistic regime. Rigorous error estimates show that this multiscale method converges uniformly in spatial/temporal discretization with respect to the small parameter for the NKGE in the nonrelativistic regime. Extension to the long-time dynamics of the NKGE with weak nonlinearity is discussed and improved uniform error bounds on time-splitting spectral method are presented based on a new technique--regularity compensation oscillation. Finally, applications to several high oscillatory dispersive partial differential equations will be discussed.
This is based on joint works with Yongyong Cai, Xuchun Dong, Yue Feng, Chunmei Su, Wenfan Yi and Xiaofei Zhao.

报告人：毕林（中国空气动力研究与发展中心）

题目： 自适应笛卡尔网格流体仿真方法

摘要： 笛卡尔网格是计算流体力学三大基础类型网格之一，与传统结构/非结构贴体网格相比，可不依赖于物面直接生成，具有自动化程度高、复杂外形适应性好、非定常/多尺度/动边界捕捉能力强等优势，天然适用于复杂流动问题的全自动仿真模拟。然而，由于笛卡尔网格的非贴体特性，存在网格与物面相对位置关系判断导致的网格生成效率问题、自适应后悬挂网格处流动模拟降阶问题、网格方向和壁面边界流动方向不一致下的附面层流动模拟难题等。空天飞行空气动力科学与技术全国重点试验室研究团队针对笛卡尔网格存在的上述固有问题，在网格数据结构与网格类型判断算法、悬挂网格高精度格式构造、非贴体网格粘性附面层虚拟单元-浸入边界梳理方法等方面取得进展。本报告将对以上工作做详细介绍。

报告人：蔡勇勇（北京师范大学）

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

摘要： 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.

报告人：陈龙（University of California at Irvine）

题目： Transformer meets boundary value inverse problems

摘要： A Transformer-based deep direct sampling method is proposed for solving a class of boundary value inverse problem. A real-time reconstruction is achieved by evaluating the learned inverse operator between carefully designed data and the reconstructed images. Specifically, inspired by direct sampling methods for inverse problems, the 1D boundary data are preprocessed by a partial differential equation-based feature map to yield 2D harmonic extensions in different frequencies as different input channels. Then, by introducing learnable non-local kernel, the approximation of direct sampling is recast to a modified attention mechanism. The proposed method is then applied to electrical impedance tomography, a well-known severely ill-posed nonlinear inverse problem. The new method achieves superior accuracy over its predecessors and contemporary operator learners, as well as shows robustness with respect to noise.

This research shall strengthen the insights that the attention mechanism, despite being invented for natural language processing tasks, offers great flexibility to be modified in conformity with the a priori mathematical knowledge, which ultimately leads to the design of more physics-compatible neural architectures. This is a joint work with Ruchi Guo (UCI) and Shuhao Cao (University of Missouri-Kansas City).

报告人：程晋（复旦大学）

题目： 从数据中学习---微分方程数值解法的创新及其应用

摘要： 学习理论的发展日新月异，为科学研究打开了一片新的天地。如何在科学计算中应用学习的思想，针对一些难点问题提出一些新的思路是目前的一个大家关心的研究方向。从另一方面讲，数学作为一门基础学科，在科学的研究中扮演着无可替代的角色。但是数学的研究与工程应用之间存在着一道鸿沟。如何针对实际问题的需求，进行相关数学研究是目前应用数学与计算数学研究的一个热点方法。在本报告，我们主要介绍了我们团队最近的一些相关的研究成果：基于机器学习的微分方程数值解的方法。针对目前数值解方法没有考虑已有精确解（基本解等）、实际工程测量的信息以及已经计算出的相关结果等信息，我们提出一种基于机器学习的数值解方法，并给出了相关的理论框架和算法。数值解模拟的结果表明我们的方法对于高波数问题有比较好的效果。

报告人：凤小兵（The University of Tennessee**）**

题目：Recent developments in fractional calculus and fractional differential equations and their numerical methods

摘要：In this talk, I shall first discuss recent developments in weak fractional calculus and fractional Sobolev spaces based on a new weak fractional derivative concept which is a natural generalization of integer order weak derivatives and helps to unify multiple existing fractional derivative concepts. I shall then introduce a class of fractional calculus of variations problems and their associated Euler-Lagrange (fractional differential) equations. This new framework/theory is based on the aforementioned theory of weak fractional derivatives and their associated fractional order Sobolev spaces. It leads to new types of fractional differential equations, including new one-side fractional Laplace operators and future value problems. Finally, I shall also briefly introduce some new finite element (and DG) methods for approximating the weak fractional derivatives and the solutions of fractional calculus of variations problems and their associated fractional differential equations.

报告人：黄云清（湘潭大学）

题目：二阶椭圆方程的自适应直接间断 Galerkin 方法

摘要：针对带有间断系数的二阶椭圆方程，基于加权平均构造合适的数值通量，进而得到相应的直接间断 Galerkin 方法，得到了能量范数下最有误差估计，进一步导出了残量型后验误差估计。注意到系数的间断性，考虑了梯度的分区域重构，采用合适的样本点，基于离散最小二乘提出了高精度梯度重构算法。基于所构造的残量型和重构型后验误差估计子，设计了自适应直接间断 Galerkin 方法，大量的数值算例展示了误差估计子和自适应算法的有效性。此报告基于与曹慧慧、易年余合作的工作。

报告人：黄忠亿（清华大学）

题目：Generalization of deepONets for learning operators arising from a class of aingularly perturbed problems

摘要：Singularly perturbed problems present inherent difficulty due to the presence of boundary/interior layers in its solution. To overcome this difficulty, we propose using deep operator networks (DeepONets). In this talk, we demonstrate for the first time the application of DeepONets to onedimensional singularly perturbed problems. We consider the convergence rate of the approximation error incurred by the operator networks in approximating the solution operator, and examine the generalization gap and empirical risk, all of which are shown to converge uniformly with respect to the perturbation parameter.

报告人：李若（北京大学）

题目：北太天元·逆数而行

摘要：北太天元数值计算通用软件（以下简称“北太天元”）是在北京大学数学科学学院、北京大学大数据分析与应用技术国家工程实验室、北京大学重庆大数据研究院的指导和支持下，由北京大学重庆大数据研究院基础软件科学研究中心自主研发的国内首款具有完全自主知识产权的科学计算软件。

北太天元聚焦科学计算领域“卡脖子”问题的解决，实现了科学计算内核根技术的突破。软件具备强大的底层数学函数库，可提供科学计算、可视化、交互式程序设计功能，支持数值计算、数据分析、数据可视化、数据优化、算法开发等场景，并通过SDK与API接口，扩展支持各类学科与行业应用，目前软件已更新至V2.3。目前已有300余所高校、100余所企事业单位开展试用，用户数量超过3万人，已连续两届在全国大学生数学建模竞赛设立“北太天元数模之星”奖项，曾获得中央电视台、重庆新闻联播等媒体宣传报道，2023年获第五届中国先进技术转化应用大赛智能制造技术创新类铜奖、CSIAM应用数学落地成果认证。

报告人：林平（University of Dundee）

题目： A thermodynamically consistent phase-field model and an energy-law preserving finite element scheme for vesicles motions and interaction

摘要： We will first show how to develop a thermodynamically consistent phase field model for the binary incompressible (quasi-incompressible) fluid. We then show how to apply the idea to model vesicle motions and deformations through a narrowed channel. We will also introduce a Lennard-Jones type of interaction potential for vesicle-vesicle and vesicle-channel wall interactions. An energy law preserving computational method is then developed for the model. A few computational examples including vesicle-wall and multi-vesicle interactions will be presented to demonstrate the model and the computational method

报告人：刘歆（中国科学院数学与系统科学研究院）

题目： Optimization models and approaches for strictly correlated electrons

摘要： In electronic structure calculations, Kohn-Sham equations rank among the most widely adopted mathematical models. However, due to the deficiency of available approximations for exchange-correlation energy, Kohn-Sham equations cannot well describe strictly correlated electrons at present. To this end, some models based on the strong-interaction limit of density functional theory have been developed in recent decades. The associated energy minimizations can be formulated as multi-marginal optimal transport problems with Coulomb cost (MMOT). Since the curse of dimensionality resides in MMOT, its low-dimensional reformulations are indispensable. In this talk, we consider the reformulation based on a Monge-like ansatz. We discuss the difficulties in the corresponding optimization problems, and also propose a global optimization approach for numerical resolution.

报告人：刘海亮（Iowa State University**）**

题目： A dynamic mass-transport method for Poisson-Nernst-Planck systems

摘要： In this talk, I will present some recent work on developing structure preserving (i.e., positivity preserving, mass conservative, and energy dissipating) methods for numerically simulating Poisson-Nernst-Planck (PNP) systems. Motivated by Benamou- Brenier's dynamic formulation of the quadratic Wasserstein metric, we introduce a Wasserstein-type distance suitable for our problem setting, we then construct a variational scheme which falls into the Jordan-- Kinderlehrer--Otto framework. The variational scheme is a first order (in time) approximation of the original PNP system. To reduce

computational cost, we further approximate the constraints and the objective function in the underlying Wasserstein-type distance, such approximations won't destroy the first order accuracy. With a standard spatial discretization, we obtain a finite dimensional strictly convex minimization problem with linear constraints. The admissible set in the variational problem is a subset of the probability space and the Wasserstein-type distance is nonnegative, therefore our scheme is a positivity preserving, mass conservative, and energy dissipating scheme.

报告人：明平兵（中国科学院数学与系统科学研究院）

题目： Large plate bending with isometry constraint: FEM vs machine learning

摘要：We study a minimization problem that arises from a plate bending model with isometry constraints. Both finite element method and machine learning based method are exploited to investigate the convergence of the minimizer, and to what degree the isometry constraints are met by the proposed methods. We found that FEM may have certain a-priori theoretical convergence guarantee, while machine learning method seems more efficient in most cases under study. This is a joint work with Li, Xiang and Liao, Yulei.

报告人：马敬堂（西南财经大学）

题目： A new implicit scheme for American put options

摘要： In this talk, we present a new implicit scheme for solving a parabolic variational inequality arising from the American put options. The discretization leads to a class of discrete elliptic variational inequalities. General results on the existence, uniqueness, comparison principle, and stability of the discrete elliptic variational inequality are established. A simple and efficient algorithm to solve the implicit discretized variational inequality is discovered. The novelty here is an explicit formula for the optimal exercise boundary. An improved algorithm is also presented to eliminate the singularity near the time to expiry. Numerical examples are carried out to show the accuracy and efficiency of the proposed algorithms. This is joint work with Xinfu Chen, Zhengyang Lu and Jinye Shen.

报告人：邱建贤（厦门大学）

题目： A robust fifth order finite difference Hermite WENO scheme for compressible Euler equations

摘要：In this presentation, we introduce a robust fifth order finite difference Hermite weighted essentially non-oscillatory (HWENO) scheme for compressible Euler equations following the HWENO with limiter (HWENO-L) scheme (J. Comput. Phys., 472:111676, 2023). The HWENO-L scheme reduced storage and increased efficiency by using restricted derivatives only for time discretizations, however, it cannot control spurious oscillations well when facing strong shocks since the derivatives are directly used in spatial discretizations without any restrictions. To address such an issue, our proposed HWENO scheme performs flux reconstructions in the finite difference framework without using the derivative value of a target cell, which can result in a simpler and more robust scheme. The resulting scheme is simpler while still achieving fifth order accuracy, so is more efficient. Besides, numerically we find it is very robust for some extreme problems even without positivity-preserving limiters. The proposed scheme also inherits

advantages of previous HWENO schemes, including arbitrary positive linear weights in the flux reconstructions, compact reconstructed stencils, and high resolution. Extensive numerical tests are performed to demonstrate the fifth order accuracy, efficiency, robustness, and high resolution of the proposed HWENO scheme.

报告人：沈捷（宁波市东方理工高等研究院）

题目： Highly efficient and accurate schemes for Navier-Stokes equations and general dissipative systems

摘要： I will first present some recent advances on the construction and analysis of new consistent splitting schemes for the time dependent Stokes equations, followed by the generalized scalar auxiliary variable (GSAV) approach to develop highly efficient and accurate schemes for a large class of complex dissipative systems. Then, by combining the GSAV approach with the new consistent splitting scheme, we construct, for the very first time, a unconditionally stable (in H^1 norm) and totally decoupled scheme with uniform second-order accuracy for the velocity and pressure, and provide a rigorous optimal error estimate. We shall also present ample numerical results to show the computational advantages of higher-order GSAV schemes.

报告人：苏春梅（清华大学）

题目： A convexity-preserving and perimeter-decreasing parametric finite element method for the area-preserving curve shortening flow

摘要： We propose and analyze a semi-discrete parametric finite element scheme for solving the area-preserving curve shortening flow. The scheme is based on Dziuk's approach (SIAM J. Numer. Anal. 36(6): 1808-1830, 1999) for the anisotropic curve shortening flow. We prove that the scheme preserves two fundamental geometric structures of the flow with an initially convex curve: (i) the convexity-preserving property, and (ii) the perimeter-decreasing property. To the best of our knowledge, the convexity-preserving property of numerical schemes which approximate the flow is rigorously proved for the first time. Furthermore, the error estimate of the semi-discrete scheme is established, and numerical results are provided to demonstrate the structure-preserving properties as well as the accuracy of the scheme. This talk is based on the joint work with Wei Jiang and Ganghui Zhang.

报告人：王立联（Nanyang Technological University）

题目： Numerical study of logarithmic Schrodinger equation

摘要： The Schrodinger equation with a logarithmic nonlinear term (LogSE): f(u)=u log(|u|^2) exhibits many distinct features and rich dynamics that make it unique among nonlinear wave equations. However, such a nonlinearity presents significant challenges in both numerical solutions and analysis. Compared with usual cubic case, the nonlinear term f(u) is non-differentiable at u=0 but only possesses certain Holder continuity. In this talk, we shall report our recent attempts in numerical study of the LogSE with a focus on time discretization via implicit-explicit scheme and time-splitting scheme and on the introduction of new tools for the error analysis. This talk is based on joint works with Jingye Yan (Jiangsu University) and Xiaolong Zhang (Hunan Normal University).

报告人：王筱平（香港中文大学（深圳）/香港科技大学）

题目：Topology optimization of flow network and applications

摘要：We propose an efficient iterative convolution thresholding method for the formulation of flow networks where the fluid is modeled by the Darcy – Stokes flow with the presence of volume sources. The method is based on the minimization of the dissipation power in the fluid region with a Darcy term. The flow network is represented by its characteristic function and the energy is approximated under this representation. The proposed method is simple and easy to implement. We prove mathematically that the iterative method has the total energy decaying property. Numerical experiments demonstrate the performance and robustness of the proposed method and interesting structures are observed.

报告人：项阳（香港科技大学）

题目：Modeling effects of randomness in high entropy alloys

摘要：High entropy alloys (HEAs) are single phase crystals that consist of random solid solutions of multiple elements in approximately equal proportions. This class of novel materials have exhibited superb mechanical properties, such as high strength which is associated with the motion of dislocations (line defects). We obtain a stochastic continuum model based on the Peierls-Nabarro framework for dislocations in an HEA from an atomistic model that incorporates the atomic level randomness and short-range order. This approach provides a fundamental explanation to the origin of the high strength of HEAs based on the stochastic effects on the intrinsic strength.

报告人：许传炬（厦门大学）

题目：Certified reduced order method for the parametrized Allen-Cahn equation

摘要：In this talk, we discuss an efficient parametrized reduced-order method for the Allen-Cahn equation. The reduced basis is constructed based on proper orthogonal decomposition and parametrized solution snapshots. Numerical analysis of the proposed method is conducted to derive error estimates for the reduced-order solutions. The impact on the accuracy of time difference quotients as snapshots is also investigated.

报告人：徐立伟（电子科技大学）

题目：On the coupling schemes of Galerkin finite element and boundary integral equation methods solving the acoustic/elastic scattering problems

摘要：In this talk, we introduce a couple of new results on coupling schemes of Galerkin finite element and boundary integral equation methods solving the acoustic/elastic scattering problems. Well-posedness of the approximate problems, analysis on the accuracy of numerical schemes, and numerical results will be presented.

报告人：应文俊（上海交通大学）

题目：一个求解 Stefan 自由边界问题的基于位势理论的直角网格方法

摘要：在这个报告中，我们将介绍一个求解Stefan自由边界问题的基于位势理论的直角网格方法。Stefan问题的自由边界会随时间推进产生极大变形，依赖表面张力系数的值，还可能长出非常复杂的指状图案。用贴体非结构网格方法求解Stefan问题的计算开销很大。这个报告中将提到的方法首先把包含不规则自由边界的矩形计算区域划分成不贴体的直角网格，不要求直角网格线与自由边界匹配。在求解整个Stefan问题的过程中，直角网格固定不变，做到了网格开销极小。在直角网格上离散Stefan问题应用基于位势理论的（涉及边界积分和体积分）方法进行离散、修正和结合快速算法进行求解。我们还将在这个报告中演示一些数值模拟结果。

报告人：袁先旭（中国空气动力研究与发展中心）

题目：智能空气动力学若干研究进展及展望

摘要：智能空气动力学是人工智能与空气动力学的结合，包含独立而明确的研究对象和研究目标，同时融入了第四研究范式（数据）和第五研究范式（智能）的独特研究方法，已逐步发展成为一门独立的交叉学科。目前在该学科领域，空天飞行空气动力科学与技术全国重点实验室研究团队结合自身在气动力预测、高速转捩和湍流方面的研究基础与特色，利用人工智能开展了若干相关研究。本报告将简要介绍相关背景，详细阐述团队通过多种智能化方法在多源数据智能融合、智能化转捩/湍流建模与预测等方面的研究进展，并对未来智能空气动力学的发展趋势与潜在挑战进行展望分析。综合来看，当前的研究成果初步展现了 AI 赋能经典流体力学难题和空气动力学工程问题的可行性，未来将融合多学科、多领域知识和方法进一步开展深入研究工作，积极推动学科的建设与发展。

报告人：赵雁翔（George Washington University）

题目：Supervised optimal transport

摘要：Optimal Transport, a theory for optimal allocation of resources, is widely used in various fields such as astrophysics, machine learning, and imaging science. However, many applications impose elementwise constraints on the transport plan which traditional optimal transport cannot enforce. Here we introduce Supervised Optimal Transport (sOT) that formulates a constrained optimal transport problem where couplings between certain elements are prohibited according to specific applications. sOT is proved to be equivalent to an 1^1 penalized optimization problem, from which efficient algorithms are designed to solve its entropy regularized formulation. We demonstrate the capability of sOT by comparing it to other variants and extensions of traditional OT in color transfer problem. We also study the barycenter problem in sOT formulation, where we discover and prove a unique reverse and portion selection (control) mechanism. Supervised optimal transport is broadly applicable to applications in which constrained transport plan is involved and the original unit should be preserved by avoiding normalization.

报告人：钟柳强（华南师范大学）

题目：二阶非线性椭圆问题有限元离散系统的迭代两网格法

摘要：首先，针对拟线性椭圆问题的协调有限元离散系统，设计和分析了相应的迭代两网格法; 其次，针对拟线性椭圆问题的内罚间断有限元离散系统，证明了有限元解的存在唯一性和先验误差估计,并设计和分析了一种迭代两网格算法，值得注意的是，该算法的有效性依赖于迭代算法初值的选取，为此需构造了一个相应的辅助变分问题. 最后，针对强非线性椭圆问题的协调有限元离散系统，设计和分析了相应的迭代两网格法. 相应的数值实验验证了上述算法的有效性。

报告人：周爱辉（中国科学院数学与系统科学研究院）

题目：第一原理电子结构模型与计算中的数学发现

摘要：第一原理电子结构计算已成为理解和探索物质机理以及预测材料性质的重要手段与工具。它可以解释实验，与实验相辅相成，从而能加速新材料的发现、设计与利用。尤其是，第一原理计算还可能替代极端条件下的实验。如何又快又好地计算大规模的电子结构是很具挑战性的课题。而电子结构模型及其数学基础与数学性质在理解、分析与设计第一原理电子结构计算方法中发挥着重要作用。我们将介绍我们小组在电子结构模型与计算研究中的一些数学发现。