

# 随机问题及相关确定性问题数值计算研讨会

一、会议时间

2024 年 6 月 28 日-2024 年 6 月 30 日

二、会议地点

南京信息工程大学明德楼 N101，N105

三、报到地点

南气宾馆（江苏省南京市江北新区宁六路 219 号）

四、会议组委会

刘文军，曹春正，陈克旺，黄瑜，王剑，汪佳玲，王廷春，吴斌，姚青云

五、会议联系人

黄瑜 13813912139；姚青云 13813611298.

六、会议日程总览

6 月 28 日 星期五		
会议报到、晚餐：自助餐		
6 月 29 日 星期六		
上午	09:00-09:15	会议开幕式
	09:15-09:30	合影
	09:30-10:30	分会报告
	10:30-10:50	茶歇
	10:50-11:50	分会报告
中午	12:00-13:30	午餐
下午	14:30-15:30	分会报告
	15:30-15:50	茶歇
	15:50-16:50	分会报告
晚上	17:30-20:00	晚餐
6 月 30 日 星期六		
自由讨论、离会		

六、会议报告安排

6 月 29 日 星期六 分会场 1：明德楼 N101				
上午	时间	报告人	题目	主持人
	09:00-09:40	吴奕飞 (天津大学)	Regularity mechanism of nonlinear Schrodinger equations with rough potential	唐庆彝 (四川大学)
	09:40-10:20	王汉权 (云南财经大学)	An asymptotic preserving scheme for the defocusing Davey-Stewartson II equation in the semiclassical limit	
	10:20-10:40	茶歇		
	10:40-11:20	蔡勇勇 (北京师范大学)	Numerical methods and analysis for highly oscillatory dispersive PDEs	王汉权 (云南财经大学)
	11:20-12:00	张勇 (天津大学)	Optimal zero-padding of kernel truncation method	
下午	14:00-14:40	袁永军 (湖南师范大学)	自旋轨道耦合 Spin-1 玻色-爱因斯坦凝聚的动力学模拟	蔡勇勇 (北京师范大学)
	14:40-15:20	冯悦 (西安交通大学)	Improved uniform error bounds on time-splitting methods for long-time dynamics of dispersive PDEs	
	15:20-15:40	茶歇		
	15:40-16:20	阮欣然 (首都师范大学)	含高阶相互作用项的 Gross-Pitaevskii 方程的基态解求解算法	张勇 (天津大学)
	16:20-17:00	易雯帆 (湖南大学)	Numerical methods for the logarithmic Dirac equation	
	17:00-17:40	陈克旺 (南京信息工程大学)	改进的 Anderson 加速算法及其应用	

6月29日 星期六 分会场2：明德楼 N105

上午	时间	报告人	题目	主持人
	09:00-09:40	徐翔 (浙江大学)	An inverse random source problem for a time fractional diffusion equation	王海兵 (东南大学)
	09:40-10:20	蒋代军 (华中师范大学)	An inverse potential problem in a variable order time-fractional diffusion equation	
	10:20-10:40	茶歇		
	10:40-11:20	王泽文 (广州航海学院、 广州交通大学(筹))	Multiple terms identification of time fractional diffusion equation with symmetric potential from nonlocal observation	吴斌 (南京信息工程大学)
	11:20-12:00	龚荣芳 (南京航空航天大学)	Determining sources in the bioluminescence tomography problem	
下午	14:00-14:40	廖洪林 (南京航空航天大学)	Average energy dissipation rates of explicit exponential Runge-Kutta methods for gradient flow problems	汪佳玲 (南京信息工程大学)
	14:40-15:20	李义宝 (西安交通大学)	Multiscale topology optimization method for lattice materials	
	15:20-15:40	茶歇		
	15:40-16:20	杨钧翔 (澳门科技大学)	Diffuse-interface modeling and computation of single/compound droplets in contact with solid	王剑 (南京信息工程大学)
	16:20-17:00	蔡文君 (南京师范大学)	Highly efficient structure-preserving algorithms for Gross-Pitaevskii equations via model reduction	
	17:00-17:40	洪旗 (南京航空航天大学)	Thermodynamically consistent hybrid computational models for fluid-particle interactions	

# 报告摘要及报告人简介

(按报告人姓氏排序)

## Highly efficient structure-preserving algorithms for Gross-Pitaevskii equations via model reduction

蔡文君 南京师范大学

**Abstract:** In this report, we design efficient structure-preserving algorithms for the Gross-Pitaevskii (GP) equation based on model order reduction strategies from the perspectives of symplectic and invariant-preserving methods. First, through spatial pseudospectral and temporal Gauss Runge-Kutta discretization, we construct a time high-order accurate symplectic full-order model for the canonical Hamiltonian structure of the GP equation. By using symplectic proper orthogonal decomposition based on Galerkin projection, combined with discrete empirical interpolation techniques, we propose a reduced-order model that not only preserves the symplectic structure but also significantly reduces computational complexity, thereby greatly decreasing the computational cost of high-order schemes. Second, for the two-dimensional rotating GP equation, we design reduced-order models that preserve either discrete energy or mass, based on canonical and non-canonical Hamiltonian structures, respectively. By integrating discrete empirical interpolation techniques and tensor methods, we further reduce the computational complexity of the nonlinear terms, enhancing the computational efficiency of high-dimensional conservative schemes. Finally, numerical experiments verify the effectiveness, conservation properties, and efficiency of the proposed methods.

**报告人简介:** 蔡文君, 南京师范大学数学科学学院教授。2014 年于南京师范大学获得博士学位, 2014 年 9 月到 2016 年 9 月在中国科学院大学计算地球动力学重点实验室从事博士后研究工作。蔡文君教授的研究兴趣主要在偏微分方程的保结构算法及其在守恒或者耗散系统中的应用。完成国家自然科学基金面上项目 1 项, 作为主要参与人完成国家重点研发计划子课题 1 项, 完成国家自然科学基金青年项目 1 项、江苏省高校自然科学重大项目 1 项, 获教育部高校科研优秀成果二等奖 (排名 4/6), 获江苏省第三届“工业与应用数学奖青年奖”, 入选第六期江苏省“333 工程”第三层次培养对象。

# Numerical methods and analysis for highly oscillatory dispersive PDEs

蔡勇勇 北京师范大学

**Abstract:** Highly oscillatory dispersive PDEs, such as Klein-Gordon equation in the non-relativistic limit, Dirac equation in the non-relativistic limit, Schrodinger equation in the semi-classical limit, arise from many different areas, e.g. computational chemistry, plasma physics, quantum mechanics. These oscillatory PDEs usually exhibit solutions with high frequency waves in time and/or in space, and are generally computational expensive. In this talk, we report some recent advances on the numerical methods and analysis for some typical highly oscillatory dispersive PDEs.

**报告人简介:** 蔡勇勇，北京师范大学教授，本科和硕士就读于北京大学，2012 年在新加坡国立大学获得博士学位，2016 年入选海外高层次人才引进计划青年项目。他先后在威斯康辛大学麦迪逊分校、马里兰大学帕克分校和普渡大学从事博士后研究工作，从 2016 年至 2019 年在北京计算科学研究中心任特聘研究员。蔡勇勇博士的研究兴趣主要是偏微分方程的数值方法及其在量子力学等领域中的应用，在 MCOM、JCP 和 SIAM 系列等期刊上发表论文 60 余篇，多次受邀参加学术会议，并在 SciCADE2019 和 ICOSAHOM2023 上作大会报告。

## 改进的 Anderson 加速算法及其应用

陈克旺 南京信息工程大学

**摘要:** Anderson 加速算法是由哈佛大学 D.G.Anderson 教授 1963 年提出，随后该加速算法得到广泛应用，但关于 Anderson 加速算法的收敛性最近才有部分结果。本次报告将介绍 Anderson 加速算法的最近进展以及其在流体计算，等几何分析以及深度学习中的应用。

**报告人简介:** 陈克旺，南京信息工程大学，讲师，博士毕业于美国佛蒙特大学，荷兰代尔夫特理工大学博士后。主要研究偏微分方程理论分析与数值计算，以及加速算法及其在等几何分析、深度学习中的应用。目前已完成国家自然科学基金青年基金项目 1 项。

# Improved uniform error bounds on time-splitting methods for long-time dynamics of dispersive PDEs

冯悦 西安交通大学

**Abstract:** In this talk, I begin with the nonlinear Klein-Gordon equation (NKGE) with weak nonlinearity, which is characterized by  $\varepsilon^2$  with  $\varepsilon \in (0, 1]$  a dimensionless parameter. Different numerical methods are applied to discretize the NKGE including finite difference methods, exponential wave integrators and time-splitting methods. Especially, we discretize the NKGE by the second-order time-splitting method in time and combine with the Fourier spectral method in space. By introducing a new technique--Regularity Compensation Oscillation (RCO) which controls the high frequency modes by the regularity of the exact solution and analyzes the low frequency modes by phase cancellation and energy method, we carry out the improved uniform error bounds for the time-splitting methods. The results have been extended to other dispersive PDEs including the (nonlinear) Schrodinger equation and Dirac equation.

**报告人简介:** 冯悦, 西安交通大学数学与统计学院教授, 博士生导师。冯悦博士于 2014 年和 2017 年在浙江大学取得学士和硕士学位, 于 2020 年在新加坡国立大学取得博士学位, 师从包维柱教授, 随后在新加坡国立大学及法国索邦大学从事博士后研究。冯悦博士近年来致力于色散偏微分方程的数值求解方法及分析方面的研究, 主要关注长时间动力学和高振荡问题的算法设计及误差估计, 相关工作发表在 SIAM Journal on Numerical Analysis, Mathematics of Computation 等计算数学权威学术期刊上。

# Determining sources in the bioluminescence tomography problem

龚荣芳 南京航空航天大学

**Abstract:** In this talk, we revisit the bioluminescence tomography (BLT) problem, where one seeks to reconstruct bioluminescence signals (an internal light source) from external measurements of the Cauchy data. In the literature, BLT is extensively studied based on diffusion approximation equation, where the distribution of peak sources is to be reconstructed and no solution uniqueness is guaranteed without adequate a priori information. Motivated by the solution uniqueness issue, a new coupled model is proposed and several theoretical results are explored.

**报告人简介：**龚荣芳，南京航空航天大学数学学院，教授、博士生导师，江苏省计算数学分会常务理事、JSIAM 理事。2009 年博士毕业于浙江大学，随后进入南航数学学院工作，期间多次赴美国、瑞典、澳大利亚、香港等地高校进行学术访问。研究方向主要包括生物光、色谱和脑成像以及 Cauchy 问题等数学物理反问题的建模、正则化理论与方法，已在 Numer. Math.、CMAME、IP、IPI、JCM 等期刊发表论文 30 多篇。主持完成国家自然科学基金、省自然科学基金等项目 7 项，当前主持国家自然科学基金面上和科技部高端外专项目各 1 项。

## **Thermodynamically consistent hybrid computational models for fluid-particle interactions**

洪旗 南京航空航天大学

**Abstract:** In this talk, we will introduce a novel computational framework designed to explore the dynamic interactions between fluid and solid particles or structures immersed in a viscous fluid medium adhering to the generalized Onsager principle. This innovative framework harnesses the power of the phase-field-embedding method, in which each solid component, whether rigid or elastic, is characterized by a volume-preserving phase field. This approach facilitates the development of a hybrid, thermodynamically consistent hydrodynamic model applicable to both rigid and elastic particles. To numerically solve this thermodynamically consistent model for elastic particles, we present a structure-preserving numerical algorithm. Notably, in the limit of an infinite elastic modulus, this algorithm converges to the one employed for modeling rigid particles. Finally, we substantiate the effectiveness, accuracy, and stability of our proposed scheme through a series of numerical experiments. These experiments not only validate the computational framework but also showcase its capabilities, reinforcing the reliability of our approach. This is a joint work with Prof. Qi Wang.

**报告人简介：**洪旗，南京航空航天大学数学学院助理教授，2019 年博士毕业于中国工程物理研究院北京应用物理与计算数学研究所。主要研究兴趣：多相复杂流体可计算建模与保结构算法。相关研究成果发表在中国科学：数学，Comput. Methods Appl. Mech. Engrg, J. Comput. Phys, Adv. Comput. Math 等学术期刊。目前主持国家自然科学基金和计算物理国家重点实验室青年基金各 1 项。

# **An inverse potential problem in a variable order time-fractional diffusion equation**

蒋代军 西安交通大学

**Abstract:** This talk deals with an inverse problem on determining a time dependent potential in a diffusion equation with temporal fractional derivative of variable order from a distributed observation. We shall study the existence, uniqueness and regularity estimates of the solution for the forward problem by utilizing the Fredholm alternative principle for compact operators. Based on a newly established coercivity for fractional derivatives of variable order, we prove a uniqueness result for the inverse potential problem. Numerically, we transform the inverse potential problem into an optimization problem with Tikhonov regularization. An iterative thresholding algorithm is proposed to find the minimizers by a newly constructed adjoint system, whose wellposedness is also verified. Several numerical experiments are presented to show the accuracy and efficiency of the proposed algorithm.

**报告人简介:** 蒋代军, 华中师范大学副教授, 博士生导师。2007 年获得华中师范大学学士学位, 2009 年和 2012 年分别获得武汉大学硕士和博士学位。蒋代军博士的研究领域包括偏微分方程反问题、稀疏优化及控制, 快速算法等, 主持国家自然科学基金项目 4 项, 在 SIAM 系列, Inverse Problems 等刊物上发表学术论文近 30 篇。

# **Multiscale topology optimization method for lattice materials**

李义宝 西安交通大学

**Abstract:** In this talk, we will introduce an efficient multiscale topology optimization method for lattice materials. In macro-scale, we present a second-order unconditionally energy stable schemes for the topology optimization problem. Using porous media approach, our objective functional composes of five terms including mechanical property, Ginzburg-Landau energy, two penalized terms for solid and the volume constraint. A Crank-Nicolson method is proposed to discrete the coupling system. We prove that our proposed scheme is unconditionally energy stable. In macro-scale, we propose a simple volume merging method for triply periodic minimal structure. A modified Allen-Cahn type equation with a correction term is proposed. The mean curvature on the surface will be



constant everywhere at the equilibrium state. Computational experiments are presented to demonstrate the efficiency of the proposed method.

**报告人简介:** 李义宝, 西安交通大学教授, 博导, 入选国家青年人才计划, 2019 年 7 月至今担任数学与统计学院党委副书记。主要从事多物理场的耦合机制、3D 打印的图形处理和拓扑优化等研究工作。自 2010 年, 在数学与力学交叉期刊发表 SCI 论文 107 篇, 获国家授权发明专利 6 项。

## **Average energy dissipation rates of explicit exponential Runge-Kutta methods for gradient flow problems**

廖洪林 南京航空航天大学

**Abstract:** We propose a unified theoretical framework to examine the energy dissipation properties at all stages of explicit exponential Runge-Kutta (EERK) methods for gradient flow problems. The main part of the novel framework is to construct the differential form of EERK method by using the difference coefficients of method and the so-called discrete orthogonal convolution kernels. As the main result, we prove that an EERK method can preserve the original energy dissipation law unconditionally if the associated differentiation matrix is positive semi-definite. A simple indicator, namely average dissipation rate, is also introduced for these multi-stage methods to evaluate the overall energy dissipation rate of an EERK method such that one can choose proper parameters in some parameterized EERK methods or compare different kinds of EERK methods. Some existing EERK methods in the literature are evaluated from the perspective of preserving the original energy dissipation law and the energy dissipation rate. Some numerical examples are also included to support our theory.

**报告人简介:** 廖洪林, 应用数学博士, 2018 年至今任教于南京航空航天大学数学学院。2010 年在东南大学获理学博士学位, 2001-2017 先后任教于原解放军理工大学、陆军工程大学。学术研究方向为偏微分方程数值解, 目前主要关注线性和非线性偏微分方程的变步长时间离散与时间自适应算法, 在 Math Comp, SIAM J Numer Anal, SIAM J Sci Comput, IMA J Numer Anal, J Comput Phys, Sci China Math 等国内外专业期刊上发表学术研究论文五十余篇。

# 含高阶相互作用项的 Gross-Pitaevskii 方程的基态解求解算法

阮欣然 首都师范大学

**摘要:** 该报告将介绍两类求解含高阶相互作用项的 Gross-Pitaevskii 方程的基态解的数值算法思想: 归一化梯度流算法与基于离散能量泛函的优化算法。经典的归一化梯度流算法在较强的高阶相互作用下具有较强的稳定性限制, 报告中将介绍特殊的技巧以减弱该限制。同时针对强高阶相互作用情形, 报告将基于密度函数构造离散化的能量, 结合凸优化算法以实现该情形下基态解的高效计算。

**报告人简介:** 阮欣然, 男, 首都师范大学数学科学学院副研究员。自 2017 年在新加坡国立大学取得博士学位以来, 先后在法国国家信息与自动化研究所、索邦大学(原巴黎六大)等地进行博士后研究。2021 年 11 月入职首都师范大学。阮欣然博士近年来围绕着波色-爱因斯坦凝聚态中的平均场模型以及生物数学中的结构种群模型进行渐近分析与算法设计, 目前已在 SIAM, Sci. Comp. J, Comp. Phys 等高水平学术期刊发表论文十余篇。

## An asymptotic preserving scheme for the defocusing Davey-Stewartson II equation in the semiclassical limit

王汉权 云南财经大学

**Abstract:** We are devoted to constructing new numerical method for the semiclassical limit of the defocusing Davey-Stewartson II equation. We introduce Wentzel-Kramers-Brillouin ansatz for the equation, and the phase-amplitude reformulation is a modified Madelung transform in fact. Meanwhile, adding some asymptotically vanishing viscosity to obtain approximatively the solution on arbitrary time intervals for  $\varepsilon > 0$ . Note that the asymptotic preserving (AP) scheme exists an non-local potential on the inverse elliptic operator, and we apply Sine spectral method to avoid the singular symbol appears in the Fourier space. The Sine spectral method not only gives spectral accuracy in space, but also minimizes the numerical dissipation in this context. Moreover, we demonstrate the system is always locally well-posed in a class of Sobolev spaces, and indeed AP. Before the formation time of oscillations, numerous experiments corroborate the fact that the time-splitting spectral method is uniformly accurate with order 2 in time and with spectral in space accuracy.

**报告人简介:** 王汉权, 男, 新加坡国立大学博士。现任中国数学会计算数学分会常务理事、云南财经大学特聘教授、统计学博士生导师、云南财经大学数学硕士生导师、云南财经大学学术委员会委员、四川大学数学学院博士生导师等。科研活动主要关注计算数学与科学工程计算方向, 感兴趣的研究领域包括计算数学及其在玻色-爱因斯坦凝聚态物理、材料中的晶体位错运动现象、基本物质(原子、分子、等离子体等)在强激光场下的物理性质与反应、非线性光学等中的应用。从事科学研究的领域包括各种偏微分方程、随机偏微分方程的数值解法(有限差分法、谱方法、谱元法等)的设计与应用, 泛函极值问题求解方法设计与应用, 最优化理论方法与应用。现主持云南省基础研究项目重点项目 1 项。已经主持完成国家自然科学基金 4 项(其中包括重大计划项目培育项目 1 项、面上项目 1 项、地区基金 1 项、青年基金 1 项), “教育部留学回国人员科研启动基金”等。发表论文 50 余篇, 完成专著与教材 4 部(其中, SCI、EI 收录的高水平研究论文有四十余篇, 在科学出版社出版专著 2 部、教材 2 本)。2013 年入选教育部新世纪优秀人才支持计划。2014 年获得“云南省有突出贡献优秀专业技术人才”称号。2017 年获得云南省自然科学奖三等奖一项。

## **Multiple terms identification of time fractional diffusion equation with symmetric potential from nonlocal observation**

王泽文 广州航海学院、广州交通大学(筹)

**Abstract:** This talk considers a simultaneous identification problem of a time-fractional diffusion equation with a symmetric potential, which aims to identify the fractional order, the potential function and the Robin coefficient from a nonlocal observation. Firstly, the existence and uniqueness of the weak solution is established for the forward problem. Then, by the asymptotic behavior of the Mittag-Leffler function, the Laplace transform, and the analytic continuation theory, uniqueness of the simultaneous identification problem is proved under some appropriate assumptions. Finally, the Levenberg-Marquardt method is employed to solve the simultaneous identification problem for finding stably approximate solutions of the fractional order, the potential function and the Robin coefficient. Numerical experiments for three test cases are given to demonstrate the effectiveness of the presented inversion method.

**报告人简介:** 王泽文, 博士, 广州航海学院与广州交通大学(筹)教授, 博士生导师; 在东华理工大学工作期间, 2011 年破格晋升教授, 2021 年晋升二级教授; 主要从事一般反问题建

模与计算等研究工作，主持承担国家自然科学基金、省自然科学基金、教育厅科技项目等项目 10 余项，入选江西省主要学科学术与技术带头人资助计划和青年科学家培养计划，获江西省自然科学二等奖 1 项，江西省高校科技成果二等奖 1 项。

## **Regularity mechanism of nonlinear Schrodinger equations with rough potential**

吴奕飞 天津大学

**Abstract:** We consider the nonlinear Schrodinger equation with rough potential, which is often referred as the disordered NLS, and arises from the background of Anderson localization. In this talk, we focus on the regularity mechanism, and its related numerical discretization of the model.

**报告人简介:** 吴奕飞，天津大学应用数学中心讲席教授、博士生导师，入选国家高层次领军人才。从事偏微分方程理论和数值计算方面的研究工作，在非线性 Schrodinger 方程、KdV 方程等整体适定性和低正则算法构造方面做出一系列研究成果。解决了菲尔兹奖获得者 T.Tao 等提出的长时间遗留问题，设计了目前为止非线性 Schrodinger 方程和 KdV 方程正则性要求最低的快速格式，在 JEMS、CMP、Adv. Math、Anal. PDE、SINUM、Numer. Math.、Math. Comp. 等学术期刊中发表论文。

## **Inverse scattering problems of the biharmonic Schrödinger operator with a first order perturbation**

徐翔 浙江大学

**Abstract:** In this talk, we will discuss an inverse scattering problems for the biharmonic Schrödinger operator in three dimensions. A stability estimate of determining the divergence-free part of the operator is derived by far-field data at multiple wavenumbers. As a consequence, we further derive a quantitative stability estimate of determining the biharmonic Schrödinger operator. Both the stability estimates improve as the upper bound of the wavenumber increases, which exhibit the phenomenon of increased stability. Moreover, we obtain the uniqueness of recovering both potential and the first order perturbation by partial far-field data. The analysis employs scattering theory to obtain an analytic domain and an upper bound for the resolvent of the fourth order elliptic operator. Notice that

due to an obstruction to uniqueness, the corresponding results do not hold in general for the Laplacian. This can be explained by the fact that the resolvent of the biharmonic operator enjoys a faster decay estimate with respect to the wavenumber compared with the Laplacian.

**报告人简介:** 徐翔, 浙江大学数学科学学院院长聘副教授。徐翔的研究主要集中在反问题的理论与计算, 共发表 SCI 论文 30 余篇, 部分论文被列为 ESI 高引论文和 Inverse Problems 亮点收录。2013 年获得曙光青年学术奖, 2014 年入选“海外高层次人才计划青年项目”、浙江省特聘专家, 2016 年入选浙江省 151 人才工程。主持国家自然科学基金委面上项目, 参与国家自然科学基金委创新群体项目、重大研究计划重点项目、国际(地区)交流合作等多项项目。目前担任浙江省数学会秘书长、中国工业与应用数学会反问题与成像专委会秘书长等。

## **Auxiliary variable viscosity splitting (AVVS) method for the incompressible fluid flows**

杨钧翔 澳门科技大学

**Abstract:** We develop a novel energy-stable linear approach, which we term as auxiliary variable viscosity splitting (AVVS) method, to efficiently solve the incompressible fluid flows. Different from the projection-type methods with pressure correction, the AVVS method adopts the viscosity splitting strategy to split the original momentum equation into an intermediate momentum equation without divergence-free constraint and a advection-free momentum equation. A time-dependent auxiliary variable which has exact value 1 is introduced to construct a supplementary equation. The new model not only inherits the same dynamics of original incompressible Navier–Stokes equations, but also facilitate us to design linearly decoupled and energy-stable time-marching scheme. Comparing with the projection-type schemes, the present method leads to an energy dissipation law with respect to kinetic energy instead of an augmented energy including velocity and pressure gradient. In each time step, only two parabolic equations with constant coefficients and one Poisson equation need to be solved. Therefore, the numerical implementation is highly efficient. Moreover, the proposed AVVS method can be directly extended to construct linear, decoupled, and energystable scheme for the turbidity current system after we slightly modify the right-hand side of supplementary equation. Extensive numerical experiments are implemented to validate the accuracy, energy stability, and capability in complex fluid simulations.

**报告人简介:** 杨钧翔, 澳门科技大学创新工程学院计算机科学与工程学院助理教授, 2021 年 8 月博士毕业于韩国高丽大学应用数学专业, 2021 年 12 月-2023 年 6 月期间在中山大学科学计算所从事科研博士后/助理研究员工作。研究兴趣为多物理场耦合问题的数学建模、相场模型、多组份流体数值模拟、三维重构与图像处理算法、数值分析等。自 2018 年起, 共参与发表 SCI 级学术论文 90 余篇, 其中以第一或通信作者身份发表 SCI 论文 68 篇, 成果主要发表在 Journal of Computational Physics, Computer Methods in Applied Mechanics and Engineering, Communications in Nonlinear Science and Numerical Simulation, Computer Physics Communication, Applied Mathematical Modelling 等计算物理与计算数学领域知名期刊。主持了国家自然科学基金青年科学基金项目、中国博士后科学基金面上项目、澳门科技大学校内研究基金项目等。曾入选 2022 年中国博士后国际交流计划引进项目。

## **Numerical methods for the logarithmic Dirac equation**

易雯帆 湖南大学

**Abstract:** In this talk, we consider numerical methods to tackle numerical challenges for solving the logarithmic Dirac equation (LogDiracE). To address this, we propose a regularized LogDiracE with the linear convergence to the LogDiracE concerning a small regularization parameter for the bounded domain case. Then, a semi-implicit finite difference method, PINN method and FNO method are introduced to consider the regularized LogDiracE. These approaches guarantee a controlled solution that facilitates reliable simulations without succumbing to the logarithmic nonlinearity challenges for the LogDiracE.

**报告人简介:** 易雯帆, 湖南大学数学学院副教授, 2016 年博士毕业于湖南师范大学, 2016-2018 年在北京计算科学研究中心从事博士后研究, 期间访问新加坡国立大学数学系一年, 2018 年入职湖南大学数学学院。主要从事偏微分方程数值计算方法及相关理论和应用的研究, 研究工作涉及非线性偏微分方程多解计算大范围收敛性算法, 及量子力学多尺度高震荡模型的高效数值方法分析及数值模拟等方面的研究, 相关工作发表在 J. Comput.Phys, Sci. China Math, Multiscale Model. Simul, IMA J. Numer. Anal, Commun. Math. Sci, J. Sci. Comput 等计算数学期刊上, 现结题国家自然科学基金青年项目 1 项, 主持湖南省教育厅重点项目 1 项。

# 自旋轨道耦合 Spin-1 玻色-爱因斯坦凝聚的动力学模拟

袁永军 湖南师范大学

**摘要:** 本报告介绍模拟自旋轨道耦合 spin-1 玻色-爱因斯坦凝聚体(SOC spin-1 BEC)动力学的高效数值算法, 并对算法的可行性进行分析。首先给出自旋轨道耦合 spin-1 玻色-爱因斯坦凝聚的总质量、总能量、总磁化强度和冷凝宽度满足的动力学规律。然后, 为 SOC spin-1 BEC 的 Gross-Pitaevskii 方程组(CGPEs)构造合适的分裂算子, 进而设计模拟 SOC spin-1 BEC 动力学的时间两步分裂法。通过对分裂的第一个子问题做傅立叶变换和证明第二个分裂子问题对应的系数矩阵为常矩阵, 得出分裂的两个子问题分别在傅立叶空间和物理空间中都为常系数一阶常微分方程组。在此基础上, 在时间方向解析求解两个分裂子问题, 并给出时间两步分裂傅立叶谱方法的二阶格式和四阶格式的算法流程。通过大量数值实验, 模拟不同参数和不同初始值下 SOC spin-1 BEC 的动态解, 验证算法在时空方向的收敛性及总质量、总能量、总磁化强度和冷凝宽度满足的动力学规律, 并发现了 SOC spin-1 BEC 一些新的物理现象。

**报告人简介:** 袁永军, 湖南师范大学教授, 湖南省青年芙蓉学者。2007 年本科毕业于湖南师范大学大学数学与应用数学专业, 2012 年博士毕业于湖南师范大学计算数学专业, 2012 年至 2015 年先后在北京计算科学研究中心和新加坡国立大学从事博士后研究工作, 2015 年 11 月进入湖南师范大学工作至今。主要从事非线性偏微分方程多解计算和玻色-爱因斯坦凝聚数值模拟方面研究, 部分工作发表在 *Mathematics of Computation*, *SIAM Journal on Scientific Computing*, *Physical Review Letters*, *Journal of Computational Physics* 和 *Physical Review A* 等杂志。主持国家自然科学基金青年基金项目 and 面上项目各 1 项。

## Optimal zero-padding of kernel truncation method

张勇 天津大学

**Abstract:** The kernel truncation method (KTM) is a commonly-used algorithm to compute the convolution-type nonlocal potential, where the convolution kernel might be singular at the origin and/or far-field and the density is smooth and fast-decaying. In KTM, in order to capture the Fourier integrand's oscillations that is brought by the kernel truncation, one needs to carry out a zero-padding of the density, which means a larger physical computation domain and a finer mesh in the Fourier space by duality. The empirical fourfold zero-padding [ Vico et al. *J. Comput. Phys.* (2016) ] puts a heavy burden on memory requirement especially for higher dimension problems. In this paper, we

derive the optimal zero-padding factor, that is,  $\sqrt{d}+1$ , for the first time together with a rigorous proof. The memory cost is greatly reduced to a small fraction, i.e.,  $\lceil[(\sqrt{d}+1)/4]\rceil^d$ , of what is needed in the original fourfold algorithm. For example, in the precomputation step, a double-precision computation on a  $256^3$  grid requires a minimum 3.4 Gb memory with the optimal threefold zero-padding, while the fourfold algorithm requires around 8 Gb where the reduction factor is around 60%. Then, we present the error estimates of the potential and density in  $d$  space dimension. Next, we re-investigate the optimal zero-padding factor for the anisotropic density. Finally, extensive numerical results are provided to confirm the accuracy, efficiency, optimal zero-padding factor for the anisotropic density, together with some applications to different types of nonlocal potential, including the 1D/2D/3D Poisson, 2D Coulomb, quasi-2D/3D Dipole-Dipole Interaction and 3D quadrupolar potential.

**报告人简介:** 张勇, 2007 年本科毕业于天津大学, 2012 年在清华大学获得博士学位。他先后在奥地利维也纳大学的 Wolfgang Pauli 研究所, 法国雷恩一大和美国纽约大学克朗所从事博士后研究工作。2015 年 7 月获得奥地利自然科学基金委支持的薛定谔基金, 2018 年入选国家海外高层次人才计划。研究兴趣主要是偏微分方程的数值计算和分析工作, 尤其是快速算法的设计和应用。迄今发表论文 30 余篇, 主要发表在包括 SIAM Journal on Scientific Computing, SIAM journal on Applied Mathematics, Journal of Computational Physics, Mathematics of Computation, Computer Physics Communication 等计算数学顶尖杂志。2014 年获得“云南省有突出贡献优秀专业技术人才”称号。2017 年获得云南省自然科学奖三等奖一项。