上海财经大学、北京师范大学珠海校区联合主办

科学计算系列报告(3)

腾讯会议：12 月 3 日周六 386-905-058　　12 月 9 日周五 743-628-986

会议设备测试：08:45-09:00		
12 月 3 日　上午报告　　时间：9:00-11:15　　腾讯会议：386-905-058		
09:00-09:45	唐庆猋	Computing ground states of spin 2 Bose-Einstein condensates by the normalized gradient flow
9:45-10:30	毛志平	DeepONet and Deep MMnet for hypersonics
10:30-11:15	黄俊涛	Structure-preserving machine learning moment closures for the radiative transfer equation
12 月 3 日　下午报告　　时间：14:00-15:30　　腾讯会议：386-905-058		
14:00-14:45	许志钦	神经网络的凝聚现象
14:45-15:30	权超禹	On H^1-stability of an L2-type method on general nonuniform meshes for subdiffusion equation
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12 月 9 日　上午报告　　时间：9:00-11:00　　腾讯会议：743-628-986		
09:00-10:00	周涛	Deep adaptive sampling for numerical PDEs
10:00-11:00	姜立建	Bayesian filtering and transfer operators

Computing ground states of spin 2 Bose-Einstein condensates by the normalized gradient flow

Qinglin Tang(唐庆彝)
四川大学

In this talk, an efficient and accurate numerical method will be proposed to compute the ground state of spin-2 Bose-Einstein condensates (BECs) by using the normalized gradient flow (NGF)or imaginary time method (ITM). The key idea is twofold. One is to find the five projection or normalization conditions that are used in the projection step of NGF/ITM, while the other one is to find a good initial data for the NGF/ITM. Based on the relations between chemical potentials and the two physical constraints givenby the conservation of the total mass and magnetization, these five projection or normalization conditions can be completely and uniquely solved out. This allows one to successfully extend the NGF/ITM to compute the ground state of spin-2 BECs. Additionally, the structures and properties of the ground states in a uniform system are analysed so as to construct efficient initial data for NGF/ITM. Numerical results will be reported to show the efficiency of our method and to demonstrate some interesting physical phenomena.

报告人简介： 唐庆彝博士毕业于新加坡国立大学，曾先后在维也纳大学、法国洛林大学等高校从事博士后研究；曾入选国家海外高层次人才计划以及四川省学术带头人及后备人选。主要从事量子物理学中的数学模型的计算方法及理论分析方面的研究；已在 SISC、JCP 等期刊上发表多篇论文。

DeepONet and DeepMMnet for hypersonics

Zhiping Mao(毛志平)
厦门大学

In this work, we shall first introduce the deep operator neural networks (DeepONets). Then, we employ the DeepONets for approximating nonlinear operators arising from high-speed flows, where the coupled multiphysics and the resulting multiscale dynamics are challenging to resolve numerically. Specifically, we predict five species in the non-equilibrium chemistry downstream of a normal shock at high Mach numbers as well as the velocity and temperature fields. We then propose a composite supervised neural network, DeepMMnet, that uses multiple pre-trained DeepONets as building blocks and scattered measurements to infer the set of all seven fields in the entire domain of interest. Two DeepMMnet architectures are tested, and we demonstrate the accuracy and capacity for efficient data assimilation with both synthetic and experimental data.

报告人简介： 毛志平，厦门大学数学科学学院教授，2009 年本科毕业于重庆大学，2015 年博士毕业于厦门大学计算数学专业，国家高层次青年人才，2015 年 10 月至 2020 年 9 月在美国布朗大学应用数学系从事博士后研究。毛志平博士主

要从事谱方法以及机器学习方面的研究，其目前在 SIREV，JCP，SISC，SINUM、CMAME 等国际高水平杂志上发表论文 20 余篇。

Structure-preserving machine learning moment closures for the radiative transfer equation

Juntao Huang (黄俊涛)
Texas Tech University

In this talk, we present our work on structure-preserving machine learning (ML) moment closure models for the radiative transfer equation. Most of the existing ML closure models are not able to guarantee the stability, which directly causes blow up in the long-time simulations. In our work, with carefully designed neural network architectures, the ML closure model can guarantee the stability (or hyperbolicity). Moreover, other mathematical properties, such as physical characteristic speeds, are also discussed. Extensive benchmark tests show the good accuracy, long-time stability, and good generalizability of our ML closure model.

报告人简介： Dr. Juntao Huang is an assistant professor at Texas Tech University. He obtained the Ph.D. degree in Applied Math in 2018 and the bachelor degree in 2013 from Tsinghua University. Prior to joining Texas Tech University in 2022, he worked as a visiting assistant professor at Michigan State University. His research interests involve the design and analysis of numerical methods for partial differential equations (PDEs) and using machine learning to assist traditional scientific computing tasks. His recent work includes structure-preserving machine learning moment closures for kinetic models and adaptive sparse grid discontinuous Galerkin (DG) methods for high-dimensional PDEs.

神经网络的凝聚现象

Zhiqin Xu (许志钦)
上海交通大学

神经网络在非线性训练过程中经常会出现参数凝聚的现象，也就是神经元会分成多个组，每组内的神经元的行为类似。本报告将介绍凝聚现象，讨论其中的机制以及其对泛化的意义。

报告人简介： 许志钦，上海交通大学自然科学研究院/数学科学学院长聘教轨副教授。2012 年本科毕业于上海交通大学致远学院。2016 年博士毕业于上海交通大学，获应用数学博士学位。2016 年至 2019 年，在纽约大学阿布扎比分校和柯

朗研究所做博士后。与合作者共同发现深度学习中的频率原则、参数凝聚和能量景观嵌入原则，发展多尺度神经网络等。以第一作者或者通讯作者身份发表论文于 JMLR，AAAI，NeurIPS，SIMODS，CiCP，CSIAM Trans. Appl. Math.，JCP，Combustion and Flame，Eur. J. Neurosci.等学术期刊和会议。第一届中国机器学习与科学应用大会和 2022 Mathematical and Scientific Machine Learning 国际会议组织者之一。现为 Journal of Machine Learning 的创刊 managing editor 之一。

On H^1-stability of an L2-type method on general nonuniform meshes for subdiffusion equation

Chaoyu Quan (权超禹)
南方科技大学

In this work the $H1$ -stability of an L2 method on general nonuniform meshes is established for the subdiffffusion equation. Under some mild constraints on the time step ratio ρk, for example $0.4573328 \le \rho k \le 3.5615528$ for all $k \ge 2$, a crucial bilinear form associated with the L2 fractional derivative operator is proved to be positive semidefifinite. As a consequence, the H 1 -stability of L2 schemes can be derived for the subdiffffusion equation. In the special case of graded mesh, such positive Semidefifiniteness holds when the grading parameter $1 < r \le 3.2016538$ and therefore the H 1 -stability of L2 schemes holds. To the best of our knowledge, this is the fifirst work on the H 1 -stability of L2 method on general nonuniform meshes for subdiffffusion equation.

报告人简介：权超禹，南方科技大学杰曼诺夫数学中心研究助理教授，主要从事溶剂化模型、相场方程高精度算法、方面的研究。2013 年本科毕业于中国科学技术大学，2017 年博士毕业于巴黎第六大学 Lions 实验室（现索邦大学），师从 Yvon Maday 和 Benjamin Stamm。目前，已在 Math. Comp.，SIAM J. Sci. Comp.，J. Comp. Phys.，M3AS 等学术期刊发表/接收论文 20 篇，主持国自然基金 2 项、广东省基金 1 项和深圳市基金 2 项。

Deep adaptive sampling for numerical PDEs

Tao Zhou(周涛)
中科院数学与系统科学研究院

Adaptive computation is of great importance in numerical simulations. The ideas for adaptive computations can be dated back to adaptive finite element methods in 1970s. In this talk, we shall first review some recent development for adaptive method with applications. Then, we shall propose a deep adaptive sampling method for solving PDEs where deep neural networks are utilized to approximate the solutions. In particular, we propose the failure informed PINNs (FI-PINNs), which can adaptively refine the training set with the goal of reducing the failure probability. Compared to the neural network approximation obtained with uniformly distributed collocation points, the developed algorithms can significantly improve the accuracy, especially for low regularity and high-dimensional problems.

报告人简介：周涛，中国科学院数学与系统科学研究院研究员。曾于瑞士洛桑联邦理工大学从事博士后研究。主要研究方向为不确定性量化、偏微分方程数值方法以及时间并行算法等，近期的主要研究课题包括深度学习与科学计算，深度生成模型及其应用等。在国际权威期刊如 SIAM Review、SINUM、JCP 等发表论文 70 余篇。2018 年获优秀青年科学基金资助，2022 年获中组部高层次人才专项资助。现担任 SIAM J Sci Comput、J Sci Comput 等国际期刊编委，国际不确定性量化期刊（International Journal for UQ）副主编。

Bayesian filtering and transfer operators

Lijian Jiang (姜立建)
同济大学数学科学学院

Bayesian filtering and transfer operators have significant connection and play important roles in stochastic dynamical systems. There exist two transfer operators: Koopman operator and Perron-Frobenius operator. In the talk, I will discuss two problems:(1) Bayesian filtering is used to correct the approximation of Koopman operator in noisy dynamical systems; (2) Perron-Frobenius operator filter is derived in Bayesian filtering. The application is investigated in data-driven modeling.

报告人简介：同济大学数学院教授，主要研究方向是多尺度问题的计算、建模和不确定性量化，统计学习。曾获国家青年人才计划支持。现任 JCAM（Journal of computational and Applied Mathematics ）,JCMDS （ Journal of Computational Mathematics and Data Science）、数值计算与计算机应用（Journal on Numerical Methods and Computer Applications）期刊编委（Associate Editor:）。在 Journal of Computational Physics, , SIAM Journal on Scientific Computing , Multiscale Modeling and Simulation，Advances in Computational Mathematics, 等重要期刊发表一系列重要论文。