The Third HKSIAM Biennial Conference
July 7 – July 11, 2025

The purpose of the HKSIAM Biennial conference is to provide a forum to expose the mathematical community to the most updated advances in industrial and applied mathematics, promoting research on various mathematical challenges arising from scientific problems and industrial applications. A key feature of the conference is our intention to invite some world-renowned mathematicians who are working at the frontiers of industrial and applied mathematics to give distinguished lectures. Another aim of the event is to bring together different groups of mathematicians working on industrial and applied mathematics in Hong Kong and to stimulate new mathematical ideas, initiate and enhance the existing collaborations between the researchers in Hong Kong and the international community to produce first-rate results in this area.

Plenary Speakers

Weizhu Bao (National University of Singapore)
Zhiming Chen (Chinese Academy of Sciences)
Patrick Ciarlet (ENSTA Paris)
Xin Guo (University of California, Berkeley)
Anders Hansen (Cambridge University)
Michael Hintermueller (Weierstrass Institute of Applied Analysis and Stochastics)
Shi Jin (Shanghai Jiaotong University)
Kui Ren (Columbia University)
Simon See (NVIDIA)
Hongkai Zhao (Duke University)

Organizing Committee

Eric Chung (Co-Chair)
Gary Choi (CUHK)
Kuang HUANG (CUHK)
Bangti Jin (Co-Chair)
Liu Liu (Communications Secretary)
Ronald Lok Ming Lui (General Secretary)
Xiaolu Tan (Communications Secretary)
Tieyong Zeng (CUHK)
Jun Zou (HKSIAM President)

Scientific Committee

Xiaojun CHEN
Ka Chun CHEUNG
Wai Ki CHING
Yayan LU
Defeng SUN
Yang WANG
Juncheng WEI
Zhouping XIN
Kun XU
Yida XU
Wenan ZANG
Xiaosheng ZHUANG

Sponsors

HKSIAM 香港工業與應用數學學會

CUHK SCI 香港中文大學理學院 FACULTY OF SCIENCE THE CHINESE UNIVERSITY OF HONG KONG

DEPARTMENT OF MATHEMATICS THE CHINESE UNIVERSITY OF HONG KONG

HKMS 香港數學學會 The Hong Kong Mathematical Society

香港中文大學新亞書院 New Asia College, The Chinese University of Hong Kong

香港培華教育基金會 Hong Kong Pei Hua Education Foundation

香港中文大學 聯合書院 UNITED COLLEGE THE CHINESE UNIVERSITY OF HONG KONG

Enquiry

Website: https://www.math.cuhk.edu.hk/conference/hksiam2025/
Address: Department of Mathematics,
The Chinese University of Hong Kong,
Shatin, Hong Kong

Contents

Introduction

The purpose of the HKSIAM Biennial conference is to provide a forum to expose the mathematical community to the most updated advances in industrial and applied mathematics, promoting research on various mathematical challenges arising from scientific problems and industrial applications. A key feature of the conference is our intention to invite some world-renowned mathematicians who are working at the frontiers of industrial and applied mathematics to give distinguished lectures. Another aim of the event is to bring together different groups of mathematicians working on industrial and applied mathematics in Hong Kong and to stimulate new mathematical ideas, initiate and enhance the existing collaborations between the researchers in Hong Kong and the international community to produce first-rate results in this area. The first and second HKSIAM Biennial conference were successfully held in January 11-15, 2021 and August 28 - Septmember 1, 2023. For more information, please see: IAS Conference on Industrial and Applied Mathematics (Jan 11-15, 2021) and The Second HKSIAM Biennial Meeting (Aug 28- Sept 1, 2023).

Scientific Background

Modern manufacturing and service industries have changed drastically due to the explosion in the knowledge economy. Fast and inexpensive computing, office products, the development and utilization of large databases, have necessitated sophisticated methods to meet new demands. Industrial and applied mathematics is the enabling factor in realizing and implementing these methods. In recent years, the mathematical community has responded to this growing need for the mathematically proved solution in the industry. Organizations such as the Fields Institute, Mitacs, and PIMS in Canada, IPAM, SIAM and the NSF in the United States, and Newton Institutes in the United Kingdom have been promoting the interaction of mathematics with industry and continuing to research on various mathematical problems arisen from economic development and technological advancement.

Industrial and applied mathematics is an inherently interdisciplinary field. In addition to mathematics, it includes subjects from fields outside mathematics such as business, computer science, medical sciences and engineering. An industrial mathematician has strong analytical and problem-solving skills

built upon a background of computing, mathematics, statistics, and basic science. Numerous reports and studies carried out by professional organizations show that there is a growing demand in the workforce for mathematics scholars with the practical skills to work with managers, engineers, etc.

Industrial and applied mathematics is a well-established field within the mathematical sciences community. Every four years there is an International Congress on Industrial and Applied Mathematics. Industrial and applied mathematics focuses on problems which come from industry and aims for solutions which are relevant to the industry, including finding the most efficient (i.e. cost-effective) way to solve the problem. With the increasing complexity and sophistication of modern industry, individuals who are able to understand technical issues, formulate precise and accurate mathematical models, implement solutions using the latest computer techniques, and convey these ideas to their co-workers who may be managers or engineers, are becoming a necessary part of many organizations and companies. Examples of areas in the industry that industrial and applied mathematics plays a key role are signal and image processing, computer graphics, computer vision, risk management, system reliability, software testing, and verification, database systems, production line optimization, and marketing research.

Conference Venue

The conference will be held in Cheng Yu Tung Building (CYT) [Point 1]. It is located next to the Hotel Hyatt Regency Hong Kong Shatin [Point 2]. It take approximately 2 minutes to walk from University MTR Station (Exit B) [Point 3]

Directions from Hyatt Regency Shatin to Conference (CYT)

Point 1: Conference Venue Cheng Yu Tung Building (CYT)
Point 2: Hyatt Regency Hong Kong Shatin
Point 3: University Station (Exit B)

Directions from ALVA Hotel to Conference (CYT)

Point 1: Conference Venue Cheng Yu Tung Building (CYT)
Point 2: University Station (Exit B)
Point 3: ALVA Hotel
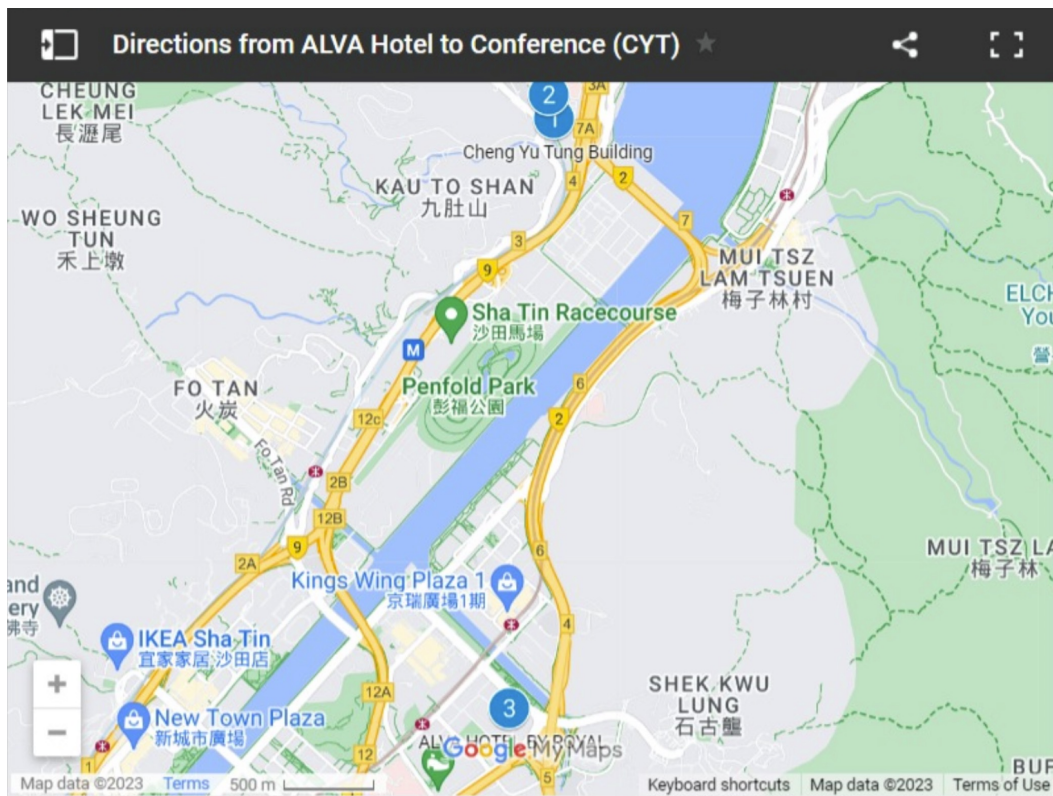
Directions from Royal Park Hotel to Conference (CYT)

Point 1: Conference Venue Cheng Yu Tung Building (CYT)
Point 2: University Station (Exit B)
Point 3: Royal Park Hotel

Lunch and Conference Banquet

Lunch : Participants will be provided with lunch box on the "Stage Restaurant" at Level 3 of the Conference Venue (CYT Building).

Banquet : The Conference Banquet will be held on Wednesday 18:30 - 20:45 at the restaurant THE STARVIEW restaurant (Address: 1/F, 1 On Ping Street, Sha Tin).

Shuttle Bus will pick up guests at 18:00 at the roundabout between CYT building and Hyatt Hotel. For return, shuttle bus will depart from THE STARVIEW restaurant at 21:00.

Banquet : THE STARVIEW restaurant (星海薈)
Address: 1/F, 1 On Ping Street, Sha Tin (沙田安平街 1 號 1 樓).

Conference Schedule

The Third HKSIAM Biennial Conference, 07-11, July 2025

Monday	Tuesday	Wednesday	Thursday	Friday
8:30 – 8:50 Registration 8:50 – 9:00 Opening Speech				
9:00 – 9:50 Zhiming Chen	9:00 – 9:50 Xin Guo	9:00 – 9:50 Weizhu Bao	9:00 – 9:50 Patrick Ciarlet	9:00 – 9:50 Shi Jin
Coffee Break	Group Photo + Coffee	9:50 – 10:40 Kui Ren	9:50 – 10:40 Hongkai Zhao	Closing Ceremony + Coffee
10:20 – 12:20 **MS01, MS02, MS10, MS07,** **MS14, MS16** (4 talks session)	10:20 – 12:20 **MS06, MS02, MS20, MS15,** **MS03, MS17** (4 talks session)	Coffee Break	Coffee Break	10:20 – 12:20 **MS08, MS13, MS20, SC03,** **MS14, MS19** (4 talks session)
		11:10 – 12:40 **MS09, MS05, MS04, MS11,** **MS12, MS19** (3 talks session)	11:10 – 12:40 **MS08, MS05, MS04, MS11** **MS12, SC01** (3 talks session)	
12:30 – 14:00 Lunch	12:30 – 14:00 Lunch	12:40 – 14:00 Lunch	12:40 – 14:00 Lunch	12:30 – 14:00 Lunch
14:00 – 14:50 Simon See	14:00 – 14:50 Anders Hansen	Free Afternoon + 17:00-18:00 HKSIAM General Meeting	14:00 – 16:00 **MS01, MS08, MS10, MS07,** **MS03, MS19** (4 talks session)	14:00 – 16:00 **SC04, MS13, MS17, MS18,** **MS12, MS19** (4 talks session)
15:00 – 16:30 **MS09, MS04, MS17, MS15,** **MS19** (3 talks session)	14:50 – 15:40 Michael Hintermueller			
	Coffee Break		Coffee Break	
16:30 – 18:00 Reception	16:10 – 18:10 **MS06, MS07, MS10, MS18,** **MS14, MS16** (4 talks session)		16:30 – 18:00 **MS08, MS09, MS11, MS12,** **SC02** (3 talks session)	Updated: 2025-07-03
		18:30 – 20:45 Banquet		

10

The Third HKSIAM Biennial Conference
Monday, 7th July 2025

Time						
8:30-8:50	Registration					
8:50-9:00	Opening Speech					
9:00 - 9:50	Plenary Session LT1 Chair: Jun ZOU	Zhiming CHEN Recent progress of high order finite element methods on arbitrarily shaped domains				
9:50-10:20	Coffee Break					
10:20-12:20	MS01, LT1	MS02, 209A	MS10, 209B	MS07, 203	MS14, 202	MS16, 201
	Yuming Ba	Xiaochun Cao	Gang Chen	Shuo Zhang	Ruchi Guo	Jianbo Cui
	Jian Huang	Tianwei Zhang	Rongfang Gong	Shuonan Wu	Lingyun Qiu	Liu Liu
	Zhichao Peng	Youzhi Zhang	Wei Gong	Xuehai Huang	Woojoo Lee	Roy He
	Lingling Ma	Zitong Yu	Yifeng Xu	Shihua Gong	Jiahua Jiang	
12:30 - 14:00	Lunch Break					
14:00 - 14:50	Plenary Session LT1 Chair: Eric CHUNG	Simon SEE From Classical Scientific Discovery to the Era of AI: A Transformational Path				
15:00 - 16:30	MS09, LT1	MS04, 209A	MS17, 209B	MS15, 203		MS19, 201
	Chenglong Bao	Jianguo Huang	Yiqi Gu	Luchan Zhang		Zuoqiang Shi
	Jian Huang	Chunmei Su	Zhengyu Huang	Tiantian Xu		Xiaobo Yin
	Zihao Hu	Seungchan Ko	Hao Liu	Xiaoxue Qin		Shuonan Wu
16:30 - 18:00	Reception					

The Third HKSIAM Biennial Conference
Tuesday, 8th July 2025

9:00 - 9:50	Plenary Session LT1 Chair: Yang XIANG	Xin GUO An alpha-potential game framework for multi-agent system				
9:50 - 10:20	Group Photo + Coffee Break					
10:20 - 12:20	MS06, LT1	MS02, 209A	MS20, 209B	MS15, 203	MS03, 202	MS17, 201
	Huaian Diao	Bo Han	Lijun Bo	Lina Zhao	Junqing Chen	Junchi Yan
	Yueguang Hu	Xiaoge Zhang	Ibrahim Ekren	Yaguang Gu	Wenjia Jing	Linlin Zhong
	Long Li	Zhiyong Yang	Said Hamadène	Wanli Yu	Sanghyeon Yu	Bin Gao
	Arpan Mukherjee	Shuren Qi	Hanxiao Wang	Xiaomin Pan	Yu Gao	Tao Xiong
12:30 - 14:00	Lunch Break					
14:00 - 15:40	Plenary Session LT1 Chair: Leevan LING	Anders HANSEN Necessary mechanisms for super AI and stopping hallucinations: The consistent reasoning paradox and the 'I don't know' function				
		Michael HINTERMUELLER A PINN-based multi-complexity solver as a PDE-constrained optimization problem				
15:40 - 16:10	Coffee Break					
16:10 - 18:10	MS06, LT1	MS07, 209A	MS10, 209B	MS18, 203	MS14, 202	MS16, 201
	Youjun Deng	Michael Neilan	Weiwei Hu	Xingding Chen	Yunho Kim	Chao Wang
	Shutong Hou	Jun Cao	Yongcun Song	Qingsong Zou	Ye Zhang	Tao Luo
	Ahcene Ghandriche	Min Zhang	Zhiyu Tan	Ruchi Guo	Soomin Jeon	Haixia Liu
	Xinlin Cao	Shudan Tian	Julius Fergy Rabago	Shihua Gong	Zhiyuan Li	Cheng Tang

The Third HKSIAM Biennial Conference
Wednesday, 9th July, 2025

9:00 - 10:40	Plenary Session LT1 Chair: Bangti JIN Ronald LUI	Weizhu BAO Structure-preserving parametric finite element methods for geometric PDEs and applications				
		Kui REN Phase Retrieval in Fresnel Regime and Nonlinear Optical Encryption				
10:40 - 11:10	Coffee Break					
11:10 - 12:40	MS09, LT1	MS05, 209A	MS04, 209B	MS11, 203	MS12, 202	MS19, 201
	Daniel Zhengyu Huang	Xin Liang	Xiaoli Li	Tao Xiong	Fenglei Fan	Zhiping Mao
	Fei Wang	Haoran Guan	Rui Ma	Xinghui Zhong	Juncai He	Yiqun Li
		Nian Shao	Xiaofeng Cai	Min Tang	Wei Huang	Xuehong Cui
12:40 - 14:00	Lunch Break					
14:00 - 18:30	Free Afternoon HKSIAM General Meeting (17:00-18:00 LT1A)					
18:30 - 20:45	Banquet					

The Third HKSIAM Biennial Conference
Thursday, 10th July 2025

9:00 - 10:40	Plenary Session LT1 Chair: Zhi ZHOU	Patrick CIARLET Solving problems with sign-changing coefficients: T-coercivity and beyond
		Hongkai ZHAO Mathematical and Computational Understanding of Neural Networks: From Representation to Learning Dynamics and From Shallow to Deep

10:40 - 11:10	Coffee Break					
11:10 - 12:40	MS08, LT1	MS05, 209A	MS04, 209B	MS11, 203	MS12, 202	SC01, 201
	Zhiwen Zhang	Wen Ting Wu	Qinglin Tang	Yanli Wang	Enming Liang	Kota TAKEDA
	Zhen Zhang	Jingyu Liu	Yue Feng	Kunlun Qi	Fanghui Liu	Yueqi WANG
	Pingyuan Wei	Hei Yin Lam	Jie Du	Jaeyong Lee	Atsushi Nitanda	Zexian LI

12:40 - 14:00	Lunch Break					
14:00 - 16:00	MS01, LT1	MS08, 209A	MS10, 209B	MS07, 203	MS03, 202	MS19, 201
	Xiaomin Pan	Yuanfei Huang	Jiajie Li	Shukai Du	Zetao Fei	Changpin Li
	Lijie Ji	Qiao Huang	Zhi Zhou	Xiang Wang	Jiaxin Zhou	Changtao Sheng
	Xiang Sun	Shenglan Yuan	Shengfeng Zhu	Ruishu Wang	Jinrui Zhang	Yufeng Nie
	Hongqiao Wang		Maolin Deng		Xinyu Liu	Xiangcheng Zheng

16:00 - 16:30	Coffee Break					
16:30 - 18:00	MS09, LT1	MS08, 209A		MS11, 203	MS12, 202	SC02, 201
	Zhiguo Wang	Shuting Gu		Zhongjian Wang	Lei Shi	Chenhao LU
	Chaozhen Wei	Weiguo Gao		Zheng Ma	Jiaye Teng	Xingguang JIN
	Huayi Wei				Jinming Weng	Qingle LIN

The Third HKSIAM Biennial Conference
Friday, 11th July 2025

9:00 - 9:50	Plenary Session LT1 Chair: Liu LIU	Shi JIN Quantum Computation of partial differential equations and related problems				
9:50 - 10:20	Closing Ceremony + Coffee Break					
10:20 - 12:20	MS08, LT1	MS13, 209A	MS20, 209B	SC03, 203	MS14, 202	MS19, 201
	Hongqiao Wang	Hao Dong	Gaoyue Guo	Zhenyi ZHU	Mikyoung Lim	Daxin Nie
	Xiaopeng Chen	Shubin Fu	Simone Scotti	Xiao MENG	Jiho Hong	Maria Lopez-Fernandez
	Chengyu Liu	Viet Ha Hoang	Jiaqiang Wen	Yixuan ZHANG	Wenlong Zhang	Yuwen Li
	Haijun Yu	Jian Huang	Lihu Xu	Tsz Ching CHOW		
12:30 - 14:00	Lunch Break					
14:00 - 16:00	SC04, LT1	MS13, 209A	MS17, 209B	MS18, 203	MS12, 202	MS19, 201
	Yuchen HUANG	Hyea Hyun Kim	Zhiwen Zhang	Chen Cui	Xiaotong Yuan	Xiaochuan Tian
	Tsz Lok IP	Mengnan Li	Yuwen Li	Fei Wang	Shao-Qun Zhang	Nicola De Nitti
	Trung Hieu GIANG	Yating Wang	Juncai He	Ying Yang	Shijun Zhang	Jieqiong Zhang
	Zhen HAO	Xiangcheng Zheng	Huayi Wei	Taishan Zeng	Chenghao Liu	Minghua Chen

Plenary Talks

Contents

Weizhu Bao
(Department of Mathematics, National University of Singapore)

Structure-preserving parametric finite element methods for geometric PDEs and applications

In this talk, I begin with a review of different geometric flows (PDEs) including mean curvature (curve shortening) flow, surface diffusion flow, Willmore flow, etc., which arise from materials science, interface dynamics in multiphase flows, biology membrane, computer graphics, geometry, etc. Different mathematical formulations and numerical methods for mean curvature flow are then discussed. In particular, an energy-stable linearly implicit parametric finite element method (PFEM) is presented in details. Then the PFEM is extended to surface diffusion flow and anisotropic surface diffusion flow, and a structure-preserving implicit PFEM is proposed. Finally, sharp interface models and their PFEM approximations are presented for solid-state dewetting. This talk is based on joint works with Harald Garcke, Wei Jiang, Yifei Li, Robert Nuernberg, Tiezheng Qian, David Srolovitz, Yan Wang and Quan Zhao.

Zhiming Chen
(Chinese Academy of Sciences)

Recent progress of high order finite element methods on arbitrarily shaped domains

We consider high-order unfitted finite element methods on Cartesian meshes with hanging nodes for elliptic interface problems, which release the work of body-fitted mesh generation and allow us to design adaptive finite element methods for solving curved geometric singularities. We will review the progress in two-dimensional problems and introduce a new high order unfitted finite element method in three-dimension that improves the numerical stability of high-order unfitted finite element methods on arbitrarily shaped smooth domains. This talk is based on joint works with Ke Li, Yong Liu, Maohui Lyu and Xueshuang Xiang.

Patrick Ciarlet
(POEMS, ENSTA, Institut Polytechnique de Paris, France)

Solving problems with sign-changing coefficients: T-coercivity and beyond

In electromagnetic theory, the effective response of specifically designed materials is modeled by strictly negative coefficients: these are the so-called negative materials. Transmission problems with discontinuous, sign-changing coefficients then occur in the presence of negative materials surrounded by classical materials. Establishing Fredholmness is well-understood thanks to the T-coercivity approach, which was first introduced for these transmission problems by Bonnet-Ben Dhia, Ciarlet and Zwölf [1].

The T-coercivity approach relies on the design of an operator T to realize the inf-sup condition and, in principle, it can be applied to any variational formulation in Hilbert spaces. If the operator is carefully chosen, it can provide useful insight for a "natural" definition of the approximation of the exact problem. The derivation of the discrete inf-sup condition then becomes elementary, at least when one considers conforming methods, that is when the discrete finite element spaces are subspaces of the exact Hilbert spaces : both the exact and the approximate problems are considered, analysed and solved at once.

For problems with sign-changing coefficients, the shape of the interface separating the two materials must be taken into account to solve the problems numerically: specific meshing rules have to be implemented to design the meshes. And, when one is solving the full Maxwell system, the operator T at hand does not lead to a "natural" discrete counterpart.

To overcome these limitations, another method has been recently developed by Ciarlet, Lassounon and Rihani [2], which relies on the use of an optimal control reformulation of the problem. On the one hand, the resulting numerical method converges without any restriction on the mesh and, on the other hand, it can be used to solve the full Maxwell system. This method is inspired by the smooth extension method, originally introduced by Fabrèges, Gouarin and Maury [3].

References

[1] A.-S. Bonnet-Ben Dhia, P. Ciarlet Jr., C.M. Zwölf. *Time harmonic wave diffraction problems in materials with sign-shifting coefficients*, J. Comput. Appl. Math., **234** (2010), pp. 1912–1919, Corrigendum p. 2616.

[2] P. Ciarlet Jr., D. Lassounon, M. Rihani. *An optimal control-based numerical method for scalar transmission problems with sign-changing coefficients*, SIAM J. Numer. Anal., **61(3)** (2023), pp. 1316–1339.

[3] B. Fabrèges, L. Gouarin, B. Maury. *A smooth extension method*, C. R. Acad. Sci. Paris, Série I, **351** (2013), pp. 361–366.

Xin Guo
(University of California, Berkeley)

An alpha-potential game framework for multi-agent system

Designing and analyzing non-cooperative multi-agent systems interacting within a shared dynamic environment is a central challenge in many existing and emerging applications, including autonomous driving, smart grid management, and e-commerce. A primary objective in these systems is for agents to reach some Nash equilibrium, where no agent benefits from changing its strategy unilaterally. However, designing algorithms for approximating or computing Nash equilibrium is generally intractable unless a certain structure of underlying multi-agent interactions can be exploited.

In this talk we will present a new paradigm for dynamic N-player non-cooperative games called alpha-potential games, where the change of a player's value function upon unilateral deviation from her strategy is equal to the change of an alpha-potential function up to an error alpha. This game framework is shown to reduce the challenging task of finding alpha-Nash equilibria for a dynamic game to minimizing the associated alpha-potential function. The latter is then shown to be a conditional McKean–Vlasov control problem. In such games, analysis of alpha reveals critical game characteristics,

including choices of admissible strategies, the intensity of interactions, and the level of heterogeneity among players. We will discuss through simple examples some recent theoretical developments, along with a few open problems for this new game framework.

Dr. Xin Guo holds the Coleman Fung Chair professorship and chairs the IEOR department at UC Berkeley. She previously held positions at Cornell (2003-2006) and IBM research (1999-2003). Her research interests and most influential works encompass stochastic analysis, controls, games, reinforcement learning, transfer learning, and generative models, alongside financial and medical data analysis. Notably, her work has been adopted by industry, including Amazon, where it has generated hundreds of millions of dollars in cost savings. She has also laid some of the mathematical foundation for FDA-approved early- cancer-detection methodology.

Anders Hansen
(Cambridge University)

Necessary mechanisms for super AI and stopping hallucinations: The consistent reasoning paradox and the 'I don't know' function

Creating Artificial Super Intelligence (ASI) (AI that surpasses human intelligence) is the ultimate challenge in AI research. This is, as we show, fundamentally linked to the problem of avoiding hallucinations (wrong, yet plausible answers) in AI. We discover a key mechanism that must be present in any ASI. This mechanism is not present in any modern chatbot and we establish that without it, ASI will never be achievable. Moreover, we reveal that AI missing this mechanism will always hallucinate. The mechanism we introduce is the computation of what we call an 'I don't know' function. An 'I don't know' function determines when an AI is correct and when it will not be able to answer with 100% confidence. The root to these findings is the Consistent Reasoning Paradox (CRP) that we discover, which is a paradox in logical reasoning. The CRP shows that the above mechanism must be present, and that – surprisingly – the weaker concept of being 'almost

sure' is impossible. In particular, an ASI cannot be 'almost sure' (say 90% sure). It will compute an 'I don't know' function and either be correct with 100% confidence, or it will not be more than 50% sure. The CRP addresses a long-standing issue that stems from Turing's famous statement that infallible AI cannot be intelligent, where he questions how much intelligence may be displayed if an AI makes no pretence at infallibility. The CRP reveals the answer – consistent reasoning requires fallibility – and thus marks a necessary fundamental shift in AI design if ASI is to ever be achieved and hallucinations to be stopped.

Michael Hintermueller
(Weierstrass Institute of Applied Analysis and Stochastics)

A PINN-based multi-complexity solver as a PDE-constrained optimization problem

We study physics-informed neural networks (PINNs) constrained by partial differential equations (PDEs) and their application in approximating multiscale PDEs. From a continuous perspective, our formulation corresponds to a non-standard PDE-constrained optimization problem with a PINN-type objective. From a discrete standpoint, the formulation represents a hybrid numerical solver that utilizes both neural networks and finite elements. We propose a function space framework for the problem and develop an algorithm for its numerical solution, combining an adjoint-based technique from optimal control with automatic differentiation. The multiscale solver is applied to a heat transfer problem with oscillating coefficients, where the neural network approximates a fine-scale problem, and a coarse-scale problem constrains the learning process. We show that incorporating coarse-scale information into the neural network training process through our modelling framework acts as a preconditioner for the low-frequency component of the fine-scale PDE, resulting in improved convergence properties and accuracy of the PINN method. The relevance of the hybrid solver to numerical homogenization is discussed.

Shi Jin
(Shanghai Jiaotong University)

Quantum Computation of partial differential equations and related problems

Quantum computers have the potential to gain algebraic and even up to exponential speed up compared with its classical counterparts, and can lead to technology revolution in the 21st century. Since quantum computers are designed based on quantum mechanics principle, they are most suitable to solve the Schrodinger equation, and linear PDEs (and ODEs) evolved by unitary operators. The most efficient quantum PDE solver is quantum simulation based on solving the Schrodinger equation. It will be interesting to explore what other problems in scientific computing, such as ODEs, PDEs, and linear algebra that arise in both classical and quantum systems, can be handled by quantum simulation.

   We will present a systematic way to develop quantum simulation algorithms for general differential equations. Our basic framework is dimension lifting, that transfers non-autonomous ODEs/PDEs systems to autonomous ones, nonlinear PDEs to linear ones, and linear ones to Schrodinger type PDEs. Our formulation allows both qubit and qumode (continuous-variable) formulations, and their hybridizations, and provides the foundation for analog quantum computing.

Kui Ren
(Columbia University)

Phase Retrieval in Fresnel Regime and Nonlinear Optical Encryption

We study an inverse problem in nonlinear optical encryption. We first show that double random phase encryption based on nonlinear optics, modeled with a nonlinear Schrödinger equation, is vulnerable to chosen-plaintext attacks (CPA). We then propose an intrinsically nonlinear encryption method by supplementing the double random phase encryption with the medium property as an additional security key. We analyze the stability of the CPA

attack on the system. Numerical simulations are presented to validate the theoretical understanding. The talk is based on joint works with Yan Cheng, Yiwei Chen, and Nathan Soedjak.

Simon See
(NVIDIA)

From Classical Scientific Discovery to the Era of AI: A Transformational Path

Scientific discovery has historically been driven by meticulous observation, hypothesis testing, and experimental validation—a methodical approach rooted in logic and empirical reasoning. Over centuries, advancements in mathematics, physics, and engineering provided the foundation for systematic inquiry, enabling breakthroughs that shaped modern civilization. With the advent of computational power in the 20th century, the research paradigm expanded to incorporate data-driven methodologies, simulation models, and automation. The emergence of artificial intelligence (AI) has now accelerated this trajectory, introducing algorithmic discovery, pattern recognition, and autonomous hypothesis generation. AI-powered systems process vast datasets at unprecedented speed, uncovering correlations beyond human capability and enabling self-adapting models in fields ranging from genomics to quantum physics. This transition from traditional scientific exploration to AI-driven discovery signifies a profound shift: knowledge generation is no longer limited by human intuition alone but augmented by machine intelligence. As AI reshapes scientific inquiry, ethical considerations, interpretability, and interdisciplinary collaboration remain essential for harnessing its potential responsibly. The fusion of human expertise with AI-driven insights marks the dawn of a new era—one where discovery is not just accelerated, but reimagined.

Hongkai Zhao
(Duke University)

Mathematical and Computational Understanding of Neural Networks: From Representation to Learning Dynamics and From Shallow to Deep

In this talk I will present both mathematical and numerical analysis as well as experiments to understand a few basic computational issues in using neural networks, as a particular form of nonlinear representation determined by the network structure and activation function, to approximate functions. I will start with frequency bias of shallow networks in terms of both representation and learning. Based on the understanding of shallow networks, we propose a structured and balanced approximation using multi-component and multi-layer neural network (MMNN) structure. While an easy modification to fully connected neural networks (FCNNs) or multi-layer perceptrons (MLPs) through the introduction of balanced multi-component structures in the network, MMNNs achieve a significant reduction of training parameters, a much more efficient training process, and a much improved accuracy compared to FCNNs or MLPs. Extensive numerical experiments are presented to illustrate the effectiveness of MMNNs in approximating functions with significant high frequency components and its automatic adaptivity in both space and frequency domain, a desirable feature for non-linear representation.

Minisymposium Talks

Contents

MS01 Statistical Inverse Problems and Model Order Reduction: Theory, Algorithms, and Applications

Organizers:
Qiuqi Li, Hunan University, qli28@hnu.edu.cn
Hongqiao Wang, Central South University, hongqiao.wang@csu.edu.cn
Lijie Ji, Shanghai University, lijieji@shu.edu.cn

Yuming Ba,
Guangdong Polytechinc Normal University
yumingba@gpnu.edu.cn

A reduced-order method based on Fourier transform for time-dependent parameterized problemsa

In this presentation, a reduced-order method based on Fourier transform is proposed for the complex dynamical systems. Here the frequendcy-domain methods is used to convert the original time-dependent parabolic equation into a frequency-dependent elliptic equation, where variable frequencies are independent. This can lead to the parallel computation for approximating the solution. Based on the frequency method, we proposed the model reduction methods to solve the frequency-dependent elliptic problems with random inputs. In this work, we first apply the proposed method to the nonlocal diffusion problems. The numerical results show that it can provide a good approximation of original problems and improve the computation efficiency. Then, we presents a Variable-separation (VS) method based on frequency-domain techniques for solving time-domain Maxwell systems with random inputs. The goal is to obtain a separated representation of the Galerkin solution to Maxwell's equations. The VS method utilizes an offline-online decomposition to efficiently solve the derived equations in the space-frequency domain. Furthermore, the frequency variable is treated as a one-dimensional random parameter, which enables the VS model to be constructed once and then reused for all frequencies involved in the inverse Fourier transform. This approach significantly enhances the computational efficiency by eliminating the need for repeated model construction.

Jian Huang,
National Center for Applied Mathematics in Hunan & Xiangtan
University
huangjian213@xtu.edu.cn

Multiscale model reduction for the time fractional thermoporoelasticity
problem in fractured and heterogeneous media

In this talk, we shall introduce the time fractional thermoporoelasticity problem in fractured and heterogeneous media. The mathematical model with a time memory formalism is described by a coupled system of equations for pressure, temperature and displacements. We use an implicit finite difference approximation for temporal discretization. We present a fine grid approximation based on the finite element method and Discrete Fracture Model (DFM) for two-dimensional model problems. Further, we use the Generalized Multiscale Finite Element Method (GMsFEM) for coarse grid approximation. The primary concept behind the proposed method is to streamline the complexity inherent in the thermoporoelasticity problem. Given that our model equation incorporates multiple fractional powers, leading to multiple unknowns with memory effects, we aim to address this intricacy by optimizing the problem's dimensionality. As a result, the solution is sought on a coarse grid, a strategic choice that not only simplifies the computational cost but also contributes to significant time savings. We present numerical results for the two-dimensional model problems in heterogeneous fractured porous media. We derive relative errors between the reference fine grid solution and the multiscale solution for different numbers of multiscale basis functions. The results confirm that the proposed method is able to achieve good accuracy with a few degrees of freedoms on the coarse grid.

Zhichao Peng,
The Hong Kong University of Science and Technology
pengzhic@ust.hk

Goal-Oriented Adaptive and Hybrid Reduced Order Modeling for Multiscale
Kinetic Transport Equations

We present novel reduced order modeling (ROM) strategies for multiscale kinetic transport equations that bridge macroscopic diffusion limits and microscopic statistical mechanics. The high-dimensional nature of these equations necessitates dimensionality reduction at the discrete level. While the system converges to a diffusion limit under strong scattering effects, it remains transport-dominated in weak scattering regimes where classical linear model order reduction (MOR) techniques may lose efficiency due to the well-known Kolmogorov barrier. To address this challenge, we design robust piecewise linear ROMs is developed. A novel goal-oriented time partitioning strategy is introduced to automatically adjusting temporal resolution based on system dynamics while maintaining insensitivity to various empirical initial partitioning choices. Moreover, we further enhance the online efficiency piecewise linear ROM by designing a hybrid ROM, which leverages auto-encoder -based nonlinear ROMs for extremely challenging transport-dominated time intervals and using computationally efficient piecewise linear reduction for remaining intervals.

Lingling Ma,
Hunan First Normal University
hudlingling@126.com

An iterative method Based on Generalized Multiscale Finite Element
Methods for Parameter-Dependent Dual Continuum model

In the report, we consider an iterative method based on Generalized Multiscale Finite Element Method (GMsFEM) to solve the dual continuum model with random inputs. The main idea of iterative methods is to reformulate the original model into another model with parameter-independent diffusion coefficients and parameter-dependent right-hand sides. Subsequently, a fixed-point iteration is used to compute the solution of the reformulated model. To quantify the statistics of the dual continnum model, we need to solve the coupled system for a large number of samples in the stochastic space. Thus the computation is prohibitively expensive. To exploit the advantages from the GMsFEM, we perform the iteration process in reduced GMsFE space to improve the computation efficiency. The proposed iterative method consisits of two stage, including an offline phase and an online phase. In offline

28

stage, we compute local multiscale basis functions in each coarse grid region based on deterministic multiscale characteristics to construct offline spaces. In online phase, a fixed-point iteration method is employed to compute the solution of the reformulated model in the offline spaces. Additionally, convergence analysis is established under some structure conditions. Finally, we present two numerical tests to show the performance of our proposed method and validate the theoretical convergence results.

Xiaomin Pan,
Shanghai University
xmpan@shu.edu.cn

Non-intrusive reduced-order modeling framework using proper orthogonal decomposition and polynomial chaos expansion

In this study, we present a novel non-intrusive reduced-order model (ROM) for solving time-dependent stochastic partial differential equations (SPDEs). Utilizing proper orthogonal decomposition (POD), we extract spatial modes from high-fidelity solutions. A dynamic model decomposition (DMD) method is then applied to vertically stacked matrices of projection coefficients for future prediction of coefficient fields. Polynomial chaos expansion (PCE) is employed to construct a mapping from random parameter inputs to the DMD-predicted coefficient field. These lead to the POD-DMD-PCE method. The innovation lies in vertically stacking projection coefficients, ensuring time-dimensional consistency in the coefficient matrix for DMD, and facilitating parameter integration for PCE analysis. This method combines the model reduction of POD with the time extrapolation strengths of DMD, effectively recovering field solutions both within and beyond the training time interval. The efficiency and time extrapolation capabilities of the proposed method are validated through various nonlinear SPDEs. These include a reaction-diffusion equation with 19 parameters, a two-dimensional heat equation with two parameters, and a one-dimensional Burgers equation with three parameters.

Lijie Ji,
Shanghai University
lijieji@shu.edu.cn

Reduced Over-Collocation Method with Adaptive Time Partitioning and
Adaptive Enrichment for Parametric Time-Dependent Equations

Abstract of the presentation: Nonlinear and nonaffine terms in parametric partial differential equations can potentially lead to a computational cost of a reduced order model that is comparable to the cost of the original full order model. To address this, the Reduced Residual Reduced Over-Collocation method (R2-ROC) is developed as a hyper-reduction method within the framework of the reduced basis method in the collocation setting. The vanilla R2-ROC method can face instability when applied to parametric fluid dynamic problems. In this talk, we introduce an adaptive time partitioning and adaptive enrichment strategy-based ROC method (AAROC). The adaptive time partitioning dynamically captures the low-rank structure, necessitating fewer reduced collocation points being sampled in each time segment. Numerical experiments on the parametric viscous Burgers' equation and lid-driven cavity problems demonstrate the efficiency, enhanced stability, and accuracy of the proposed AAROC method.

Xiang Sun,
Ocean University of China
sunxiang@ouc.edu.cn

Deep Learning-Based Reduced-Order Modeling for Parameterized
Convection-Dominated Partial Differential Equations

Reduced-order modeling of fluid flows has been an active area of research. It approximates the evolution of physical systems in time in terms of coherent patterns and structures that generally consist of a dimensionality reduction mechanism and a dynamical model in the reduced state space. This paper proposes a deep learning-based reduced-order modeling composed of β-variational autoencoder, multilayer perceptron, and transformer architectures for problems governed by the parameterized convection-dominated partial differential equations. In our approach, β-variational autoencoder is

utilized as a dimensionality reduction mechanism, transformer is trained to predict the future state of the system, and multilayer perceptron is applied to learn the relationship between different parameter values and latent space representations. Therefore, the future state of the system can be obtained in the online phase. The proposed method is tested on several benchmark convection-dominated partial differential equations, such as Burgers' equation, traffic flow problem, shallow water equation and Navier-Stokes equation. The results demonstrate the applicability and effectiveness of the proposed reduced-order modeling method for convection-dominated partial differential equations.

Hongqiao Wang,
Central South University
Hongqiao.Wang@csu.edu.cn

Accelerated Bayesian Optimal Experimental Design via Conditional Density Estimation and Informative Data

The Design of Experiments (DOEs) is a fundamental scientific methodology that provides researchers with systematic principles and techniques to enhance the validity, reliability, and efficiency of experimental outcomes. In this study, we explore optimal experimental design within a Bayesian framework, utilizing Bayes' theorem to reformulate the utility expectation—originally expressed as a nested double integral—into an independent double integral form, significantly improving numerical efficiency. To further accelerate the computation of the proposed utility expectation, conditional density estimation is employed to approximate the ratio of two Gaussian random fields, while covariance serves as a selection criterion to identify informative data-set during model fitting and integral evaluation. In scenarios characterized by low simulation efficiency and high costs of raw data acquisition, key challenges such as surrogate modeling, failure probability estimation, and parameter inference are systematically restructured within the Bayesian experimental design framework. The effectiveness of the proposed methodology is validated through both theoretical analysis and practical applications, demonstrating its potential for enhancing experimental efficiency and decision-making under uncertainty.

MS02 Trustworthy ML: Theory and Applications

Organizers: Shuren Qi, Fenglei Fan, Youzhi Zhang, and Xiaoge Zhang

Xiaochun Cao
Sun Yat-sen University
caoxiachun@mail.sysu.edu.cn

Attribution-based Safety in Agent Decision-making

Ensuring the safety of agent decision-making is a critical challenge in artificial intelligence, with significant implications for improving decision reliability, safety monitoring, and risk prevention. Attribution techniques, as a core component of explainability, face the key question of whether they can effectively enhance decision safety and reliability. Prior research shows that attribution analysis not only clarifies model decision processes but also plays a vital role in model quality monitoring and risk control. High-quality explanations are crucial, as models with better performance often exhibit more reasonable attribution distributions, which help identify decision anomalies. Certain training strategies can also improve the reasonableness of attributions. This talk systematically explores attribution-based safety in agent decision-making across three areas: interpretable attribution techniques, attribution-guided training, and attribution-based anomaly monitoring and correction. We first review attribution methods at the input, parameter, and data levels to identify factors influencing decisions and provide theoretical support. Next, we analyze existing attribution-guided training methods and their effects on attribution reasonableness and model performance. Finally, we investigate whether attribution distributions correlate with decision reliability in deployment, explore how monitoring attribution anomalies can enhance safety, and assess low-cost online correction methods for decision failures. Our goal is to offer theoretical foundations and technical pathways for safer agent decision-making, supporting future research and implementation. We also evaluate attribution techniques in embodied and non-embodied agent scenarios, assess their maturity, and outline future trends.

Bio: Xiaochun Cao is the Dean of School of Cyber Science and Technology, Sun Yat-sen University. His research interests include: artificial intelligence especially computer vision, and content analysis in cyber space, etc. He received the B.E. and M.E. degrees both in computer science from Beihang University (BUAA), China, and the Ph.D. degree in computer science from the University of Central Florida, USA, with his dissertation nominated for the university level Outstanding Dissertation Award. After graduation, he spent about three years at ObjectVideo Inc. as a Research Scientist. Before joining SYSU, he was a professor at Institute of Information Engineering, Chinese Academy of Sciences. He has authored and coauthored over 300 journal and conference papers. In 2004 and 2010, he was the recipients of the Piero Zamperoni best student paper award at the International Conference on Pattern Recognition. Dr. Cao was the recipients of Outstanding Young Scientists Fund and Excellent Young Scientists Fund of National Natural Science Foundation of China, in 2020 and 2014, respectively. He is on the editorial boards of IEEE Transactions on Pattern Analysis and Machine Intelligence, IEEE Transactions on Image Processing, IEEE Transactions on Multimedia, and Acta Electronica Sinica. He was on the editorial board of IEEE Transactions on Circuits and Systems for Video Technology.

Tianwei Zhang
Nanyang Technological University
tianwei.zhang@ntu.edu.sg

Safety Benchmarking and Testing of Multimodal Large Language Models

Multimodal Large Language Models (MLLMs), epitomized by ChatGPT, Stable Diffusion and Heygen, have made remarkable strides in very recent years. They significantly simplify the tasks of creating high-quality content in various modalities such as images, videos, and coherent text based on users' demands. However, the widespread adoption of generative models has also raised ethical and societal concerns. Issues related to data privacy, bias in AI algorithms, and the potential for model misuse have become subjects of intense debate. In this talk, I will introduce some works towards the safety benchmarking and testing of MLLMs. These studies accentuate the pressing challenges and opportunities in securing large model ecosystems.

Bio: Tianwei Zhang is currently an associate professor at College of Computing and Data Science, Nanyang Technological University, Singapore. He is the deputy director of cyber security research centre @ NTU, and associate director of NTU Centre Computational Technologies for Finance. He received his Bachelor's degree at Peking University in 2011, and Ph.D degree at Princeton University in 2017. He has been involved in the organization committee of numerous technical conferences. He serves on the editorial board of IEEE Transactions on Circuits and Systems for Video Technology (TCSVT) since 2021, and receives the best editor award in 2023. His research focuses on building efficient and trustworthy computer systems. He has published more than 150 papers in top-tier security, AI, and system conferences and journals. He has received several research awards, including Distinguished Paper Award @ ASPLOS'23, Distinguished Paper Award @ ACL'24, Distinguished Artifact Award @ Usenix Security'24, Distinguished Artifact Award @ CCS'24.

Youzhi Zhang
Hong Kong Institute of Science & Innovation
youzhi.zhang.lgc@gmail.com

A Game-theoretic Approach for Trustworthy AI

Progress in AI has often been measured by the mastery of games, and game-theoretical AI systems have been applied to solve many real-world problems as well. Game theory is an important tool for trustworthiness, especially security. In this talk, I will first present the game-theoretic approach for public security, especially about a real-world problem of urban network security games, where law enforcement officers must respond quickly to apprehend a criminal who is choosing an escape route while the criminal strategically selects a path to evade capture. Based on that, I will show how game theory can be used for trustworthy AI.

Bio: Youzhi Zhang is an associate professor of CAIR, HKISI-CAS and was an assistant professor during August 2022 - April 2025. Before joining CAIR, he was a postdoctoral researcher at the Northwestern University, USA, working with Professor V.S. Subrahmanian. From August 2020 to August 2021, he was a postdoctoral researcher at the Dartmouth College, USA,

working with Professor V.S. Subrahmanian. He received the Ph.D degree in Computer Science from the Nanyang Technological University, Singapore, where he was advised by Professor Bo An. Prior to that, he received the Bachelor and Master degrees from the Sun Yat-sen University, China. His research interests include artificial intelligence, multi-agent systems, computational game theory, multi-agent reinforcement learning, optimization, and decision making in complex environments including security and healthcare. For contributions to algorithms for equilibrium computation in multiplayer games and their applications, he won the Ph.D Best Thesis Award from the School of Computer Science and Engineering, Nanyang Technological University in 2021.

Zitong Yu
Great Bay University
yuzitong@gbu.edu.cn

Subtle Visual Computing

Subtle visual signals, though often imperceptible to the human eye, contain subtle yet crucial information that can reveal hidden patterns within visual data. By applying advanced computer vision and representation learning techniques, we can unlock the potential of these signals to better understand and interpret complex environments. This ability to detect and analyze subtle signals has profound implications across various fields, e.g., 1) from medicine, where early identification of minute anomalies in medical imaging can lead to life-saving interventions, 2) from industry, where spotting micro-defects in production lines can prevent costly failures, 3) from affective computing, where understanding micro-expression and micro-gesture under human interaction scenarios can benefit the deception detection. In this talk, we will introduce foundation models and methods to detect and decode these 'subtle visual signals' on representative downstream applications.

Bio: Zitong Yu received the Ph.D. degree in Computer Science and Engineering from the University of Oulu, Finland, in 2022. Currently, he is an Assistant Professor at Great Bay University, China. He was a Postdoctoral researcher at ROSE Lab, Nanyang Technological University. He was a visiting scholar at TVG, University of Oxford, from July to November 2021. He

is a Senior Member of IEEE. His research focus on subtle visual computing. He has published more than 40 works on top-tier journals and conferences such as TPAMI/IJCV/CVPR/ICCV/ECCV, and received 6200 google citations. He was AC/SPC of ACM MM'25, ICME'23, BMVC'24/25, IJCB'24, and IJCAI'25. He organized the 1st Workshop & Challenge on Subtle Visual Computing on ACM MM'25 and Special Issue Subtle Visual Computing on Machine Intelligence Research. He won the 1st Place in the ChaLearn Multi-Modal Face Anti-spoofing Attack Detection Challenge with CVPR'20. He was a recipient of IAPR Best Student Paper Award, IEEE Finland Section Best Student Conference Paper Awar, second prize of the IEEE Finland Jt. Chapter SP/CAS Best Paper Award, Best Paper Candidate of ICME'24, Best Paper Honorable Mention Award of CCBR'24, and World's Top 2% Scientists 2023/2024 by Stanford.

Bo Han
Hong Kong Baptist University
bhanml@comp.hkbu.edu.hk

Exploring Trustworthy Foundation Models:
Benchmarking, Finetuning and Reasoning

In the current landscape of machine learning, where foundation models must navigate imperfect real-world conditions such as noisy data and unexpected inputs, ensuring their trustworthiness through rigorous benchmarking, safety-focused finetuning, and robust reasoning is more critical than ever. In this talk, I will focus on three recent research advancements that collectively advance these dimensions, offering a comprehensive approach to building trustworthy foundation models. For benchmarking, I will introduce CounterAnimal, a dataset designed to systematically evaluate CLIP's vulnerability to realistic spurious correlations, revealing that scaling models or data quality can mitigate these biases, yet scaling data alone does not effectively address them. Transitioning to finetuning, we delve deep into the process of unlearning undesirable model behaviors. We propose a general framework to examine and understand the limitations of current unlearning methods and suggest enhanced revisions for more effective unlearning. Furthermore, addressing reasoning, we investigate the reasoning robustness under noisy rationales by constructing the NoRa dataset and propose contrastive denoising

with noisy chain-of-thought, a method that markedly improves denoising-reasoning capabilities by contrasting noisy inputs with minimal clean supervision.

Bio: Bo Han is currently an Associate Professor in Machine Learning and a Director of Trustworthy Machine Learning and Reasoning Group at Hong Kong Baptist University, and a BAIHO Visiting Scientist of Imperfect Information Learning Team at RIKEN Center for Advanced Intelligence Project (RIKEN AIP), where his research focuses on machine learning, deep learning, foundation models, and their applications. He was a Visiting Research Scholar at MBZUAI MLD (2024), a Visiting Faculty Researcher at Microsoft Research (2022) and Alibaba DAMO Academy (2021), and a Postdoc Fellow at RIKEN AIP (2019-2020). He received his Ph.D. degree in Computer Science from University of Technology Sydney (2015-2019). He has co-authored three machine learning monographs, including Machine Learning with Noisy Labels (MIT Press), Trustworthy Machine Learning under Imperfect Data (Springer Nature), and Trustworthy Machine Learning from Data to Models (Foundations and Trends). He has served as Senior Area Chair of NeurIPS, and Area Chairs of NeurIPS, ICML and ICLR. He has also served as Associate Editors of IEEE TPAMI, MLJ and JAIR, and Editorial Board Members of JMLR and MLJ. He received paper awards, including Outstanding Paper Award at NeurIPS, Most Influential Paper at NeurIPS, and Outstanding Student Paper Award at NeurIPS Workshop, and service awards, including Notable Area Chair at NeurIPS, Outstanding Area Chair at ICLR, and Outstanding Associate Editor at IEEE TNNLS. He received the RGC Early CAREER Scheme, IEEE AI's 10 to Watch Award, IJCAI Early Career Spotlight, INNS Aharon Katzir Young Investigator Award, RIKEN BAIHO Award, Dean's Award for Outstanding Achievement, Microsoft Research StarTrack Scholars Program, and Faculty Research Awards from ByteDance, Baidu, Alibaba and Tencent.

Xiaoge Zhang
The Hong Kong Polytechnic University
xiaoge.zhang@polyu.edu.hk

Implementing Trust in Non-Small Cell Lung Cancer Diagnosis with a Conformalized Uncertainty-Aware AI Framework in Whole-Slide Images

Ensuring trustworthiness is fundamental to the development of artificial intelligence (AI) that is considered societally responsible, particularly in cancer diagnostics, where a misdiagnosis can have dire consequences. Current digital pathology AI models lack systematic solutions to address trustworthiness concerns arising from model limitations and data discrepancies between model deployment and development environments. To address this issue, we developed TRUECAM, a framework designed to ensure both data and model trustworthiness in non-small cell lung cancer subtyping with whole-slide images. TRUECAM integrates 1) a spectral-normalized neural Gaussian process for identifying out-of-scope inputs and 2) an ambiguity-guided elimination of tiles to filter out highly ambiguous regions, addressing data trustworthiness, as well as 3) conformal prediction to ensure controlled error rates. We systematically evaluated the framework across multiple large-scale cancer datasets, leveraging both task-specific and foundation models, illustrate that an AI model wrapped with TRUECAM significantly outperforms models that lack such guidance, in terms of classification accuracy, robustness, interpretability, and data efficiency, while also achieving improvements in fairness. These findings highlight TRUECAM as a versatile wrapper framework for digital pathology AI models with diverse architectural designs, promoting their responsible and effective applications in real-world settings.

Bio: Xiaoge Zhang is an Assistant Professor in the Department of Industrial and Systems Engineering (ISE) at The Hong Kong Polytechnic University. His research interests center on risk management, reliability engineering, and trustworthiness assurance of AI/ML-powered intelligent systems using uncertainty quantification, knowledge-enabled AI, and fail-safe measures. He received his Ph.D. in Systems Engineering and Operations Research at Vanderbilt University, Nashville, Tennessee, United States in 2019. He has won multiple awards, including Peter G. Hoadley Best Paper Award, Chinese Government Award for Outstanding Self-Financed Students Studying Abroad, Bravo Zulu Award, Pao Chung Chen Fellowship, among others. He has published more than 80 papers in leading academic journals, such as

Nature Communications, IEEE Transactions on Artificial Intelligence, IEEE Transactions on Information Forensics and Security, IEEE Transactions on Reliability, IEEE Transactions on Cybernetics, IEEE Transactions on Industrial Informatics, IEEE Transactions on Automation Science and Engineering, Reliability Engineering & Systems Safety, Risk Analysis, Decision Support Systems, and Annals of Operations Research, among others. He is on the editorial board of Journal of Organizational Computing and Electronic Commerce. He is a member of INFORMS, IEEE and IISE.

Zhiyong Yang
University of Chinese Academy of Sciences
yangzhiyong21@ucas.ac.cn

Pursuing a Proper Allocation of the Probability Mass in Knowledge Distillation

Knowledge Distillation (KD) transfers knowledge from a large teacher model to a smaller student model by minimizing the divergence between their output distributions, typically using forward Kullback-Leibler divergence (FKLD) or reverse KLD (RKLD). It has become an effective training paradigm due to the broader supervision information provided by the teacher distribution compared to one-hot labels. In this talk, we identify that the core challenge in KD lies in balancing two mode-concentration effects: the Hardness-Concentration effect, which refers to focusing on modes with large errors, and the Confidence-Concentration effect, which refers to focusing on modes with high student confidence.

Through an analysis of how probabilities are reassigned during gradient updates, we observe that these two effects are entangled in FKLD and RKLD, but in extreme forms. Specifically, both are too weak in FKLD, causing the student to fail to concentrate on the target class. In contrast, both are too strong in RKLD, causing the student to overly emphasize the target class while ignoring the broader distributional information from the teacher.

To address this imbalance, we propose ABKD, a generic framework with α-β-divergence. Our theoretical results show that ABKD offers a smooth interpolation between FKLD and RKLD, achieving a better trade-off between these effects. Extensive experiments on 17 language/vision datasets with 12 teacher-student settings confirm its efficacy.

Bio: Zhiyong Yang received the MSc degree in computer science and technology from the University of Science and Technology Beijing (USTB), in 2017, and the PhD degree from the University of Chinese Academy of Sciences (UCAS), in 2021. He is currently a tenure-track assistant professor with the UCAS. His research interests lie in machine learning and learning theory, with special focus on AUC optimization, meta-learning/multi-task learning, and learning theory for recommender systems. He has authored or coauthored several academic papers in top-tier international conferences and journals including T-PAMI/ICML/NeurIPS/CVPR. He served as a reviewer for several top-tier journals and conferences such as T-PAMI, ICML, NeurIPS, and ICLR.

Shuren Qi
The Chinese University of Hong Kong
shurenqi@cuhk.edu.hk

Rethink Deep Learning with Invariance in Data Representation

Integrating invariance into data representations is a principled design in intelligent systems. Representations play a fundamental role, where systems and applications are both built on meaningful representations of digital inputs (rather than the raw data). In fact, the proper design/learning of such representations relies on priors w.r.t. the task of interest. Here, the concept of symmetry from the Erlangen Program may be the most fruitful prior — informally, a symmetry of a system is a transformation that leaves a certain property of the system invariant. Symmetry priors are ubiquitous, e.g., translation as a symmetry of the object classification, where object category is invariant under translation.

The quest for invariance is as old as pattern recognition itself. Invariant design has been the cornerstone of various representations in the era before deep learning, such as the SIFT. As we enter the early era of deep learning, the invariance principle is largely ignored and replaced by a data-driven paradigm, such as the CNN. However, this neglect did not last long before they encountered bottlenecks regarding robustness, interpretability, efficiency, and so on. The invariance principle has returned in the era of rethinking deep learning, forming a new field known as Geometric Deep Learning (GDL).

In this talk, I will give a historical perspective of the invariance in data representations. More importantly, I will introduce research dilemmas, promising works, future directions, and our contributions.

Bio: Shuren Qi is currently a Postdoctoral Fellow with Department of Mathematics, The Chinese University of Hong Kong. His research focuses on Geometric Deep Learning, with applications in Trustworthy AI and Science AI. He has authored 12 papers in top-tier journals and conferences, such as IEEE TPAMI and USENIX Security. His works offer some new designs of invariant representations — from global to local and hierarchical assumptions. More information is available at https://shurenqi.github.io/.

MS03 Wave Propagation in Novel Materials and its Application in Inverse Problems and Imaging

Organizer: Hai Zhang

Junqing Chen,
Tsinghua University
jqchen@tsinghua.edu.cn

Calculating the propagating modes of electromagnetic wave in periodic structures

When the electromagnetic wave incidents on the periodic structures, beside the scattering field, some propagating modes which are traveling in the periodic medium could be generated. We study the calculating of the propagating modes. We formulate the problem as a nonlinear eigenvalue problem in an unbounded periodic domain. Then we use perfectly matched layers to truncate the unbounded domain, recast the problem to a quadratic eigenvalue problem, and prove the approximation property of the truncation. Finally, we formulate the quadratic eigenvalue problem to a general eigenvalue problem, use the finite element method to discrete the truncation problem, and show numerical examples to verify theoretical results.

Wenjia Jing
Tsinghua University
wjjing@tsinghua.edu.cn

Dynamics of wave packets near a Dirac point in the subwavelength regime

It is known that Dirac dispersion cones exist at subwavelength scales in bubbly honeycomb phononic crystals. In this talk we will present the time-evolution of wave packets that are spectrally concentrated near such a Dirac point. It turns out that the wave packets remain spectrally close to the Dirac point while the envelopes evolve according to a 2D Dirac system up to a long time. The subwavelength scale affects the description naturally. The talk is based on a joint work with H. Ammari and X. Fu.

Sanghyeon Yu
Korea University
sanghyeon_yu@korea.ac.kr

Wave propagation near geometric singularities

Concentrating light at the nanoscale is one of the greatest challenge in optics. If conventional optical devices are used, one cannot focus light into a spot smaller than a few hundred of nanometers due to the diffraction limit. Nano-optics overcomes this fundamental difficulty using various optical nanostructures having 'geometrical singularities' on their surfaces. Light can be strongly localized near the geometric singularity point and it is of high importance to understand this singular phenomenon quantitatively for nano-optics applications. Its mathematical analysis requires to solve the PDE spectral problem for an elliptic operator where two key assumptions break down: uniform ellipticity and boundary smoothness, resulting in the singular behavior of solutions. It In this talk, we discuss how to characterize the singularity of solutions to the spectral PDE towards a mathematical theory of nano-optics.

Yu GAO,
Department of Mathematics, The Hong Kong University of
Science and Technology
yugaomath@gmail.com

Optimal Design of Broadband Plasmonic Nanoparticles via Reduced-Order Modeling

In this talk, we present an optimal design problem for broadband absorption materials composed of plasmonic nanoparticles, with broad applications across engineering and physics. The design process poses significant computational challenges, including multi-particle interactions, frequency responses across resonant and broadband regimes, non-convex optimization, and shape derivative computations. To address these challenges, we develop a general optimization framework based on integral equations, introducing a parameterized formulation that avoids direct shape derivative calculations. For computational efficiency, we employ reduced-order modeling, first simplifying

the problem using elliptical particles before generalizing to arbitrary shapes with larger parameters. Further acceleration is achieved through a shape-dependent reduced basis method: the forward problem is solved using eigenfunctions of the Neumann-Poincaré (NP) operator, while the adjoint problem leverages the eigenfunctions of the dual NP operator—both approaches rigorously handle integral equation singularities. To overcome non-convex optimization difficulties, we propose an initialization strategy under weak particle interactions, which estimates the number and size of nanoparticles as an initial guess before gradient-based refinement. Numerical experiments demonstrate the method's accuracy, efficiency, robustness, and flexibility in achieving optimal material designs.

Zetao FEI,
Ecole Polytechnique
zetao.fei@polytechnique.edu

Model-based Super-resolution: Towards a Unified Framework for Super-resolution

In mathematics, a super-resolution problem can be formulated as acquiring high-frequency data from low-frequency measurements. This extrapolation problem in the frequency domain is well-known to be unstable. We propose the model-based super-resolution framework (Model-SR) to address this ill-posedness. Within this framework, we can recover the signal by solving a nonlinear leastsquare problem and achieve super-resolution. Theoretically, the resolution-enhancing map is proved to have Lipschitz continuity under mild conditions, leading to a stable solution to the super-resolution problem. We apply the general theory to three concrete models and give the stability estimates for each model. Numerical experiments are conducted to show the super-resolution behavior of the proposed framework. The model-based mathematical framework can be extended to problems with similar structures.

Jiaxin Zhou,
Department of Mathematics, City University of Hong Kong
jiaxzhou@cityu.edu.hk

Super-Resolution Imaging via Resonant Subwavelength Coaxial Annular Holes

This work presents a mathematical analysis of resonances for an array of subwavelength coaxial annular holes and a new super-resolution imaging approach using the resonant structure. By employing a multiscale analytical framework based on a combination of the integral equation in the exterior domain and the waveguide mode expansion inside the small three-dimensional holes, we derive asymptotic expansions of complex-valued scattering resonances for the underlying subwavelength structure and analyze the electromagnetic field amplification at the resonant frequencies. In particular, it is shown that the resonant modes oscillate on a subwavelength scale in the near field if the annular holes are placed close to each other. By leveraging this observation, we develop a novel super-resolution imaging approach that utilizes resonant modes through the subwavelength resonant structure as the illuminate pattern and present a numerical reconstruction algorithm to solve the underlying inverse problem. Numerical examples show that a ten-fold improvement can be achieved in image resolution with the new imaging method.

Jinrui Zhang,
Zhejiang University
zhangjinrui@zju.edu.cn

Selective focusing of multiple particles in homogeneous and layered medium

Inverse scattering of multiple particles has a wide range of applications. In this talk, we apply the DORT (Decomposition of the Time Reversal Operator) method to this imaging problem, enabling selective focusing on each particle using far field measurements under different boundary conditions. Specifically, we show that under suitable conditions, each particle with various boundary generates several significant eigenvalues with the corresponding

eigenfunctions producing incident waves that focus selectively on the associated particle. Extension to inverse scattering in layered medium is also given.

Xinyu Liu,
Hong Kong University of Science and Technology
xliuem@connect.ust.hk

Model Selection and Parameter Estimation of One-Dimensional Gaussian Mixture Models

Mixture models are widely employed across various fields to model data and signals originating from sub-populations or distinct sources. Among these models, the Gaussian mixture model (GMM) has emerged as one of the most extensively studied and widely applied models. In this talk, we discuss the challenge of learning one-dimensional Gaussian mixture models (GMMs) with a specific focus on estimating both the model order and the mixing distribution from i.i.d. samples. We introduce the computational resolution limit (CRL), a novel concept that helps quantify the lower bound on the sampling complexity for exactly recovering the model order. Notably, this concept can also be extended to the estimation of the GMM means. We propose an algorithm that leverages Fourier measurements to estimate both the model order and the mixing distribution. Our analysis shows that the algorithm's sampling complexity matches the established lower bound, confirming its optimality. Numerical experiments further demonstrate that our approach outperforms conventional methods in terms of efficiency and accuracy. Both the concept and algorithm can be extended to the high-dimensional GMMs.

MS04 Recent development on advanced numerical schemes for challenging PDEs

Organizers: Lina Zhao

Jianguo Huang,
Shanghai Jiao Tong University
jghuang@sjtu.edu.cn

A locking-free virtual element method for 3D linear elasticity problems

In this talk, we will focus on proposing and analyzing a new locking-free lowest order virtual element method for the linear elasticity problem in three dimensions. Concretely speaking, a virtual element function on a polyhedron K is harmonic, while its restriction on the boundary of K is a continuous piecewise linear function with respect to an auxiliary triangulation. Such construction requires no further 3D partition of K. Under some reasonable mesh assumptions, we derive the inverse inequality, the norm equivalence and the error estimate of the interpolation operator for the underlying virtual element. Using these results combined with a rigorous analysis, we establish a robust error estimate in H1 norm for the proposed method. Finally, we perform numerical results to demonstrate theoretical findings. The talk is based on a joint work with Wenxuan Wang from Shanghai Jiao Tong University.

Chunmei Su,
Tsinghua University
sucm13@163.com

Temporal high-order structure-preserving parametric finite element methods for curvature flows

Firstly we propose a series of temporal high-order parametric finite element methods to simulate curvature flows. Particularly, for those flows with multiple geometric structures, e.g., surface diffusion which decreases the area and preserves the volume, we propose a type of structure-preserving methods by incorporating two scalar Lagrange multipliers and two evolution equations involving the area and volume, respectively. These schemes can effectively

preserve the structure at a fully discrete level. Extensive numerical experiments demonstrate that our methods achieve the desired temporal accuracy, as measured by the manifold distance, while simultaneously preserving the geometric structure of the surface diffusion.

Seungchan Ko,
Inha University
scko@inha.ac.kr

Analysis and approximation of generalized Newtonian fluids with
non-standard growth conditions

In this talk, we consider a system of nonlinear partial differential equations modeling the motion of an incompressible non-Newtonian fluid with non-standard growth conditions. For this model, a fluid can change its rheological properties through various external stimuli (e.g. electric or magnetic fields, temperature, light, pH value, concentrations of chemical molecules). Due to the variable dependency of the power-law index, establishing compactness results cannot be achieved by standard techniques and requires additional technical treatments. In this talk, we discuss mathematical results regarding the well-posedness of weak and strong solutions of such models. And then we construct a finite element approximation for the model and perform the mathematical analysis of the numerical method.

Xiaoli Li,
Shandong University
xiaolimath@sdu.edu.cn

Several structure-preserving schemes for the Q-tensor flow

In this paper, we propose two efficient fully-discrete schemes for Q-tensor flow by using the first- and second-order stabilized exponential scalar auxiliary variable approach in time and the finite difference method for spatial discretization. The modified discrete energy dissipation laws are unconditionally satisfied for both two constructed schemes. A particular feature

is that, for two-dimensional (2D) and a kind of three-dimensional (3D) Q-tensor flows, the unconditional maximum-bound-principle (MBP) preservation of the constructed first-order scheme is successfully established, and the proposed second-order scheme preserves the discrete MBP property with a mild restriction on the time-step sizes. Furthermore, we rigorously derive the corresponding error estimates for the fully-discrete second-order schemes by using the built-in stability results.Finally, various numerical examples validating the theoretical results, such as the orientation of liquid crystal in 2D and 3D, are presented for the constructed schemes.

Rui Ma,
Beijing Institute of Technology
rui.ma@bit.edu.cn

Mixed finite element methods for elastic multi-structures

First, this talk will introduce a mixed finite element method for the problem of two coupled plates. By introducing the union of stresses and moments as an auxiliary variable, which is of significant interest in practical applications, a mixed formulation is developed and its well-posedness is established. Based on the mixed formulation, a mixed finite element method is presented along with an illustrative example. Second, this talk will consider the coupled problem of a three-dimensional elastic body and a Kirchhoff plate. The Hellinger–Reissner formulation is adopted for the body by introducing stress as an auxiliary variable, while the displacement-based formulation is employed for the plate. This approach enables accurate stress approximations and allows for non-matching meshes at the interface. Discrete stability and error estimates are derived for both conforming and nonconforming finite element discretizations.

Xiaofeng Cai,
Beijing Normal University
xfcai@bnu.edu.cn

High-Dimensional High-Order Conservative Semi-Lagrangian Discontinuous Galerkin Method for Nonlinear Vlasov Equations

The semi-Lagrangian method, by tracking the evolution of the solution along fluid trajectories, effectively overcomes the CFL time-step restriction of traditional Eulerian schemes and has, in recent years, been widely applied to the numerical solution of high-dimensional nonlinear Hamiltonian systems such as the kinetic Vlasov equation in plasma physics. To address the challenge of simultaneously achieving high-order spatial accuracy, exact mass and energy conservation, and the ability to take large time steps in two or more dimensions, we propose a genuinely high-dimensional conservative semi-Lagrangian discontinuous Galerkin (SLDG) method. This scheme inherits the high-order accuracy and local conservation properties of discontinuous Galerkin finite elements, and by exploiting characteristic tracing in the full phase space, it enables explicit, large-CFL time stepping without dimensional splitting errors. Moreover, to satisfy the temporal accuracy demands of nonlinear transport, we couple the high-dimensional SLDG spatial discretization with a class of high-order, Lie group–based exponential Runge–Kutta integrators, yielding a fully nonlinear SLDG algorithm. Numerical experiments on classical benchmarks demonstrate the proposed method's significant advantages in spatial accuracy, conservation of invariants, and computational efficiency.

Qinglin Tang,
Sichuan University
qinglin_tang@163.com

A linearly implicit and energy conservative method for the logarithmic
Klein-Gordon equation

In this talk, we first propose a local Lagrangian regularization (LLR) method to regularize the logarithmic Klein-Gordon equation (LogKGE) to avoid singularity caused by the logarithmic nonlinearity of the LogKGE, thus leading to a LLR logarithmic Klein-Gordon equation (LLRLogKGE) with a small regularization parameter $0 < \epsilon \ll 1$ to approximate the LogKGE with error at $O(\epsilon)$. Then, we will propose a linearly implicit Fourier pseudo-spectral scheme to solve the LLRLogKGE. The scheme can preserve the original total energy at discrete level. Ample numerical results will be also presented to validate the scheme.

Yue Feng,
Xi'an Jiaotong University
yue.feng@xjtu.edu.cn

Explicit Symmetric Low-Regularity Integrator for the Nonlinear Schrodinger Equation

The numerical approximation of low-regularity solutions to the nonlinear Schrodinger equation (NLSE) is notoriously difficult and even more so if structure-preserving schemes are sought. Recent works have been successful in establishing symmetric low-regularity integrators for NLSE. However, so far, all prior symmetric low-regularity algorithms are fully implicit, and therefore require the solution of a nonlinear equation at each time step, leading to significant numerical cost in the iteration. In this work, we introduce the first fully explicit (multi-step) symmetric low-regularity integrators for NLSE. We demonstrate the construction of an entire class of such schemes which notably can be used to symmetrise (in explicit form) a large amount of existing low-regularity integrators. We provide rigorous convergence analysis of our schemes and numerical examples demonstrating both the favourable structure preservation properties obtained with our novel schemes, and the significant reduction in computational cost over implicit methods.

Jie Du,
East China Normal University
jdu@math.ecnu.edu.cn

Well-balanced positivity-preserving high-order discontinuous Galerkin methods for Euler equations with gravitation

We develop high order discontinuous Galerkin (DG) methods with Lax-Friedrich fluxes for Euler equations under gravitational fields. Such problems may yield steady-state solutions and the density and pressure are positive. There were plenty of previous works developing either well-balanced (WB) schemes to preserve the steady states or positivity-preserving (PP) schemes to get positive density and pressure. However, it is rather difficult to construct WB PP schemes with Lax-Friedrich fluxes, due to the penalty term in the flux. In fact, for general PP DG methods, the penalty coefficient must

be sufficiently large, while the WB scheme requires that to be zero. This contradiction can hardly be fixed following the original design of the PP technique. In this talk, we reformulate the source term such that it balances with the flux term when the steady state has reached. To obtain positive numerical density and pressure, we choose a special penalty coefficient in the Lax-Friedrich flux, which is zero at the steady state. The technique works for general steady-state solutions with zero velocities. Numerical experiments are given to show the performance of the proposed methods.

MS05 Recent Advances in Randomized Numerical Linear Algebra

Organizers: Hei Yin Lam, Nian Shao

Xin Liang
Beijing Institute of Mathematical Sciences and Applications
liangxin@bimsa.cn

On the optimality of the Oja's algorithm for online PCA

In this talk we analyze the behavior of the Oja's algorithm for online/streaming principal component subspace estimation. It is proved that with high probability it performs an efficient, gap-free, global convergence rate to approximate an principal component subspace for any sub-Gaussian distribution. Moreover, it is the first time to show that the convergence rate, namely the upper bound of the approximation, exactly matches the lower bound of an approximation obtained by the offline/classical PCA up to a constant factor.

This is a joint work with Zhen-Chen Guo (Nankai), Li Wang (UTA), Ren-Cang Li (UTA), Wen-Wei Lin (NJCAM).

Haoran Guan,
The Hong Kong Polytechnic University
21037226R@connect.polyu.hk

Deterministic and randomized LU-Householder CholeskyQR

In this talk, we show LU-Householder CholeskyQR (LHC) for QR factorization of full-rank tall-skinny matrices. Similar to LU-CholeskyQR, LHC does not require a sufficient condition of $\kappa_2(X)$ for the input tall-skinny matrix $X \in \mathbb{R}^{m \times n}$. This characteristic ensures the algorithm's reliability in the real-world applications, which is different from other CholeskyQR-type algorithms. To address the issue of numerical breakdown in Cholesky factorization of LU-CholeskyQR when the L-factor is ill-conditioned, LHC employs HouseholderQR to generate the upper-triangular factor alternatively. In order to accelerate LHC for tall-skinny matrices, we incorporate the latest sketching techniques to develop randomized versions of LHC, SLHC with

single-sketching and SSLHC with multi-sketching. To ensure numerical stability, LHC2, SLHC3, and SSLHC3 are constructed with CholeskyQR(2) after the preconditioning steps. We provide rounding error analysis for these new algorithms. Numerical experiments demonstrate the better applicability of our new algorithms compared to LU-CholeskyQR2 while maintaining numerical stability. With the sketching technique, our randomized algorithms, SLHC3 and SSLHC3, show significant acceleration over LHC2 in our tests. Among them, SLHC3 with the Gaussian sketch can deal with more ill-conditioned X with different m and n for X. SSLHC3 with multi-sketching is applicable when $\frac{m}{n}$ is large enough and is more efficient than SLHC3. Both of them are robust enough after numerous experiments.

Nian Shao
École Polytechnique Fédérale de Lausanne
nian.shao@epfl.ch

A randomized small-block Lanczos method for large-scale null space computations

Computing the null space of a large sparse matrix A is a challenging computational problem, especially if the nullity—the dimension of the null space—is not small. When using a block Lanczos method for this purpose, conventional wisdom suggests to use a block size d that is not smaller than the nullity. In this work, we show how randomness can be utilized to allow for smaller d without sacrificing convergence or reliability. Even $d = 1$, corresponding to the standard single-vector Lanczos method, becomes a safe choice. This is achieved by using a small random diagonal perturbation, which moves the zero eigenvalues of $A^{\mathsf{T}}A$ away from each other, and a random initial guess. We analyze the effect of the perturbation on the attainable quality of the null space and derive convergence results that establish robust convergence for $d = 1$. As demonstrated by our numerical experiments, a smaller block size combined with restarting and partial reorthogonalization results in reduced memory requirements and computational effort. It also allows for the incremental computation of the null space, without requiring a priori knowledge of the nullity. Our algorithm is best suited for situations

when the nullity of A is moderately large. In particular, this excludes matrices with many more columns than rows. This is a joint work with Daniel Kressner (EPFL).

Wen-Ting Wu,
Beijing Institute of Technology
wuwenting@bit.edu.cn

Randomized-Gauss-Seidel-type and randomized-Kaczmarz-type methods

The randomized-Gauss-Seidel-type and randomized-Kaczmarz-type methods are representative and effective randomized projection iteration methods for solving large-scale systems of linear equations. In this talk, we find the intrinsic connection between these two types of methods. We also point out that the randomized extended Gauss-Seidel method is actually mathematically equivalent to the randomized extended Kaczmarz method. In addition, by classifying a linear system into four cases according to its consistency and the column-rank of its coefficient matrix, we give the preferred method among the randomized Kaczmarz method, the randomized Gauss-Seidel method, the randomized extended Kaczmarz method, and the randomized extended Gauss-Seidel method in each case.

Jingyu Liu,
Fudan University
jyliu22@m.fudan.edu.cn

A Fast Direct Solver for Nonuniform Discrete Fourier Transform of Type 3

Nonuniform discrete Fourier transform (NUDFT) and its inverse are widely used in various fields of scientific computing. In this talk, we introduce a novel fast direct inversion method for type 3 NUDFT. The proposed method approximates the type 3 NUDFT matrix as a product of a type 2 NUDFT matrix and an HSS matrix, where the type 2 NUDFT matrix is further decomposed as the product of an HSS matrix and uniform DFT matrix as proposed by Wilber et al. Based on the decomposition of the type 3 NUDFT

matrix, both matrix forward application and backward inversion could be accomplished in quasi-linear complexity. Our fast backward inversion can serve as a fast direct solver or as an efficient preconditioner. Additionally, we provide an error bound for the approximation under specific sample distributions. Numerical results are presented to verify the relevant theoretical properties and demonstrate the efficiency of the proposed methods.

Hei Yin Lam,
École Polytechnique Fédérale de Lausanne
hysan.lam@epfl.ch

Randomized low-rank Runge-Kutta methods

This work proposes and analyzes a new class of numerical integrators for computing low-rank approximations to solutions of matrix differential equation. We combine an explicit Runge-Kutta method with repeated randomized low-rank approximation to keep the rank of the stages limited. The so-called generalized Nyström method is particularly well suited for this purpose; it builds low-rank approximations from random sketches of the discretized dynamics. In contrast, all existing dynamical low-rank approximation methods are deterministic and usually perform tangent space projections to limit rank growth. Using such tangential projections can result in larger error compared to approximating the dynamics directly. Moreover, sketching allows for increased flexibility and efficiency by choosing structured random matrices adapted to the structure of the matrix differential equation. Under suitable assumptions, we establish moment and tail bounds on the error of our randomized low-rank Runge-Kutta methods. When combining the classical Runge-Kutta method with generalized Nyström, we obtain a method called Rand RK4, which exhibits fourth-order convergence numerically – up to the low-rank approximation error. For a modified variant of Rand RK4, we also establish fourth-order convergence theoretically. Numerical experiments for a range of examples from the literature demonstrate that randomized low-rank Runge-Kutta methods compare favorably with two popular dynamical low-rank approximation methods, in terms of robustness and speed of convergence.

This is a joint work with Gianluca Ceruti and Daniel Kressner.

MS06 Wave Propagation with Resonant Perturbations: Theory and Applications

Organizers: Xinlin Cao, Mourad Sini

Huaian Diao,
Jilin University, Changchun, China
diao@jlu.edu.cn

On quasi-Minnaert resonances in elasticity and their applications to stress concentrations

In this talk, we shall introduce a novel quasi-Minnaert resonance for an elastic hard inclusion embedded in a soft homogeneous medium in the sub-wavelength regime. The quasi-Minnaert resonance consists of boundary localization and surface resonance for the generated internal total and external scattered wave fields associated with the hard inclusion. It possesses similar quantitative behaviours as those for the classical Minnaert resonance due to high-contrast material structures, but occurs for a continuous spectrum of frequencies instead of certain discrete Minnaert resonant frequencies. We present a comprehensive analysis to uncover the physical origin and the mechanism of this new physical phenomenon. It is shown that the delicate high-contrast material structures and the properly tailored incident waves which are coupled together in a subtle manner play a crucial role in ensuring such phenomena. The stress concentration phenomena in both the internal total field and the scattered field components are also rigorously established.

Yueguang HU,
City University of Hong Kong,
yueghu2-c@my.cityu.edu.hk

Acoustic Boundary Conditions Arising from High-Contrast Material Inclusions and Related Field Concentration Problem

This presentation examines the asymptotic behaviors of time-harmonic acoustic wave caused by incident wave interacting with inhomogeneous medium

inclusions possessing high-contrast material parameters. We derive precise asymptotic estimates and develop several effective models for acoustic obstacle scattering when material parameters reach extreme values. Additionally, I will discuss some related field concentration problem in wave scattering systems.

Long Li,
Radon Institute, Austrian Academy of Sciences
long.li@ricam.oeaw.ac.at

Uniform Space and Time Behavior for Acoustic Resonators

We discuss the time-domain acoustic wave propagation in the presence of a subwavelength resonator modeling a Microbubble. A uniform point-approximation expansion of the wave field—valid in both space and time—is derived. The leading-order behavior consists of two components:

(1) The primary wave, representing the field generated in the absence of the bubble;

(2) The resonant wave, arising from the interaction between the bubble and the background medium. It describes a spatial Dirac source modulated in time by a solution to a 1D second-order Cauchy problem, where the propagation and attenuation parameters correspond to the real and imaginary parts of the Minnaert resonance.

We show that the lifetime of the resonant wave is inversely proportional to the imaginary part of the relevant subwavelength resonance (here, the Minnaert resonance), while its oscillation period is determined by the real part.

Arpan Mukherjee,
MSU-BIT, Shenzhen, China
arpan.mukherjee@ricam.oeaw.ac.at

Time-Domain Analysis for Dispersive Effective Models

We develop a unified time-domain framework for modeling acoustic wave propagation in bubbly media, avoiding Fourier transforms to handle general incident waves (not restricted to band-limited signals). The derived effective models account for dispersion caused by the subwavelength Minnaert resonance of bubbles. Key results include:

(1) A dispersive effective medium theory derived directly in the time domain. The model is governed by an integro-differential equation with a time-convolution term representing the memory effect of bubble resonances. Unlike classical homogenization methods, periodicity in bubble arrangement is not required. Instead, the local density of bubble clusters is controlled by a non-negative continuous function K, which directly shapes the effective medium properties. This flexibility enables applications in materials design and imaging.

(2) An effective transmission condition for acoustic waves interacting with subwavelength resonators distributed on a smooth, bounded hypersurface (flat or curved). The condition connects the jump in the normal derivative of the acoustic field to a time-convolution of its second derivative with a sinusoidal kernel. The kernel's period depends on the Minnaert resonance frequency. Three distinct acoustic regimes emerge:

- *High resonance*: The surface transmits waves without reflection;
- *Moderate resonance*: The surface behaves as a dispersive screen with memory;
- *Low resonance*: The surface acts as a partially reflective barrier with negligible memory.

The models combine spatial adaptability (via K) and temporal dispersion, providing a versatile tool for controlling acoustic waves.

Youjun Deng,
Central South University, China
youjundeng@csu.edu.cn

Spectral Theory of Neumann-Poincare Type Operators
for Anisotropic Geometry and its Applications

In this talk, we shall present some recent results on spectral properties of Neumann-Poincare (NP) type operators for anisotropic geometry, especially nanorod shape geometry. We shall also present some main potential applications in inverse problems such as imaging, cloaking and resonance by using anisotropic geometry.

Shutong Hou,
Southeast University, China
230228431@seu.edu.cn

A Novel Approach for an Inverse Source Problem of the Wave Equation

We address the inverse problem of reconstructing the source term in a bounded domain for the time-domain wave equation. A small droplet with high contrast is injected into the medium, and then the difference in the wave fields before and after injecting the droplet is utilized to develop a novel reconstruction approach. First, we analyze the asymptotic behavior of the wave field after injecting the droplet by using the time-domain integral equation method. Then, on the basis of this analysis, the wave field before injecting the droplet is reconstructed by utilizing the external measurements. Next, the source term is reconstructed through numerical differentiation of the wave field before the droplet injection. A key advantage of our approach is that it only requires measurements at a fixed point over a period of time. Additionally, to show the performance of our approach for the inverse problem, we also develop an efficient algorithm to solve the time-domain Lippmann-Schwinger equation for the corresponding forward problem. Numerical experiments in three dimensions are presented to demonstrate the effectiveness of the proposed approach.

Ahcene Ghandriche,
Nanjing Center for Applied Math, Nanjing, China
gh.hsen@njcam.org.cn

Optical Inversion Using Plasmonic Contrast Agents

In this talk, we will introduce a new technique for reconstructing the permittivity distribution of a given domain (medium) using remotely measured electromagnetic fields. Our idea is to utilize remote fields that are measured before and after injecting, one by one in the medium, plasmonic nano-particles. Such a technique is known in the context of imaging using contrast agents, where nano-particles play the role of contrast agents in optical imaging.

Xinlin Cao,
The Hong Kong Polytechnic University
xinlin.cao@polyu.edu.hk

Electromagnetic Waves Generated by a Hybrid Dieletric-Plasmonic Dimer

In this talk, we are concerned with the electromagnetic wave propagation in the presence of a hybrid dimer composed of two closely coupled nano-particles: one plasmonic and the other dielectric. We found out that such a hybrid dimer can polarize both the incident electric and magnetic fields. Consequently, they have the potential to modify both the electric permittivity and magnetic permeability of the surrounding medium if the two nano-particles share common resonant frequencies. We derive the asymptotic expansion of the fields generated by these hybrid dimers in the subwavelength regime, for incident frequencies near their shared resonant frequencies, confirming these findings.

MS07 Finite element methods, complexes and applications

Organizers: Long Chen (UCI, lchen7@uci.edu),
Jun Hu (Peking University, hujun@math.pku.edu.cn),
Ruchi Guo (Sichuan University, ruchiguo@scu.edu.cn)

Shuo Zhang,
Chinese Academy of Sciences,
szhang@lsec.cc.ac.cn

Minimal finite element spaces for differential k-forms on cubical meshes

In this talk, we present a unified family of finite element spaces for differential k-forms on $\mathbb{R}^n$ cubical meshes, $0 \leqslant k \leqslant n$, $n \geqslant 1$. The spaces each employs the Whitney forms for piecewise shape functions, and thus each is of minimal degree. The approximation and consistency are proved for the spaces with respect to $H\Lambda^k$ problems. The Park-Sheen element which uses piecewise linear element space for H^1 problems on cubical meshes is included in the family for 0-forms. Discrete de Rham complexes and commutative diagrams are established associated with the spaces.

Shuonan Wu,
Peking University,
snwu@math.pku.edu.cn

A stabilized nonconforming finite element method for the surface biharmonic problem

This talk presents a novel stabilized nonconforming finite element method for solving the surface biharmonic problem. The method extends the New-Zienkiewicz-type (NZT) element to polyhedral (approximated) surfaces by employing the Piola transform to define the connection of vertex gradients between adjacent elements. Key features of the surface NZT finite element space include its H1-relative conformity and the weak H(div) conformity of the surface gradient, allowing for stabilization without the need for artificial

parameters. Assuming that the exact solution and the dual problem possess only H3 regularity, we establish optimal error estimates in the energy norm and provide, for the first time, a detailed analysis yielding optimal second-order convergence in the broken H1 norm. Numerical experiments are provided to support the theoretical results, and they suggest that the stabilization term may not be necessary.

Xuehai Huang,
Shanghai University of Finance and Economics
xuehai@sufe.edu.cn

Linear Mixed Finite Element Method with a Third-Order Tensor for Strain Gradient Elasticity

An optimal and robust low-order mixed finite element method with a third-order tensor is developed for the strain gradient elasticity (SGE) model in arbitrary dimensions, achieving optimal convergence rates. The method discretizes the third-order stress gradient tensor using a low-order H(div) tensor element and the displacement using the linear Crouzeix–Raviart element. Optimal error estimates, uniform with respect to both the mesh size and the Lamé coefficient, are established based on an L^2-bounded interpolation operator for third-order tensors. Finally, numerical experiments in both two and three dimensions are presented to verify the theoretical results.

Shihua Gong,
CUHK-Shenzhen
gongshihua@cuhk.edu.cn

High order methods and robust block preconditioners for the fluid-rigid body interaction

We consider numerical algorithms for particulate flows, which involve the interactions between rigid particles and incompressible flows. In this talk, we will discuss computational challenges for this coupled system, including handling the moving interface between circular particles and flows, and

addressing bottlenecks in large-scale and long-duration simulations. Our algorithms use arbitrary Eulerian-Lagrangian mapping to track the moving interface and distributed Lagrange multipliers to enforce the rigid-body motion. The advantages of our algorithms include featuring accurate quadrature, and maintaining a sharp interface, with the potential for high-order methods. At the end of the talk, we will discuss the stability analysis of the variational problems, which leads to robust parallel solvers for the linearized systems. We will also present some simulation results of particulate flows in microfluidics.

Micheal Nelian,
University of Pittsburgh
neilan@pitt.edu

Finite Element Complexes for the Surface Stokes Problem

In this talk, we discuss a C^0 interior penalty method for the fourth-order stream function formulation of the surface Stokes problem. The scheme utilizes continuous, piecewise polynomial spaces defined on an approximate surface. The discretization is positive definite and converges optimally in the isoparametric setting. A notable feature of the scheme is that it does not explicitly depend on the Gauss curvature of the surface, thus allowing simpler implementation. This is achieved by exploiting the relationship between Lagrange and BDM elements through a discrete complex defined on the approximate surface.

Limin Ma,
Wuhan University
limin18@whu.edu.cn

Supercloseness and Asymptotic Analysis for the nonconforming
Crouzeix-Raviart element

We consider numerical algorithms for particulate flows, which involve the interactions between rigid particles and incompressible flows. In this talk,

we will discuss computational challenges for this coupled system, including handling the moving interface between circular particles and flows, and addressing bottlenecks in large-scale and long-duration simulations. Our algorithms use arbitrary Eulerian-Lagrangian mapping to track the moving interface and distributed Lagrange multipliers to enforce the rigid-body motion. The advantages of our algorithms include featuring accurate quadrature, and maintaining a sharp interface, with the potential for high-order methods. At the end of the talk, we will discuss the stability analysis of the variational problems, which leads to robust parallel solvers for the linearized systems. We will also present some simulation results of particulate flows in microfluidics.

Min Zhang,
Beijing Forestry University,
zhangminD01@bjfu.edu.cn

A family of conforming finite element divdiv complexes on cuboid meshes

This talk introduces the first family of conforming finite element divdiv complexes on cuboid meshes. The complex exhibits exactness on a contractible domain in the sense that the kernel space of each successive discrete map is the range of the previous one. This allows for algebraic structure-preserving finite element discretization of both the biharmonic equation and the linearized Einstein-Bianchi system. The convergence of optimal order is established and validated through numerical examples.

Shudan Tian,
Xiangtan University,
shudan.tian@xtu.edu.cn

Mixed Finite element method for stress gradient elasticity problem

In this talk, I will introduce several mixed finite element pairs for linear stress gradient elasticity problems. We prove the discrete inf-sup condition and analyze certain singular points. Numerical experiments are presented to validate the theoretical results.

Shukai Du,
Syracuse University
sdu113@syr.edu

Accelerating finite element-type methods with machine learning on substructures

Machine learning and data-driven approaches have shown potential in accelerating numerical simulations, such as numerical weather prediction and molecular dynamics. However, they often suffer from high training costs, limited data availability, or unreliable generalization. In contrast, traditional physics-based numerical methods, such as finite element methods, are grounded in solid theoretical foundations and have proven effective across a wide range of problems. Yet, they still face challenges in high-dimensional settings (e.g., radiative transfer, Boltzmann equations), which require effective model reduction techniques, and in applications involving repeated queries (e.g., inverse problems, ensemble forecasting), where computational efficiency is crucial. In this talk, we present our recent efforts on developing a new class of methods that aims to combine the strengths of finite element-type techniques and machine learning. The approach has two key components: (1) reducing the model complexity of finite element through static condensation and accelerating computation using machine learning, and (2) mitigating the high training costs and data demands of machine learning models by training on substructures. Specifically, I will discuss how this new approach can be naturally derived as a data-driven augmentation of hybridizable discontinuous Galerkin methods.

Xiang Wang,
Jilin University,
wxjldx@jlu.edu.cn

Constructions of the Finite Volume Element Method with a Two-layer Dual Strategy

We introduce a two-layer dual strategy that can avoid main common drawbacks of the existing high-order finite volume element (FVE) schemes. The existing high-order FVE schemes are complicated to construct since the

number of the dual elements in each primary element used in their construction increases with a rate $O((k+1)^2)$, where k is the order of the scheme. Moreover, all kth-order FVE schemes require a higher regularity H^{k+2} than the approximation theory for the L^2 theory. Furthermore, all FVE schemes lose local conservation properties over boundary dual elements when dealing with Dirichlet boundary conditions. The proposed FVE-2L schemes has a much simpler construction since they have a fixed number (four) of dual elements in each primary element. They also reduce the regularity requirement for the L^2 theory to H^{k+1} and preserve the local conservation law on all dual elements of the second dual layer for both flux and equation forms.

Ruishu Wang,
Jilin University,
wangrs_math@jlu.edu.cn

A Primal Staggered Discontinuous Galerkin Method on Polytopal Meshes

We present a novel staggered discontinuous Galerkin (SDG) method for polytopal meshes. This approach employs a primal-dual grid framework to ensure local flux conservation, thereby enhancing both stability and accuracy. The method is hybridizable, reducing the degrees of freedom compared to existing techniques. Additionally, it establishes connections to other numerical methods on polytopal meshes, offering a versatile and efficient solution for complex geometric problems.

Jun Cao,
Toronto Metropolitan University,
jcao@torontomu.ca

An IBM-Based Numerical Framework for Study of Tornadic Wind Dynamics

A tornado combines three co-existing kinematic components - updraft, translation, and rotation - producing a fully three-dimensional, transient flow

field. Accurately prescribing boundary conditions for such a system in conventional CFD frameworks is challenging, which helps explain the scarcity of truly three-dimensional numerical studies on tornado–building interactions.

Motivated by recent advances in the immersed-boundary method (IBM), we re-tailored Rankine Combined Vortex Model (RCVM). Using the "relative-motion" principle, the model treats the building as virtually translating toward a pinned, purely rotational flow. At a sufficiently distant outer boundary, the flow is therefore time-invariant, eliminating the costly boundary-condition updates required in the original RCVM and greatly accelerating computation.

In this study we extend the re-tailored RCVM to three dimensions by incorporating a logarithmic vertical profile for velocity variation. The resulting 3-D tornado inflow is embedded in a high-order finite-difference turbulence solver equipped with an IBM treatment of the moving building, yielding a practical and powerful tool for simulating tornado–structure interaction.

A case study on a prismatic building shows that the vertical (uplift) force component dominates the load spectrum in all three directions, corroborating field observations of the "uprooting" effect seen in many tornado disasters.

MS08 Stochastic Dynamical Systems and Machine Learning

Organizers: Xiang ZHOU, Yuanfei HUANG

Zhiwen ZHANG,
The University of Hong Kong
zhangzw@hku.hk

Stochastic Interacting Particle Field Methods in the Computation of Chemotaxis and Haptotaxis

In this talk, I will present the latest developments in the stochastic interacting particle field (SIPF) methods. The methodology originates from the Lagrangian framework. It is used in the computation of asymptotic behaviors of PDEs, such as the effective diffusivities and KPP front speed. Then we turn to the interacting particle methods for elliptic-type Keller–Segel equations. Very recently, we have further extended our research on SIPF methods, facilitating the computation of parabolic-type Keller–Segel and haptotaxis equations. If time permits, I will also discuss how these results interact with the field of generative modeling.

Zhen ZHANG,
Southern University of Science and Technology
zhangz@sustech.edu.cn

Neural Evolutionary Kernel Method for Evolutionary PDEs

This work introduces a novel method named the Neural Evolutionary Kernel Method (NEKM) for solving a class of evolutionary PDEs through DNNs based kernels. By using operator splitting and boundary integral techniques, we propose particular neural network architectures which approximate evolutionary kernels of solutions and preserve structures of time-dependent PDEs. Mathematical prior knowledge are naturally built into these DNNs based kernels through convolutional representation with pre-trained Green functions, leading to serious reduction in the number of parameters in the NEKM and

very efficient training processes. Experimental results demonstrate the efficiency and accuracy of the NEKM in solving many typical evolutionary PDEs in complex domains and on manifolds, showcasing its promising potential for applications in data driven scientific computing.

Pingyuan WEI,
Southeast University
pwei@seu.edu.cn

Metastable Transitions in Periodically Perturbed Langevin Systems under Small Noise

In this talk, we will discuss the noise-induced rare transitions in periodically driven systems. The maximum likelihood paths (MLPs) are often sought in order to reveal the transition mechanism. We show that MLPs between metastable periodic states can persist under small nonautonomous forcing, given appropriate conditions. Furthermore, we obtain a closed-form explicit expression for approximating the change in transition rates. These results are derived using standard perturbation techniques for the Euler-Lagrange equation, Melnikov theory, and a linear-theory calculation. Our methods provide a route toward a detailed understanding of the interaction between periodic forcing and noise in rather general systems. This talk is based on joint work with Ying Chao and Jinqiao Duan.

Yuanfei HUANG,
City University of Hong Kong
yhuan26@cityu.edu.hk

Entropy Production in Non-Gaussian Active Matter: Theory and Algorithm

We present a general framework for deriving entropy production rates in active matter systems driven by non-Gaussian active fluctuations. Using the probability flow equivalence technique, we derive an entropy production formula and show that it satisfies the integral fluctuation theorem $\langle \exp[-\Delta s_{\text{tot}} + B_{\text{act}}] \rangle = 1$ and the generalized second law $\langle \Delta s_{\text{tot}} \rangle \geq \langle B_{\text{act}} \rangle$, where B_{act}

characterizes active fluctuations. Our results are valid for arbitrary initial conditions, covering both steady-state and transient regimes, and reduce to standard stochastic thermodynamics when $B_{\text{act}} = 0$. We also propose a deep learning-based method, leveraging the Lévy score function, to efficiently compute entropy production. This approach is validated on two systems: a Brownian particle in a periodic active bath and an active polymer system with active and passive components. Our framework unifies the analysis of entropy production in active matter and provides practical computational tools for studying nonequilibrium behaviors. This work is in collaboration with Chengyu LIU, Bing MIAO, and Xiang ZHOU.

Qiao HUANG,
Southeast University
qiao.huang@seu.edu.cn

Second-order Hamilton–Jacobi–Bellman equations at the crossroads of stochastic geometric mechanics and stochastic thermodynamics

This talk systematically investigates the mathematical structure of path measures, both from a measure-theoretical perspective and through stochastic differential equations. The realization of path measures as Langevin systems hinges on the pivotal role of second-order Hamilton–Jacobi–Bellman equations, which form the foundation of stochastic geometric mechanics and applications in stochastic thermodynamics. We explore the emergence of the Onsager–Machlup functional in large deviation theory, the rates of entropy production in irreversible thermodynamic processes, entropy minimization problems encoded in stochastic geometric mechanics, and the identification of Langevin systems from most probable paths.

Shenglan YUAN,
Great Bay University
shenglanyuan@gbu.edu.cn

Rare events in a stochastic vegetation-water dynamical system based on machine learning

Stochastic vegetation-water dynamical systems are fundamental to understanding ecological stability, biodiversity conservation, water resource sustainability, and climate change adaptation. In this study, we introduce an innovative machine learning framework for analyzing rare events in stochastic vegetation-water systems driven by multiplicative Gaussian noise. By integrating the Freidlin-Wentzell large deviation theory with deep learning techniques, we establish rigorous asymptotic formulations for both the quasipotential and mean first exit time. Leveraging vector field decomposition principles, we develop a novel neural network architecture capable of accurately computing the most probable transition paths and mean first exit times across diverse boundary conditions, including both non-characteristic and characteristic scenarios. Our findings demonstrate that the proposed method significantly enhances the predictive capabilities for early detection of vegetation degradation, thereby offering robust theoretical foundations and advanced computational tools for ecological management and conservation strategies. Furthermore, this approach establishes a scalable framework for investigating more complex, high-dimensional stochastic dynamical systems, opening new avenues for research in ecological modeling and environmental forecasting.

Shuting GU,
Shenzhen Technology University
gushuting@sztu.edu.cn

Iterative Proximal Minimization Formulation for saddle points search

Saddle points play a central role in the study of activated processes in gradient flows driven by free energy. In this talk, we introduce an Iterative Proximal Minimization (IPM) formulation for saddle point computation. This approach modifies the original Iterative Minimization Formulation (IMF) by adding a proximal penalty term to the auxiliary functional in the IMF. The modification addresses two key challenges: the strong dependence of convergence on the initial guess and the divergence of the IMF caused by the excessive inner iterations. Numerical experiments on the Ginzburg-Landau and Landau-Brazovskii free energies demonstrate the improved efficiency and robustness of the proposed method.

Weiguo GAO,
Fudan University
wggao@fudan.edu.cn

How Do Flow Matching Models Memorize and Generalize in Sample Data Subspaces?

Real-world data is often assumed to lie within a low-dimensional structure embedded in high-dimensional space. In practical settings, we observe only a finite set of samples, forming what we refer to as the sample data subspace. It serves an essential approximation supporting tasks such as dimensionality reduction and generation. A major challenge lies in whether generative models can reliably synthesize samples that stay within this subspace rather than drifting away from the underlying structure. In this work, we provide theoretical insights into this challenge by leveraging Flow Matching models, which transform a simple prior into a complex target distribution via a learned velocity field. By treating the real data distribution as discrete, we derive analytical expressions for the optimal velocity field under a Gaussian prior, showing that generated samples memorize real data points and represent the sample data subspace exactly. To generalize to suboptimal scenarios, we introduce the Orthogonal Subspace Decomposition Network (OSDNet), which systematically decomposes the velocity field into subspace and off-subspace components. Our analysis shows that the off-subspace component decays, while the subspace component generalizes within the sample data subspace, ensuring generated samples preserve both proximity and diversity. This is joint work with Ming Li.

Hongqiao WANG,
Central South University
hongqiao.wang@csu.edu.cn

Active learning for minimum energy path with Gaussian process surrogate

We present a Bayesian framework to estimate the Minimum Energy Path (MEP) and saddle point from noisy, computationally expensive energy function evaluations. Gaussian process regression (GPR) serves as a surrogate model for the energy function, while a tailored likelihood function evaluates

73

the consistency of candidate paths with observed data and the GPR approximation. Combined with a prior, this enables Bayesian computation of the MEP posterior. To refine the surrogate, we propose an active learning strategy that iteratively designs new evaluation points—prioritizing regions of high uncertainty—and updates the dataset. Iterations cease upon MEP posterior convergence. The method's efficacy is validated through two numerical benchmarks, demonstrating accurate recovery of MEPs and saddle points with minimal energy evaluations.

Xiaopeng CHEN,
Shantou University
xpchen@stu.edu.cn

Positivity-preserving Numerical Algorithms for Stochastic Differential Equations Driven by Fractional Brownian Motion

In fields such as finance and ecology, stochastic differential equations (SDEs) must strictly preserve the positivity of solutions to align with practical significance. However, traditional numerical methods exhibit limitations in addressing such issues. This paper focuses on the construction of positivity-preserving numerical algorithms for SDEs driven by fractional Brownian motion (fBm) with non-Markovian systems. Specifically, the proposed algorithm is applied to the Cox-Ingersoll-Ross (CIR) model driven by fBm, and numerical simulations are conducted to analyze its first moment and second moment.

Chengyu LIU,
City University of Hong Kong
cliu687-c@my.cityu.edu.hk

Generative Path Method for Wasserstein Gradient Flow

Wasserstein gradient flow (WGF) describes the evolution of probability distributions as a gradient flow of a given free energy functional in the Wasserstein space of probability measures, with wide applications in machine learning, computational physics, and biology, as well as other scientific fields. We

propose a novel generative-path framework by formulating the gradient flow as a path-finding variational problem on the Wasserstein space by leveraging the Least Action Principle for interactive diffusion particles. Our variational method directly optimizes the entire gradient path from an arbitrary initial probability distribution to the unknown equilibrium probability distribution, which is geometrically represented by a discrete chain of probability distributions ("images"). We incorporate the technique of normalizing flow, which uses a sequence of stacked invertible residual neural network blocks to map the initial distribution to the equilibrium distribution, to represent this chain for Wasserstein gradient path. By connecting the sequence of "images" along the chain to the sequence of residual blocks in the normalizing flow networks, we are effectively able to generate the whole gradient path by training one single generative network for normalizing flow, and even without any *prior* knowledge of the final equilibrium state. Numerical experiments on benchmark problems, including Fokker-Planck equations, aggregation-drift equations, aggregation-diffusion equations, demonstrate that our method achieves significant improvements in computational efficiency and stability while accurately capturing complex probability flows.

Haijun YU,
Chinese Academy of Sciences
hyu@lsec.cc.ac.cn

A Gradient-Oriented Diffusion Sampling Method for Deep Partial
Differential Equation Solvers

In recent years, deep learning methods for the forward and inverse problems of partial differential equations have received increasing attention. The numerical errors of these methods can generally be decomposed into three parts: network approximation error, data sampling error, and training error. Among them, the data sampling error usually plays a dominant role in the total error. For cases where the smoothness of the solution is relatively uniform and the domain geometry is relatively simple, we can adopt Gaussian sampling to reduce sampling error. However, for complex domains, high-dimensional problems, and situations where the smoothness of the solution is highly non-uniform in spatial distribution, adaptive sampling is a mainstream approach to reducing sampling errors. Many scholars have focused

on this issue and proposed a variety of adaptive sampling methods, but there is still no perfect solution currently. In this talk, we introduce a gradient-oriented diffusion sampling method. This method borrows the idea of moving mesh methods, uses the gradient information of the solution as an indicator for points movement, and moves the sampling points by solving a stochastic diffusion equation. This approach can avoid the large computational cost caused by optimizing the sampling points using the PINN's residual of the equation, and has good sampling efficiency for high-dimensional non-uniform problems. We have applied this method to elliptic steady-state problems, nonlinear parabolic problems (phase-field equations), and the incompressible Navier-Stokes equations. The numerical results show that our method is significantly superior to the commonly used existing adaptive sampling methods.

MS09 Advances in Optimization Theory and Numerical Methods for Nonlinear Systems

Organizers: Long Chen (University of California, Irvine),
Hao Luo (Chongqing Normal University),
Jingrong Wei (The Chinese University of Hong Kong)

Chenglong Bao
Yau Mathematical Sciences Center, Tsinghua University
clbao@tsinghua.edu.cn

A stochastic gradient descent method with global convergence for minimizing nearly convex functions

This talk proposes a stochastic gradient descent method with an adaptive Gaussian noise term for minimizing nonconvex differentiable functions. In both probability space and state space, our theoretical analysis shows that for a class of nonconvex functions, represented by nearly convex functions, the proposed algorithm converges linearly to a certain neighborhood of the global optimal solution whose diameter depends on the variance of the gradient and the deviation between the estimated lower bound and the optimal value. Specifically, when full gradient information is utilized and the sharp lower bound of the objective function is available, the algorithm converges linearly to the global optimal solution. Furthermore, we propose a double-loop method that alternatively updates the lower bound estimate of the optimal value and the sequence, achieving the convergence to a neighborhood of the global optimal solution depending only on the variance of the gradient, provided that the lower bound estimate is asymptotically accurate.

Jian Huang
Xiangtan University, China
huangjian213@xtu.edu.cn

Numerical discretization of a Darcy-Forchheimer flow with variable density and heat transfer

In this talk, we shall introduce a heat transfer scenario in Darcy-Forchheimer porous media with variable density. The block-centered finite difference method is applied to discretize the non-isothermal flow equations governing the system. Specifically, the pressure field is modeled using the nonlinear Darcy-Forchheimer formulation, while the density and temperature are described by convection-dominated diffusion equations, which are treated via the characteristic method. Theoretical analyses are rigorously developed for pressure, velocity, density, temperature, and auxiliary flux across non-uniform grids. Several numerical experiments are carried out to illustrate the merits of our method by comparing numerical results to analytical solutions.

Zihao Hu
The Hong Kong University of Science and Technology
zihaohu@ust.hk

Extragradient Type Methods for Riemannian Variational Inequality Problems

In this work, we consider monotone Riemannian Variational Inequality Problems (RVIPs), which encompass both Riemannian convex optimization and minimax optimization as particular cases. In Euclidean space, the last-iterates of both the extragradient (EG) and past extragradient (PEG) methods converge to the solution of monotone variational inequality problems at a rate of $O\left(\frac{1}{\sqrt{T}}\right)$ [1]. However, analogous behavior on Riemannian manifolds remains open. To bridge this gap, we introduce the Riemannian extragradient (REG) and Riemannian past extragradient (RPEG) methods. We show that both exhibit $O\left(\frac{1}{\sqrt{T}}\right)$ last-iterate convergence and $O\left(\frac{1}{T}\right)$ average-iterate convergence, aligning with observations in the Euclidean case. These results are enabled by judiciously addressing the holonomy effect so that additional complications in Riemannian cases can be reduced and the Euclidean proof inspired by the performance estimation problem (PEP) technique, or the sum-of-squares (SOS) technique can be applied again.

78

Daniel Zhengyu Huang
Beijing International Center for Mathematical Research, Center
for Machine Learning Research, Peking University, China
huangdz@bicmr.pku.edu.cn

Stable Derivative Free Gaussian Mixture Variational Inference for Bayesian Inverse Problems

This paper is concerned with the approximation of probability distributions known up to normalization constants, with a focus on Bayesian inference for large-scale inverse problems in scientific computing. In this context, key challenges include costly repeated evaluations of forward models, multimodality, and inaccessible gradients for the forward model. To address them, we develop a variational inference framework that combines Fisher-Rao natural gradient with specialized quadrature rules to enable derivative free updates of Gaussian mixture variational families. The resulting method, termed Derivative Free Gaussian Mixture Variational Inference (DF-GMVI), guarantees covariance positivity and affine invariance, offering a stable and efficient framework for approximating complex posterior distributions. The effectiveness of DF-GMVI is demonstrated through numerical experiments on challenging scenarios, including distributions with multiple modes, infinitely many modes, and curved modes in spaces with up to 100 dimensions. The method's practicality is further demonstrated in a large-scale application, where it successfully recovers the initial conditions of the Navier-Stokes equations from solution data at positive times.

Fei Wang
Xi'an Jiaotong University
feiwang.xjtu@xjtu.edu.cn

DeepONet Augmented by Randomized Neural Networks for Efficient Operator Learning in PDEs

Deep operator networks (DeepONets) represent a powerful class of data-driven methods for operator learning, demonstrating strong approximation capabilities for a wide range of linear and nonlinear operators. They have

shown promising performance in learning operators that govern partial differential equations (PDEs), including diffusion-reaction systems and Burgers' equations. However, the accuracy of DeepONets is often constrained by computational limitations and optimization challenges inherent in training deep neural networks. Furthermore, the computational cost associated with training these networks is typically very high. To address these challenges, we leverage randomized neural networks (RaNNs), in which the parameters of the hidden layers remain fixed following random initialization. RaNNs compute the output layer parameters using the least-squares method, significantly reducing training time and mitigating optimization errors. In this work, we integrate DeepONets with RaNNs to propose RaNN-DeepONets, a hybrid architecture designed to balance accuracy and efficiency. Furthermore, to mitigate the need for extensive data preparation, we introduce the concept of physics-informed RaNN-DeepONets. Instead of relying on data generated through other time-consuming numerical methods, we incorporate PDE information directly into the training process. We evaluate the proposed model on three benchmark PDE problems: diffusion-reaction dynamics, Burgers' equation, and the Darcy flow problem. Through these tests, we assess its ability to learn nonlinear operators with varying input types. When compared to the standard DeepONet framework, RaNN-DeepONets achieves comparable accuracy while reducing computational costs by orders of magnitude. These results highlight the potential of RaNN-DeepONets as an efficient alternative for operator learning in PDE-based systems.

Zhiguo Wang
Sichuan University
wangzhiguo@scu.edu.cn

Diffusion Models for Chance-Constrained Optimization

Chance-constrained optimization arises in a variety of applications but remains challenging due to two fundamental difficulties: the non-convexity of the feasible region, which complicates global optimization, and the uncertainty in the underlying distribution, which is typically accessible only through finite samples. In this talk, we introduce a general framework for Diffusion Models with Gradient Guidance, presenting both first-order and

80

second-order formulations of the guidance mechanism. We establish theoretical guarantees for convergence under mild conditions. Building on this, we propose a generative approach—DiffOpt—to sample from the chance-constrained feasible set and identify global minimizers of target objectives via gradient guidance. Experimental results demonstrate the superior performance of DiffOpt in probabilistically robust waveform design under imperfect channel state information (CSI).

Chaozhen Wei
University of Electronic Science and Technology of China
cwei4@uestc.edu.cn

An efficient primal dual algorithm for generalized Wasserstein gradient flows

In this talk, I will present a novel numerical approach for computing a class of minimizing movement schemes with nonlinear mobility transport distances, and apply it to computing Wasserstein gradient flows arising widely in applications in material sciences such as phase separation, grain growth, solid-state wetting/dewetting and thin film surfactant dynamics. By leveraging the variational structure, along with the dynamical characterization of the Wasserstein-like transport distance, we construct a fully discrete scheme that ends up with a minimization problem with convex objective function and linear constraint, which can be solved by primal dual operator splitting schemes and its variant versions. Our method has built-in positivity or bounds preserving, mass conservation, and entropy decreasing properties, and overcomes stability issue due to the strong nonlinearity and degeneracy. I will show a suite of simulation examples to demonstrate the effectiveness of our algorithm.

Huayi Wei
Xiangtan University
weihuayi@xtu.edu.cn

FEALPy: A Cross-Platform Intelligent CAX Engine with Scalable Tensor Computation for Multi-Method Simulations

FEALPy is a cross-platform, intelligent CAX engine designed to advance multi-method simulations through scalable tensor computation. While originally rooted in finite element algorithms, FEALPy now supports a wide array of numerical methods including finite difference, finite volume, particle methods, and more. The platform's core lies in its unified mesh interface, enabling seamless transitions between different mesh types and dimensions without the need to modify the underlying code. FEALPy integrates machine learning algorithms, combining traditional CAX methods with AI to accelerate the development of next-generation intelligent CAX applications. With its multi-backend tensor computation engine, supporting libraries such as Numpy, PyTorch, and JAX, FEALPy is adaptable to modern heterogeneous hardware systems. Faithful to its mission, FEALPy aims to provide reliable, robust support for researchers and engineers, promoting innovation in CAX methods and paving the way for cutting-edge industrial applications. This presentation presents FEALPy's architecture, key technologies, and diverse application scenarios, positioning it as a steadfast companion in the field of intelligent CAX.

References

[1] Cai, Y., Oikonomou, A. and Zheng, W., 2022. Finite-time last-iterate convergence for learning in multi-player games. Advances in Neural Information Processing Systems, 35, pp.33904-33919.

MS10 Recent Advances in PDE-constrained Optimization

Organizers: Wei Gong, Zhi Zhou, and Shengfeng Zhu

Gang Chen
Sichuan University
cglwdm@scu.edu.cn

A finite element method for distributed control of indefinite time-harmonic Maxwell's equations

We study the problem of approximating the distributed optimal control problem governed by the indefinite time-harmonic Maxwell's equations with the Nédélec's finite elements. First, we derive the wavenumber explicit regularity result. Second, we present the error analysis, for which the state and the control can reach the optimal order of approximation, with constant independent of the wavenumber. Then, to solve the indefinite system, we give a method based on the classical AMS preconditioner and prove that the converges of this method are dependent on the wave number but independent of the mesh size. Numerical experiments confirm our theoretical results.

Rongfang Gong
Nanjing University of Aeronautics and Astronautics
grf_math@nuaa.edu.cn

Uniquely determining sources in bioluminescence tomography

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, several theoretical results where the light sources are in the shape of C^2 domains or polyhedral- or corona-shaped are explored, followed by a new shape optimization approach for the source identification.

One particular characteristic of the optimal algorithm is the decoupling of the source strength and the source support. Some numerical experiments are implemented for the verification of theoretical results.

Wei Gong
Chinese Academy of Sciences
grf_wgong@lsec.cc.ac.cn

A novel shape optimization approach for source identification in elliptic equations

In this talk, we propose a novel shape optimization approach for the source identification of elliptic equations. This identification problem arises from two application backgrounds: actuator placement in PDE-constrained optimal controls and the regularized least-squares formulation of source identifications. The optimization problem seeks both the source strength and its support. By eliminating the variable associated with the source strength, we reduce the problem to a shape optimization problem for a coupled elliptic system, known as the first-order optimality system. As a model problem, we derive the shape derivative for the regularized least-squares formulation of the inverse source problem and propose a gradient descent shape optimization algorithm, implemented using the level-set method. Several numerical experiments are presented to demonstrate the efficiency of our proposed algorithms.

Yifeng Xu
Shanghai Normal University
yfxu@shnu.edu.cn

A finite element method for phase-field dependent topology optimization in Stokes flow

My presentation is concerned with finite element approximations of a phase-field parameterized topology optimization problem governed by the Stokes equations. The discrete minimizing phase field is sought in the usual

conforming linear finite element space while the nonconforming linear finite elements (Crouzeix-Raviart elements) and piecewise constants are used to approximate the velocity field and the pressure field respectively. Convergence of the resulting finite element method will be discussed for the uniform and the adaptive mesh refinement strategies respectively. Promising numerical results by the two proposed schemes applied to several examples are also reported. This is a joint work with Prof. Bangti Jin at The Chinese University of Hong Kong, Jing Li and Prof. Shengfeng Zhu, both at East China Normal University.

Weiwei Hu[a], Ming-Jun Lai[b] and Hao-Ning Wu[c]
University of Georgia[a,b,c]
Weiwei.Hu@uga.edu[a], hnwu@uga.edu[b], mjlai@uga.edu[c]

Mixing by incompressible flows based on optimal transport

We consider the fluid mixing problem by incompressible flows based on the method of optimal transport. The inhomogeneous distribution of a passive scalar field is governed by the transport equation with a constraint on the final state. Specifically, the velocity field is assumed to be induced by a finite set of cellular flows which can be controlled in time. Rigorous proof of existence of a globally optimal solution is presented and numerical experiments are conducted to demonstrate the effectiveness of our control design.

Yongcun Song,
City University of Hong Kong
ysong307@gmail.com

Physics-informed neural networks for non-smooth PDE-constrained optimization problems

Abstract: We study the application of well-known physics-informed neural networks (PINNs) for solving non-smooth PDE-constrained optimization problems. First, we consider a class of PDE-constrained optimization problems where additional nonsmooth regularization is employed for constraints on the control or design variables. To solve such problems, we combine the alternating direction method of multipliers (ADMM) and PINNs and propose

the ADMM-PINNs algorithmic framework, which unties the PDE constraints and the nonsmooth regularization terms for iterations. Accordingly, at each iteration, one of the resulting subproblems is a smooth PDE-constrained optimization, which PINNs can efficiently solve, and the other is a simple nonsmooth optimization problem that usually has a closed-form solution or can be efficiently solved by various standard optimization algorithms or pre-trained neural networks. Then, we consider the optimal control of PDEs with interfaces. We employ the recently developed discontinuity-capturing neural network to tackle the non-smoothness of the PDEs with interfaces and propose hard-constraint PINNs for solving such optimal control problems. The hard-constraint PINNs ensure both the boundary and interface conditions are satisfied strictly, and meanwhile, they are decoupled from the learning of the PDEs. All these PINNs methods are mesh-free, easy to implement, and scalable to different PDE settings. Various numerical results are reported to validate the effectiveness and efficiency of the proposed PINNs methods.

Zhiyu Tan
Xiamen University
zhiyutan@xmu.edu.cn

On Lagrange multipliers of constrained optimization in Hilbert spaces

In this paper we introduce the essential Lagrange multiplier and establish the solid mathematical foundation of constrained optimization in Hilbert spaces with sharp results on the mathematical foundation of quadratic programming based methods such as the SQP method, the necessary and sufficient conditions for the existence and uniqueness of Lagrange multipliers, the essential difference of the theory of Lagrange multipliers in finite and infinite-dimensional spaces and an essential characterization of the convergence of the classical augmented Lagrangian method. They are achieved by a newly developed decomposition framework for Lagrange multipliers of the Karush-Kuhn-Tucker system of constrained optimization problems in Hilbert spaces, which is totally different from the existing theories based on separation theorems.

Julius Fergy Rabago
Kanazawa University, Japan
jftrabago@gmail.com

Inverse Geometry via Shape Optimization: Numerical Solution and
Well-Posedness from a Moving Boundary Framework

This talk revisits a toy inverse geometry problem formulated via shape optimization. We present a simple numerical method and study a related Hele-Shaw-type moving boundary problem, establishing short-time existence and uniqueness of a classical solution. The analysis provides a conceptual framework that also supports the stability of numerical schemes for similar shape optimization problems. This is joint work with Masato Kimura (Kanazawa University, Japan).

Jiajie Li
Shanghai Jiao Tong University
lijiajie20120233@163.com

Shape and topology optimization of supercapacitor electrode to maximize
charge storage

This work proposes a shape optimization approach for electrode morphology to maximize charge storage in supercapacitors. The ionic distributions and electric potential are modeled by the steady-state Poisson–Nernst–Planck system. Shape sensitivity analysis is performed to derive the Eulerian derivative in both volumetric and boundary expressions. An optimal electrode morphology is obtained through gradient flow algorithms. The steady-state Poisson–Nernst–Planck system is efficiently solved by the Gummel fixed-point scheme with finite-element discretization, in which exponential coefficients with large variation are tackled with inverse averaging techniques. Extensive numerical experiments are performed to demonstrate the effectiveness of the proposed optimization model and corresponding numerical methods in enhancing charge storage in supercapacitors. It is expected that the proposed shape optimization approach provides a promising tool in the design of electrode morphology from a perspective of charge storage enhancement.

Zhi Zhou
The Hong Kong Polytechnic University
zhi.zhou@polyu.edu.hk

Numerical analysis of quantitative photoacoustic tomography in a diffusive regime

In this talk, we consider the numerical analysis of quantitative photoacoustic tomography, which is modeled as an inverse problem to quantitatively reconstruct the diffusion and absorption coefficients in a second-order elliptic equation, utilizing multiple internal measurements. We establish a conditional stability in L^2 norm, under a provable nonzero condition, assuming randomly chosen boundary excitation data. Building upon this conditional stability, we propose and analyze a numerical reconstruction scheme based on an output least squares formulation, employing finite element discretization. We provide an a priori error estimate for the numerical reconstruction, serving as a guideline for selecting computational parameters. Several numerical examples will presented to illustrate the theoretical results.

Shengfeng Zhu
East China Normal University
sfzhu@math.ecnu.edu.cn

Efficient identification of geometric inverse sources of parabolic problems by model order reduction

We investigate reduced-order models (ROMs) for efficiently solving geometric inverse source problems in parabolic equations. To reconstruct source supports in diffusion processes, a reduced-order approach combining proper orthogonal decomposition (POD) and incremental singular value decomposition (ISVD) is proposed. This method significantly reduces the computational complexity and storage requirements typically associated with numerical shape and topology optimization. Numerical experiments are conducted to validate the effectiveness and efficiency of the proposed methodology. This a joint work with Xindi Hu and Yangwen Zhang.

Maolin Deng
The Chinese University of Hong Kong
mldeng@math.cuhk.edu.hk

Neural Network for discrete EIT solved by weights

In this work, we develop a novel neural network (NN) approach to solve the discrete inverse conductivity problem of recovering the conductivity profile on network edges from the discrete Dirichlet-to-Neumann map on a square lattice. The novelty of the approach lies in the fact that the sought-after conductivity is not provided directly as the output of the NN but is instead encoded in the weights of the post-trainig NN in the second layer. Hence the weights of the trained NN acquire a clear physical meaning, which contrasts with most existing neural network approaches, where the weights are typically not interpretable. This work represents a step toward designing NNs with interpretable post-training weights. Numerically, we observe that the method outperforms the conventional Curtis-Morrow algorithm and constrained approach for both noisy full and partial data.

MS11 Recent Developments of Numerical Methods and Modeling for Kinetic and Related Equations

Organizers: Liu Liu, Zhichao Peng

Tao Xiong,
University of Science and Technology of China,
taoxiong@ustc.edu.cn

Efficient Asymptotic Preserving Methods based on Characteristics for Frequency-dependent Radiative Transfer Equation

n this work, we try to develop an efficient asymptotic preserving method for frequency-dependent radiative transfer equations. Due to the optical opacity is frequency and temperature dependent, it varies from 0 to infinity, so that across three different regimes. We apply the characteristic based approach to get a revised model, and we modify it so that it can capture the free streaming regime. The new approximated model is solved by an asymptotic preserving Monte-Carlo method, in which we only solve a spatial dependent macroscopic equation (not frequency dependent). Based on the available macroscopic variables, it provides the emission source for the microscopic equation, which is then solved the Monte-Carlo method. The new method allows large time steps for all frequency regimes. Numerical experiments are given to demonstrate the effectiveness and efficiency of our approach.

Zheng Ma,
Shanghai Jiao Tong University,
zhengma@sjtu.edu.cn

DeepRTE: Pre-trained Attention-based Neural Network for Radiative Tranfer

Abstract: In this study, we propose a novel neural network approach, termed DeepRTE, to address the steady-state Radiative Transfer Equation (RTE). The RTE is a differential-integral equation that governs the propagation of radiation through a participating medium, with applications spanning

diverse domains such as neutron transport, atmospheric radiative transfer, heat transfer, and optical imaging. Our proposed DeepRTE framework leverages pre-trained attention-based neural networks to solve the RTE with high accuracy and computational efficiency. The efficacy of the proposed approach is substantiated through comprehensive numerical experiments. vspace1cm

Min Tang,
Shanghai Jiaotong University,
tangmin@sjtu.edu.cn

Random Source iteration method to mitigate the ray effect

The commonly used velocity discretization for simulating the radiative transport equation (RTE) is the discrete ordinates method (DOM). One of the long-standing drawbacks of DOM is the phenomenon known as the ray effect. Due to the high dimensionality of the RTE, DOM results in a large algebraic system to solve. The Source Iteration (SI) method is the most standard iterative method for solving this system. In this talk, by introducing randomness into the SI method, we propose a novel random source iteration (RSI) method that offers a new way to mitigate the ray effect without increasing the computational cost. We have rigorously proved that RSI is unbiased with respect to the SI method and that its variance is uniformly bounded across iteration steps; thus, the convergence order with respect to the number of samples is $1/2$. Furthermore, we prove that the RSI iteration process, as a Markov chain, is ergodic under mild assumptions. Numerical examples are presented to demonstrate the convergence of RSI and its effectiveness in mitigating the ray effect.

Yanli Wang,
Beijing Computational Science Research Center,
ylwang@csrc.ac.cn

Adaptive Sparse Discrete Velocity Method for the Boltzmann-BGK Equation

In this work, we introduce a Adaptive Sparse Discrete Velocity Method (ASDVM) for solving the Boltzmann-BGK equation. The distribution function is decomposed into two parts: an equilibrium component represented

by the Maxwellian distribution and a non-equilibrium component. Discrete velocity points are allocated only to the non-equilibrium part, resulting in a significantly reduced number of velocity points, particularly in near-continuous regimes, which greatly lowers the computational cost compared to conventional discrete velocity methods. The discretization of the microscopic velocity space is dynamically and adaptively adjusted based on the non-equilibrium component of the distribution. Several numerical examples are presented to validate the efficiency and accuracy of the proposed ASDVM.

Kunlun Qi,
University of Minnesota,
kqi@umn.edu

A fast Fourier spectral method for wave kinetic equation

The central object in wave turbulence theory is the wave kinetic equation (WKE), which is an evolution equation for wave action density and acts as the wave analog of the Boltzmann kinetic equations for particle interactions. Despite recent exciting progress in the theoretical aspects of the WKE, numerical developments have lagged behind. In this talk, I will introduce a fast Fourier spectral method for solving the WKE. The key idea lies in reformulating the high-dimensional nonlinear wave kinetic operator as a spherical integral, analogous to the classical Boltzmann collision operator. The conservation of mass and momentum leads to a double convolution structure in Fourier space, which can be efficiently handled by the fast Fourier transform (FFT), reducing the computational cost from $O(N^3d)$ to $O(MN^dlogN)$ with N-frequency nodes and $M \ll N^d$ in d-dimensions. The accuracy and efficiency of the proposed method can be demonstrated through several numerical tests in both 2D and 3D, revealing and conjecturing some interesting and unique features of this equation.

Jaeyong Lee,
Chung-Ang University,
jaeyong@cau.ac.kr

Deep Learning Approaches for Solving Kinetic Equations

Recent advances in deep learning have introduced powerful tools for solving kinetic equations, which often suffer from high computational costs due to nonlinearity and dimensionality. In this talk, we present deep learning-based approaches to solve two important kinetic models: the Vlasov-Poisson-Fokker-Planck equation and the Fokker-Planck-Landau equation. We also introduce FourierSpecNet, a neural network framework that incorporates spectral structure to efficiently approximate the Boltzmann collision operator. The method enables resolution-invariant learning and fast inference.

Zhongjian Wang,
Nanyang Technological University,
zhongjian.wang@ntu.edu.sg

Neuron Monge map estimation with convergence guarantee

In this talk, I will discuss our recent approach in neuron nets approximation to Monge map (optimal transport). Our starting point is the DeepParticle methods in learning probalistic solutions of multiscale PDEs. Then we will develop a new learning objective based on the DeepParticle framework. Under mild assumptions of the target distribution, we show validity of the new objective under L2 metric of prior. We further illustrate the effectiveness under more general assumptions, by several numerical experiments including distributions with disjoint supports and parametrized distributions.

Xinghui Zhong,
Zhejiang University,
zhongxh@zju.edu.cn

Energy-Conserving Discontinuous Galerkin Methods for Vlasov Systems

We propose energy-conserving numerical schemes for the Vlasov-type systems. Those equations are fundamental models in the simulation of plasma physics. The total energy is an important physical quantity that is conserved by those models. Our methods are the first Eulerian solver that can preserve fully discrete total energy conservation. The main features of our methods include energy-conservative temporal and spatial discretization. We validate our schemes by rigorous derivations and benchmark numerical examples.

MS12 Understanding the Learning of Deep Networks: Expressivity, Optimization, and Generalization

Organizers (Alphabetical): Fenglei Fan, Wei Huang, Shaoqun Zhang, Shijun Zhang

Fenglei Fan
Department of Data Science, City University of Hong Kong
fenglfan@cityu.edu.hk

Width and Depth Equivalence: from the Perspective of Dynamic System

While classic studies proved that wide networks allow universal approximation, recent research and successes of deep learning demonstrate the power of deep networks. Based on a symmetric consideration, we investigate if the design of artificial neural networks should have a directional preference, and what the mechanism of interaction is between the width and depth of a network. Inspired by the De Morgan law, we address this fundamental question by establishing a quasi-equivalence between the width and depth of ReLU networks from the perspective of the dynamic system. Based on our findings, a deep network has a wide equivalent, and vice versa, subject to an arbitrarily small error.

Juncai He
Yau Mathematical Sciences Center, Tsinghua University
jche@tsinghua.edu.cn

On the Expressivity of Neural Networks and Its Applications

In this talk, I will present some recent results on the expressivity of neural networks and its applications. First, we will illustrate the connections

95

between linear finite elements and ReLU DNNs, as well as between spectral methods and ReLU^k DNNs. Second, we will share our latest findings regarding the open question of whether DNNs can precisely recover piecewise polynomials of arbitrary order on any simplicial mesh in any dimension. Then, we will discuss a specific result on the optimal expressivity of ReLU DNNs and its application, combining it with the Kolmogorov-Arnold representation theorem. Finally, I will offer a remark on the study of convolutional neural networks from an expressivity perspective.

Wei Huang
RIKEN Center of Advanced Intelligence, Japan
wei.huang.vr@riken.jp

On the Comparison between Multi-modal and Single-modal Contrastive Learning

Multi-modal contrastive learning with language supervision has presented a paradigm shift in modern machine learning. By pre-training on a web-scale dataset, multi-modal contrastive learning can learn high-quality representations that exhibit impressive robustness and transferability. Despite its empirical success, the theoretical understanding is still in its infancy, especially regarding its comparison with single-modal contrastive learning. In this work, we introduce a feature learning theory framework that provides a theoretical foundation for understanding the differences between multi-modal and single-modal contrastive learning. Through a trajectory-based optimization analysis and generalization characterization on downstream tasks, we identify the critical factor, which is the signal-to-noise ratio (SNR), that impacts the generalizability in downstream tasks of both multi-modal and single-modal contrastive learning. Through the cooperation between the two modalities, multi-modal learning can achieve better feature learning, leading to improvements in performance in downstream tasks compared to single-modal learning. Our analysis provides a unified framework that can characterize the optimization and generalization of both single-modal and multi-modal contrastive learning.

Enming Liang
Department of Data Science, City University of Hong Kong
eliang4@cityu.edu.hk

Homeomorphic Projection to Ensure Neural-Network Solution Feasibility
for Constrained Optimization

There has been growing interest in employing neural networks (NNs) to directly solve constrained optimization problems with low run-time complexity. However, it is non-trivial to ensure NN solutions strictly satisfy problem constraints due to inherent NN prediction errors. Existing feasibility-ensuring methods are either computationally expensive or lack performance guarantee. In this paper, we propose Homeomorphic Projection as a low-complexity scheme to guarantee NN solution feasibility for optimization over a general set homeomorphic to a unit ball, covering all compact convex sets and certain classes of non-convex sets. The idea is to (i) learn a minimum distortion homeomorphic mapping between the constraint set and a unit ball using a bi-Lipschitz invertible NN (INN), and then (ii) perform a simple bisection operation concerning the unit ball such that the INN-mapped final solution is feasible with respect to the constraint set with minor distortion-induced optimality loss. We prove the feasibility guarantee and bounded optimality loss under mild conditions. Simulation results, including those for non-convex AC-OPF problems in power grid operation, show that homeomorphic projection outperforms existing methods in solution feasibility and run-time complexity while achieving similar optimality loss.

Fanghui Liu
Department of Mathematics, University of Warwick
fanghui.liu@warwick.ac.uk

Norm-based capacity in machine learning: Generalization, deterministic
equivalence and function spaces

Machine learning (ML) generally operates in high-dimensions, of which the performance is characterized by learning efficiency—both theoretically (statistical and computational efficiency) and empirically (practical efficient ML). A fundamental question in ML theory and practice is how the test error

(generalization) evolves with sample size and model capcity (e.g., model size), shaping key concepts such as the bias-variance trade-offs, double descent, and scaling laws.

In this talk, I will discuss how the test error will behave if a more suitable metric than model size for model capacity is used. To be specific, I will present a unified perspective via deterministic equivalence on generalization by analyzing how norm-based model capacity control reshapes our understanding of these foundational concepts: there is no bias-variance trade-offs; phase transition exists from under-parameterized regimes to over-parameterized regimes while double descent doesn't exist; scaling law is formulated as a multiplication style under norm-based capacity. Additionally, I will briefly discuss which norm is suitable for neural networks and what are the fundamental limits of learning efficiency imposed by such norm-based capacity from the perspective of function space. Talks are based on https://arxiv.org/abs/2502.01585 and https://arxiv.org/abs/2404.18769

Atsushi Nitanda
A*STAR Centre for Frontier AI and Research (A*STAR CFAR)
atsushi_nitanda@cfar.a-star.edu.sg

Propagation of Chaos for Mean-Field Langevin Dynamics and its
Application to Model Ensemble

Mean-field Langevin dynamics (MFLD) is an optimization method derived by taking the mean-field limit of noisy gradient descent for two-layer neural networks in the mean-field regime. Recently, the propagation of chaos (PoC) for MFLD has gained attention as it provides a quantitative characterization of the optimization complexity in terms of the number of particles and iterations. A remarkable progress by Chen et al. (2022) showed that the approximation error due to finite particles remains uniform in time and diminishes as the number of particles increases. In this work, by refining the defective log-Sobolev inequality, a key result from that earlier work, under the neural network training setting, we establish an improved PoC result for MFLD, which removes the exponential dependence on the regularization coefficient from the particle approximation term of the optimization complexity. As an application, we propose a PoC-based model ensemble strategy with theoretical guarantees.

Lei Shi
School of Mathematical Sciences, Fudan University
leishi@fudan.edu.cn

Learning Theory of Classification with Deep Neural Networks

Deep neural networks have achieved remarkable success in various binary classification tasks. Despite their practical effectiveness, theoretical understanding of their generalization in binary classification remains limited. In this talk, I will present our recent progress on classification using deep neural networks.

Jiaye Teng
Shanghai University of Finance and Economics
tengjiaye@sufe.edu.cn

A Mathematically Provable Two-Stage Training Dynamics in Transformers

Transformers may exhibit two-stage training dynamics during the real-world training process. For instance, when training GPT-2 on Counterfact dataset, the answers progress from syntactically incorrect to syntactically correct to semantically correct. However, existing theoretical analyses hardly account for this two-stage phenomenon. In this paper, we theoretically demonstrate how such two-stage training dynamics occur in transformers. Specifically, we analyze the dynamics of transformers using feature learning techniques under in-context learning regimes, based on a disentangled two-type feature structure. Such disentanglement of feature structure is general in practice, e.g., natural languages contain syntax and semantics, and proteins contain primary and secondary structures. To our best known, this is the first rigorous result regarding a two-stage optimization process in transformers. Additionally, a corollary indicates that such a two-stage process is closely related to the spectral properties of the attention weights, which accords well with empirical findings.

Jinming Weng
Jilin University
jinmingwen1@163.com

Randomized Orthogonal Matching Pursuit Algorithm with Adaptive Partial Selection for Sparse Signal Recovery

The orthogonal matching pursuit (OMP) algorithm, known for its exceptional ability to reconstruct sparse signals, is a widely employed algorithm in compressed sensing. Numerous studies have provided theoretical analyses supporting its capability for achieving exact recovery. However, when applied to large-scale sparse signal recovery, the OMP algorithm incurs substantial computational overhead, leading to prolonged running time. To address this challenge, in this talk, we will introduce a Randomized OMP with Adaptive Partial Selection (AROMP) algorithm to mitigate computational overhead and reduce runtime. The novelty of the AROMP algorithm lies in its utilization of a randomized index selection method rather than a greedy approach to select the index in each iteration. Subsequently, we will theoretically characterize the gap between AROMP and OMP for exactly recovering an s-sparse signal and show that the gap decreases as the number of comparisons K increases, sparsity s decreases, or signal dimension n decreases. We will also show some experimental results to illustrate the efficiency and effectiveness of our proposed method on sparse signal recovery, face recognition tasks, and image reconstruction tasks. This is joint work with Changhao Li, Qianyu Shu and Zhengchun Zhou.

Xiaotong Yuan
School of Intelligence Science and Technology
Nanjing University
xtyuan@nju.edu.cn

Derandomized Online-to-Non-convex Conversion for Stochastic Weakly Convex Optimization

Online-to-non-convex conversion (O2NC)) is a randomized method for producing Goldstein (δ, ϵ)-stationary points of non-smooth non-convex functions with optimal oracle complexity $O(\delta^{-1}\epsilon^{-3})$. Subject to *random scaling* on the update, O2NC recapitulates the stochastic gradient descent with

momentum (SGDM) algorithm popularly used for training neural networks. Random scaling, however, conflicts with virtually all practical algorithms. So a natural question arises: Can we derandomize O2NC to achieve the same optimal rate but without randomization? On the negative side, the general answer is *no* due to the impossibility result of Jordan et al. (COLT 2023) showing that no dimension-free rate can be achieved by deterministic algorithms. On the positive side, as we are going to deliver in this talk that the answer is *yes* when the functions are weakly convex. To this end, we present a novel O2NC framework that deterministically converts a *periodic* online gradient descent algorithm to a stochastic weakly convex optimizer. Remarkably, the derandomized algorithm converges at an optimal rate which is invariant to the weak-convexity parameter as long as it is no larger than $O(\delta^{-1/2}\epsilon^{-1.5})$. In other words, the higher stationarity of solution is required, the weaker convexity can be tolerated by our algorithm.

Shao-Qun Zhang
Nanjing University
zhangsq@lamda.nju.edu.cn

Recent Studies on Spiking Neural Networks

Recent years have emerged a surge of interest in spiking neural networks (SNNs). The performance of SNNs hinges not only on searching apposite architectures and connection weights, similar to conventional artificial neural networks, but also on the meticulous configuration of their intrinsic structures. In this talk, we introduce our studies on theoretical characterizations of SNNs. We begin this talk with an interesting finding relative to bifurcation in SNNs, and then delve deep into the intrinsic structures of SNNs. Our findings elucidate why the efficacy of SNNs hinges heavily on the configuration of intrinsic structures and lead to a recommendation that enhancing the adaptability of these structures contributes to improving the overall performance and applicability of SNNs. Based on these findings, we further provide comprehensive theoretical investigations on SNNs, including approximation, complexity, efficiency, and generalization. Specifically, we prove the first generalization bound relative to SNNs that the stochastic spiking neurons maintain generalization bounds with an exponential reduction in

Rademacher complexity. Empirical experiments conducted on various real-world datasets affirm the effectiveness of our proposed methods.

Shijun Zhang
Department of Applied Mathematics, Hong Kong Polytechnic University
shijun.zhang@polyu.edu.hk

Tackling High-Frequency Challenges: From Shallow to Multi-Layer Neural Networks

This talk explores the limitations of shallow neural networks in addressing high-frequency challenges and introduces a novel solution through a multi-layer, multi-component neural network (MMNN) architecture. We demonstrate that shallow networks behave like low-pass filters, struggling with high-frequency components due to machine precision constraints and slow learning dynamics. The MMNN architecture overcomes these obstacles by efficiently decomposing complex functions, achieving substantial improvements in accuracy and computational efficiency. Numerical experiments validate the effectiveness of this approach in capturing fine details in oscillatory functions.

Student Forum

Chenghao Liu
Department of Data Science, City University of Hong Kong
chenghao9926@gmail.com

Characterizing ResNet's Universal Approximation Capability

Since its debut in 2016, ResNet has become arguably the most favorable architecture in deep neural network (DNN) design. It effectively addresses the gradient vanishing/exploding issue in DNN training, allowing engineers to fully unleash DNN's potential in tackling challenging problems in various domains. Despite its practical success, an essential theoretical question remains largely open: how well/best can ResNet approximate functions? In

this paper, we answer this question for several important function classes, including polynomials and smooth functions. In particular, we show that ResNet with constant width can approximate Lipschitz continuous function with a Lipschitz constant μ using $\mathcal{O}(c(d)(\varepsilon/\mu)^{-d/2})$ tunable weights, where $c(d)$ is a constant depending on the input dimension d and $\epsilon > 0$ is the target approximation error. Further, we extend such a result to Lebesgue-integrable functions with the upper bound characterized by the modulus of continuity. These results indicate a factor of d reduction in the number of tunable weights compared with the classical results for ReLU networks. Our results are also order-optimal in ε, thus achieving optimal approximation rate, as they match a generalized lower bound derived in this paper. This work adds to the theoretical justifications for ResNet's stellar practical performance.

MS13 Novel Numerical Methods in Multiscale Models

Organizers: Wing Tat Leung, Yating Wang

Hyea Hyun Kim
Kyung Hee University
hhkim@khu.ac.kr

Iterative algorithms for neural network approximation to PDEs by domain decomposition methods

Domain decomposition methods are applied for neural network approximations to PDEs in order to achieve efficient and scalable solutions. The problem domain is partitioned into overlapping or nonoverlapping subdomains and local neural networks are then introduced to approximate the solution in each subdomain, where each local problem is solved independently for a provided boundary condition. This solution procedure with independent local problems requires a suitable update formula on the boundary conditions to achieve a convergent approximate solution. As a result, an iterative algorithm for neural network approximation can be obtained, where the local problem training can be done efficiently by utilizing a multiprocessor parallel computation with communication between neighboring network solutions only in the update of the iterates. In this talk, several iterative algorithms will be presented based on the design of the update formula and further acceleration schemes will be also discussed with various numerical experimental results.

Viet Ha Hoang
Nanyang Technological University
vhhoang@ntu.edu.sg

A hierarchical approach for multicontinuum homogenization in high contrast media

The multicontinuum homogenization method solves a series of constrained cell problems to capture localized information for each continuum. However, solving all these cell problems on very fine grids at every macroscopic point

is computationally expensive. We propose a hierarchical multicontinuum homogenization framework, which defines hierarchical macroscopic points and solve the constrained problems on grids of varying resolutions. We assume that the local solutions can be represented as a combination of a linear interpolation of local solutions from preceding levels and an additional correction term. This combination is substituted into the original constrained problems, and the correction term is resolved using finite element grids of varying sizes, depending on the level of the macropoint. We establish that our approach incurs a substantial computational saving cost. Numerical experiments validate the effectiveness of the proposed method in media with slowly varying properties, underscoring its potential for efficient multiscale modeling.

This is a joint work with Wei Xie, Yin Yang and Yunqing Huang

Xiangcheng Zheng
Shandong University
xzheng@sdu.edu.cn

Analysis and computation for multiscale Abel kernel and related nonlocal models

We consider the variable-exponent Abel kernel and demonstrate its multiscale nature in modeling crossover dynamics from the initial quasi-exponential behavior to long-term power-law behavior. Then we apply this to subdiffusion, diffusion-wave equation and integro-differential equation that model different multiscale phenomena. Both mathematical and numerical analysis will be considered for each model, with numerical simulations indicating the crossover dynamics of the models.

Shubin Fu
Eastern Institute for Advanced Study
shubinfu@eias.ac.cn

Multiscale subspaces and their relationships with preconditioners

In this talk, I will introduce the basic ideas of constructing multiscale subspaces and how these subspaces can be leveraged to develop efficient preconditioners. Specifically, I will discuss their applications in Darcy's flow in highly heterogeneous and fractured media, compressible flow and transport, elasticity problems, and the Helmholtz equation.

Jian Huang
National Center for Applied Mathematics in Hunan & Xiangtan University, China
huangjian213@xtu.edu.cn

Multicontinuum homogenization for coupled flow and transport equations

In this talk, we present the derivation of a multicontinuum model for the coupled flow and transport equations by applying multicontinuum homogenization. We perform the multicontinuum expansion for both flow and transport solutions and formulate novel coupled constraint cell problems to capture the multiscale property, where oversampled regions are utilized to avoid boundary effects. Assuming the smoothness of macroscopic variables, we obtain a multicontinuum system composed of macroscopic elliptic equations and convection-diffusion-reaction equations with homogenized effective properties. Finally, we present numerical results for various coefficient fields and boundary conditions to validate our proposed algorithm.

Hao Dong
Xidian University
donghaoxd@xidian.edu.cn

Higher-order multi-scale method and it convergence analysis for multi-field coupling problems of composite structures

Under extreme thermo-mechanical coupling environments, the material properties of composites change significantly with temperature, exhibiting complex nonlinear thermo-mechanical coupling behaviors. To effectively and finely simulate the nonlinear thermo-mechanical coupling problems of composite structures, this report develops a novel higher-order multi-scale computational method with high-accuracy and efficient computational performance. Firstly, on the basis of multi-scale asymptotic analysis and Taylor series approach, a new higher-order multi-scale computational model is established to accurately analyze the nonlinear thermo-mechanical coupling behaviors in composite structures. Then, under certain simplifications and assumptions, the convergence estimate of the higher-order multi-scale asymptotic solutions is obtained. Next, based on the established higher-order

multi-scale computational model, a two-stage multi-scale algorithm is developed to efficiently simulate time-dependent nonlinear thermo-mechanical coupling problems of composite structures. Subsequently, extensive numerical experiments demonstrate that the proposed approach has competitive advantages for solving the nonlinear thermo-mechanical coupling problems of composite structures, which has exceptional numerical accuracy and less computational cost. Finally, some progresses in multi-scale computation of nonlinear thermo-electrical coupling problems of composite structures and deep learning simulation of multi-scale problems of composite structures are introduced.

Yating Wang
Xi'an Jiaotong University
yatingwang@xjtu.edu.cn

Efficient temporal splitting scheme for high contrast multiscale problems

In this talk, we propose a parallel algorithm based on the temporal splitting scheme fot the multiscale flow problem. The idea is first to evolve the partially explicit system using a coarse time step size, then correct the solution on each coarse time interval with some fine propagators. This procedure is then performed iteratively till convergence. We analyze the stability and convergence of the proposed algorithm. The numerical experiments demonstrate that the proposed algorithm achieves high numerical accuracy for high-contrast problems and converges in a relatively small number of iterations. The number of iterations stays stable as the number of coarse intervals increases, thus significantly improving computational efficiency through parallel processing.

Mengnan Li
Nanjing University of Posts and Telecommunications
mengnanli@njupt.edu.cn

Data-driven reduced-order modeling for nonautonomous dynamical systems in multiscale media

In this talk, we present data-driven reduced-order modeling for nonautonomous dynamical systems in multiscale media. The Koopman operator has received extensive attention as an effective data-driven technique, which can transform the nonlinear dynamical systems into linear systems through acting on observation function spaces. Different from the case of autonomous dynamical systems, the Koopman operator family of nonautonomous dynamical systems significantly depend on a time pair. In order to effectively estimate the time-dependent Koopman operators, a moving time window is used to decompose the snapshot data, and the extended dynamic mode decomposition method is applied to computing the Koopman operators in each local temporal domain. Many physical properties in multiscale media often vary in very different scales. In order to capture multiscale information well, the dimension of collected data may be high. To accurately construct the models of dynamical systems in multiscale media, we use high spatial dimension of observation data. It is challenging to compute the Koopman operators using the very high dimensional data. Thus, the strategy of reduced-order modeling is proposed to treat the difficulty. The proposed reduced-order modeling includes two stages: offline stage and online stage. In offline stage, a blockwise low rank decomposition is used to reduce the spatial dimension of initial snapshot data. For the nonautonomous dynamical systems, real-time observation data may be required to update the Koopman operators. The online reduced-order modeling is proposed to correct the offline reduced-order modeling. Three methods are developed for the online reduced-order modeling: fully online, semi-online and adaptive online. The adaptive online method automatically selects the fully online or semi-online and can achieve a good trade-off between modeling accuracy and efficiency.

MS14 Theory and Application on Inverse Problems and Imaging

Organizer: Jiho Hong

Ruchi Guo,
Sichuan University
ruchiguo@scu.edu.cn

Transformer and the application to inverse problems

A Transformer-based deep direct sampling method is proposed for electrical impedance tomography, a well-known severely ill-posed nonlinear boundary value inverse problem. We give a specific example to a fundamental question: whether and how one can benefit from the theoretical structure of a mathematical problem to develop task-oriented and structure-conforming deep neural networks? Specifically, inspired by direct sampling methods for inverse problems, the 1D boundary data in different frequencies are preprocessed by a partial differential equation-based feature map to yield 2D harmonic extensions as different input channels. Then, by introducing learnable non-local kernels, the direct sampling is recast to a modified attention mechanism. The new method achieves superior accuracy over its predecessors and contemporary operator learners and shows robustness to noises in benchmarks. This research shall strengthen the insights that, despite being invented for natural language processing tasks, the attention mechanism 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.

Lingyun Qiu,
Tsinghua University
lyqiu@tsinghua.edu.cn

Sediment Concentration Estimation via Multiscale Inverse Problem and Stochastic Homogenization

In this work, we present a novel approach for sediment concentration measurement in water flow, modeled as a multiscale inverse medium problem. To address the multiscale nature of the sediment distribution, we treat it as an inhomogeneous random field and use the homogenization theory in deriving the effective medium model. The inverse problem is formulated as the reconstruction of the effective medium model, specifically, the sediment concentration, from partial boundary measurements. Additionally, we develop numerical algorithms to improve the efficiency and accuracy of solving this inverse problem. Our numerical experiments demonstrate the effectiveness of the proposed model and methods in producing accurate sediment concentration estimates, offering new insights into sediment measurement in complex environments.

Woojoo Lee,
Korea Advanced Institute of Science and Technology
es3777@kaist.ac.kr

Bayesian optimization for tracking a moving target in inverse scattering problems

We study the inverse scattering problem of tracking the location and orientation of a moving target from far-field data generated by a single incident field. Our approach formulates the problem as the optimization of a misfit functional comparing measured and simulated far-field data. In both two- and three-dimensional settings, we derive formulas describing the far-field data under translation and rotation of the target and prove the local Lipschitz continuity of the far-field data with respect to the rotation angle at the true value. These results are combined with Bayesian optimization to reduce the number of objective function evaluations during tracking. The tracking framework is developed for both two- and three-dimensional targets, and when the shape is unknown, machine learning is used to infer the target's shape. Numerical examples involving randomly generated shapes and trajectories illustrate the performance of the proposed method.

Jiahua Jiang,
University of Birmingham
j.jiang.3@bham.ac.uk

Illuminating Accuracy with Learning-guided Refinement: A Warm-basis
Iterative Method for Fluorescence Molecular Tomography

Fluorescence Molecular Tomography (FMT) is a non-invasive optical imaging technology widely used in biomedical research to reconstruct the volumetric distribution of fluorescent targets by measuring fluorescence signals emitted from the surface. FMT reconstruction faces significant accuracy challenges due to limited light penetration and strong photon scattering, which degrade depth resolution and worsen the inverse problem's ill-posedness. Iterative methods struggle with poor Z-resolution despite advanced regularization, while operator-learning approaches can improve depth recovery but rely on large, high-quality paired datasets that are often impractical to acquire experimentally. Moreover, directly using the prediction from a trained deep learning model as an initial guess does not always lead to improved reconstructions. We present a warm-basis iterative projection method (WB-IPM) for solving 3D FMT problems, where the initial basis is obtained by a trained neural network, and then the reconstruction is refined by an augmented flexible hybrid projection method. Theoretical results show that, under reasonable conditions, our method can achieve a lower error bound than standard flexible hybrid projection methods. We demonstrate the effectiveness of our method on both numerical and real experiments.

Yunho Kim,
Ulsan National Institute of Science and Technology
yunhokim@unist.ac.kr

Space-time summation-by-parts for the wave equation

In this talk, I will present a recent development of SBP (Summation-By-Parts) in time and space for the wave equation. To the best of my knowledge, there has not been a proper extension of SBP to both time and space. I will discuss both theoretical and numerical results. I will also present an application of the method for photoacoustic imaging.

Ye Zhang,
Beijing Institute of Technology & Shenzhen MSU-BIT University
ye.zhang@smbu.edu.cn

On the universal approximation theorems for neural networks for ill-posed inverse problems

We establish universal approximation theorems for neural networks applied to general nonlinear ill-posed operator equations. In addition to the approximation error, the measurement error is also taken into account in our error estimation. We introduce the expanding neural network method as a novel iterative regularization scheme and prove its regularization properties under different a priori assumptions about the exact solutions. Within this framework, the number of neurons serves as the regularization parameter. We demonstrate that for data with high noise levels, a small network architecture is sufficient to obtain a stable solution, whereas a larger architecture may compromise stability due to overfitting. Furthermore, under standard assumptions in regularization theory, we derive convergence rate results for neural networks in the context of variational regularization. Several numerical examples are presented to illustrate the robustness of the proposed neural network-based algorithms.

Soomin Jeon,
Dong-A University
soominjeon@dau.ac.kr

SVD-Based Spectral Methods for Data Efficiency in Imaging and Learning

Singular Value Decomposition (SVD) plays a fundamental role in modern applied mathematics, particularly in tasks involving data reduction and efficient representation. In this talk, we present two distinct applications of SVD that address practical challenges in medical imaging and machine learning. The first application focuses on medical image compression, where we propose an adaptive rank selection strategy to achieve compact yet clinically meaningful representations of image data. The second application explores active learning through the lens of Neural Tangent Kernels (NTKs), employing spectral analysis of NTK matrices to identify the most informative data batches for training. In both cases, SVD serves as a unifying analytical tool

for optimizing information content and computational efficiency. These results demonstrate the versatility of spectral methods in solving high-impact problems across domains.

Zhiyuan Li,
Ningbo University
lizhiyuan@nbu.edu.cn

Hölder stable recovery of the source of fractional wave equations

In this talk, we are devoted to the inverse source problem in fractional wave equation, with the aid of extra measurement data on partial boundary. Stability results are obtained by using bi-orthogonal basis for the Mittag-Leffler functions provided that the measurement time is large enough.

Mikyoung Lim,
Korea Advanced Institute of Science and Technology
mklim@kaist.ac.kr

Estimates for neural approximation via wavelet frame theory

We introduce a wavelet-based framework for analyzing the universal approximation properties of neural networks. By leveraging wavelet frame theory on spaces of homogeneous type, we establish sufficient conditions on activation functions that ensure the corresponding neural networks satisfy the so-called averaging kernel conditions. Under these conditions, neural networks can approximate any function in a specific function space associated with the activation functions, with explicit error estimates. Our results accommodate various smooth, possibly oscillatory activations, and further extend to non-smooth activations. This work is a collaboration with Youngmi Hur and Hyojae Lim.

Jiho Hong,
The Chinese University of Hong Kong
jihohong@cuhk.edu.hk

Unique Determination of Variable Order of Time Fractional Diffusion from One Boundary Measurement

We consider the inverse problem to recover the order of time derivation for subdiffusion using one boundary measurement. The order of time derivation represents the speed of diffusion and is assumed to be a function of the space variable in 1D, 2D and 3D. For this new inverse problem, we introduce the uniqueness and stability results. The proofs are based on the asymptotic relations of the Laplace transform of the boundary data. We briefly introduce two approaches to prove the asymptotic relations: an elementary proof of gluing and the Neumann series argument using the well-developed properties of resolvent operators. This is a collaborative work with Bangti Jin and Yavar Kian.

Wenlong Zhang,
Southern University of Science and Technology
zhangwl@sustech.edu.cn

Convergence Estimates of Inverse Source Problems with Boundary Measurement

In this work, we investigate the Tikhonov-type regularized solutions and their finite element solutions to the inverse space-dependent source problem from boundary measurement data. Firstly, with the classical source condition, we establish the convergence of regularized solutions and their finite element solutions under the standard L^2 norm. The error estimates present explicit dependence on the critical parameters like noise level, regularization parameter, mesh size and time step size. Next, based on our proposed weak norm, we get the conditional stability of Lipschitz type for the inverse problem, then the first order convergence of regularized solutions can be derived in the sense of weak norm. We get this convergence without any source condition. Moreover, this work is further carried out for the scattered data.

We suppose the observation points are scattered and the point-wise measurement data come with independent sub-Gaussian random noises. Then we give the stochastic convergence of regularized solutions and propose an efficiently iterative algorithm to determine the optimal regularization parameter. Numerical experiments are presented to demonstrate the effectiveness of the proposed algorithms.

MS15 Numerical Methods and Computational Modeling in Fluid Dynamics and Materials Science

Organizers: Xiaoxue Qin, Xiaomin Pan

Luchan Zhang,
Shenzhen University
zhanglc@szu.edu.cn

Dynamics of grain boundaries based on underlying microstructure

Grain boundaries are surface defects in crystalline materials. Dynamic properties of grain boundaries play vital roles in the mechanical and plastic behaviors of polycrystalline materials. The properties of grain boundaries strongly depend on their microscopic structures. We present continuum models for the dynamics of grain boundaries based on the continuum distribution of the line defects (dislocations or disconnections) on them. The long-range elastic interaction between the line defects is included in the continuum models to maintain stable microstructure on grain boundaries during the evolution. The continuum models is able to describe both normal motion and tangential translation of the grain boundaries due to both coupling and sliding effects that were observed in atomistic simulations and experiments.

Tiantian Xu,
Yonsei University
tian0917@yonsei.ac.kr

A data-driven reduced-order model for swimming optimization of a self-propelled filament

Flapping motions of wings or fins are commonly used by animals to generate lift or thrust, enabling efficient locomotion in fluid environments. To optimize the swimming performance of a self-propelled flexible filament for bioinspired applications, we develop a computational framework integrating high-fidelity simulation and reduced-order modeling. The fluid–structure interaction is resolved using a monolithic immersed boundary method, which eliminates the need for mesh regeneration during flapping motion. Proper

orthogonal decomposition (POD) is employed to extract dominant flow features, and a transformer-based neural network is trained to capture the nonlinear mapping between input parameters and POD coefficients. This POD-transformer model significantly reduces computational cost while retaining high accuracy. Validation against full-order simulations demonstrates the robustness of the surrogate model across various material properties and operating conditions. A genetic algorithm is used to maximize swimming speed, where an optimal solution set is found. This framework offers a scalable and accurate approach for optimizing bioinspired propulsion, with potential extensions to broader fluid–structure interaction problems.

Xiaoxue Qin,
Shanghai University
qinxiaoxue@shu.edu.cn

A Three-dimensional Continuum Simulation Method for Grain Boundary

We have developed a range of continuum models that describe the structure and dynamics of low angle grain boundaries in three dimensions. The static model minimizes grain boundary energy according to Frank's formula constraints, while the dynamic model includes the motion and reactions of dislocations. We have developed numerical algorithms based on the projection method. In comparing our simulation results with atomistic simulations, it is evident that our model accurately predicts the dislocation structure, energy profiles of grain boundaries, and their dynamics. These findings highlight the potential of continuum models to enhance the understanding of material behavior and solid mechanics.

Lina Zhao,
City University of Hong Kong
linazha@cityu.edu.hk

A novel multipoint stress control volume method for linear elasticity on quadrilateral grids

In this talk, I will present a novel control volume method that is locally conservative and locking-free for linear elasticity problem on quadrilateral grids. The symmetry of stress is weakly imposed through the introduction of a Lagrange multiplier. As such, the method involves three unknowns: stress, displacement and rotation. To ensure the well-posedness of the scheme, a pair of carefully defined finite element spaces is used for the stress, displacement and rotation such that the inf-sup condition holds. An appealing feature of the method is that piecewise constant functions are used for the approximations of stress, displacement and rotation, which greatly simplifies the implementation. In particular, the stress space is defined delicately such that the stress bilinear form is localized around each vertex, which allows for the local elimination of the stress, resulting in a cell-centered system. The convergence analysis will be shown for the scheme. Several numerical experiments will be performed to verify the performance of the proposed scheme.

Yaguang Gu,
South China University of Technology
guyaguang@scut.edu.cn

Bound- and Positivity-preserving Affine-invariant WENO Scheme for the Five-equation Model of Two-medium Flows

Numerical study on compressible two-medium flows has been a hot issue in recent decades due to broad applications in gas bubble dynamics, underwater explosion, inertial confinement fusion, and so on. In this study, we present a fifth order finite difference path-conservative alternative WENO scheme with central-upwind numerical flux (PCCU-AWENO) for the five-equation transport model of two-medium flows with the stiffened gas equation of state. We propose a uniformly high order flux-based bound- and positivity-preserving (BP-P) limiters for the scheme, while preserving the equilibrium solutions simultaneously. Once the BP-P limiters are used, oscillations may be generated at material interface. To this end, we introduce the affine-invariant WENO interpolations, which take care of structures in small scales. In addition, we will explain how to choose a proper family of paths for the non-conservative product to improve BP-P CFL conditions. Finally, numerical examples are shown to verify robustness and effectiveness of the PCCU-AWENO scheme.

Wanli Yu,
Jiangsu Ocean University
yuwanli@jou.edu.cn

A Compressible Multiphase Flow Model with Immersed Boundary Method
for Near-Field Underwater Explosion Dynamics

In this study, we present a novel solver for simulating compressible multi-fluid multiphase flow in near-field underwater explosions. The developed solver uses a modified version of six-equation reduced model of a diffuse-interface method combined immersed boundary method (IBM). We discretize the equation system using a Godunov-type scheme with a two phase HLLC approximate Riemann solver and a MUSCL-Hancock primitive scheme with TVD limiters, achieving second-order extension. Both the dimensional splitting and fractional-step methods are used to model one-dimensional operators, splitting them into sequential operators. A ghost cell IBM is used to embed complex terrain into the simulation domain. The immersed boundary surfaces are defined as point clouds, capable of exhibiting structured or unstructured patterns. IB objects are represented as level sets within the computational domain, and computational geometry concepts are employed to classify points as outside, nearby, or inside the immersed boundary. The signed distance computation method is then applied to define the object surfaces. The inverse distance weighting interpolation method is utilized to evaluate the interpolation cell. The zero normal velocity at the solid boundary is enforced to reconstruct the ghost cell. Test cases have been executed to authenticate the proposed model for simulating the interaction between UNDEXs and solid obstacles. The compressible multi-fluid model combined with IBM is well validated and proven to be precise in representing shockwave-structure interaction, enhancing its applicability in engineering scenarios.

Xiaomin Pan,
Shanghai University
xmpan@shu.edu.cn

Unconditionally energy-stable and accurate schemes based on hyperbolic
tangent scalar auxiliary variable approach for gradient flows

119

In this paper, we extend the selection of auxiliary variables by proposing a hyperbolic tangent scalar auxiliary variable (tanh-SAV) approach for solving gradient flows. The proposed tanh-SAV schemes introduce an auxiliary variable based on the hyperbolic tangent function, providing a well-defined formulation that enables the construction of decoupled, linear, and efficient numerical schemes. We demonstrate the construction of first-order, second-order, and higher-order unconditionally energy-stable schemes, utilizing either the Crank–Nicolson method or a k-step backward differentiation formula for time discretization. Only one constant coefficient equation needs to be solved per time step. Furthermore, the theoretical analysis demonstrates the discrete energy stability of the proposed numerical schemes and proves the positivity property of the auxiliary variable. In addition, we provide numerical simulations of one- and two-dimensional Cahn–Hilliard, Allen–Cahn, and phase-field crystal models. The results demonstrate that, consistent with the theoretical analysis, the proposed schemes preserve the positivity of auxiliary variable, maintain excellent stability, and achieve the desired temporal accuracy.

MS16 Recent Advances in Mechanism-Informed Data-Driven Methods: Theories and Applications

Organizers: Dong Wang, Hao Liu

Zheng Ma,
Shanghai Jiao Tong University
zhengma@sjtu.edu.cn

Solving PDE Inverse Problems with Generative Models and Their Applications

In recent years, with the development of deep learning, many methods have been successfully applied to solving inverse problems of partial differential equations (PDEs). However, most current deep learning-based inversion methods either require paired data for support or necessitate retraining the neural network when the conditions of the inverse problem change, significantly reducing inversion efficiency and limiting its scope of application. To overcome this limitation, we propose an unsupervised inversion method specifically designed for PDE inverse problems by integrating score-based generative diffusion models. Our research is based on the Bayesian inversion framework, transforming the task of solving the posterior distribution into a conditional generative process realized by solving the reverse-time stochastic differential equation. Additionally, to enhance the accuracy of inversion results, we introduce a diffusion posterior sampling inversion algorithm based on ordinary differential equations. This algorithm stems from the marginal probability density function characteristics of two different forward generative processes satisfying the same Fokker-Planck equation. Through a series of experiments on various PDEs, we validate the efficiency and robustness of the proposed method.

Jianbo Cui,
The Hong Kong Polytechnic University
jianbo.cui@polyu.edu.hk

A Supervised Learning Scheme for Computing Hamilton-Jacobi Equation
via Density Coupling

We propose a supervised learning scheme for the first order Hamilton-Jacobi PDEs in high dimensions. The scheme is designed by using the geometric structure of Wasserstein Hamiltonian flows via a density coupling strategy. It is equivalently posed as a regression problem using the Bregman divergence, which provides the loss function in learning while the data is generated through the particle formulation of Wasserstein Hamiltonian flow. We prove a posterior estimate on L1 residual of the proposed scheme based on the coupling density. Furthermore, the proposed scheme can be used to describe the behaviors of Hamilton-Jacobi PDEs beyond the singularity formations on the support of coupling density. Several numerical examples with different Hamiltonians are provided to support our findings.

Liu Liu,
The Chinese University of Hong Kong
lliu@math.cuhk.edu.hk

A Multi-Fidelity Method in Velocity Discretization for the Boltzmann
Equation

In this work, we develop a new multi-fidelity method for the Boltzmann equation which can reduce significantly the computational cost in velocity discretization. Different from previous work on multi-fidelity method that was designed to solve corresponding uncertainty quantification problems, we are interested to study the deterministic problems, including both linear transport and non-linear Boltzmann-type equations under different scales. The asymptotic-preserving property of proposed numerical scheme will be provided, in addition to analyzing the local consistency errors. Several numerical examples for linear transport and nonlinear Boltzmann models will be shown, in order to validate the efficiency and accuracy of our new method. This is a joint work with Nicolas Crouseilles and Zhen Hao.

Roy He,
City University of Hong Kong
royhe2@cityu.edu.hk

Identifying Differential Equations from Single Noisy Trajectories with Sparsity Control

Identifying differential equations (ODEs or PDEs) from single noisy trajectory data is a rising research field with important applications in various fields. It can automatically find the differential equations satisfied by the observational data, and the identified models can be used to validate theory or to discover new dynamics. Different frameworks have been proposed in the literature. In this talk, we will first review recent theoretical results, and then focus on a stream of works based on optimizations with l0-sparsity restriction.

Chao Wang,
Southern University of Science and Technology
wangc6@sustech.edu.cn

Variational Bayesian Network for Depth Estimation and Image Restoration from a Defocused Image

Depth estimation and image restoration from a single defocused image are two fundamental yet interdependent problems in computer vision. Existing works often address these tasks separately, overlooking their intrinsic connections through optical physics principles and lacking rigorous mathematical foundations. To bridge this gap, we introduce a new framework that combines both tasks using a physics-informed optimization process. Our supervised method models the defocused image as a function of the depth map and an all-in-focus (AiF) image based on optical principles. The depth map helps guide the AiF image recovery, while the AiF image helps regularize the depth map through the reconstruction error. To solve our model, we develop a variational inference algorithm where all expected posterior distributions are parameterized as deep neural networks to improve flexibility. Experiments demonstrate the superior performance of our method in both depth

estimation and image restoration, highlighting the benefits of integrating physical principles with data-driven learning.

Tao Luo,
Shanghai Jiao Tong University
luotao41@sjtu.edu.cn

Quantifying Training Difficulty and Accelerating Convergence in Neural Network-Based PDE Solvers

In this talk, we first introduce the concept of implicit bias in deep learning. We then discuss the implicit biases present in common neural network-based PDE solvers, offering new insights into the optimization and generalization of these algorithms. Finally, we present data-driven approaches for solving multi-scale PDE problems, and discuss the associated implicit biases, optimization, and generalization issues.

Haixia Liu,
Huazhong University of Science and Technology
liuhaixia@hust.edu.cn

A Novel First-Order Preconditioned Algorithm for Total Variation Minimization

Total variation minimization is a variational problem famous for preserving the edges, and has been proved as one of the most successful models in many applications, such as image processing and network sciences. Due to its importance in many applications, numerous efficient algorithms (i.e., primal-dual algorithm by Chambolle and Pock (J. Math. Imaging Vis., 2011), split Bregman method by Goldstein and Osher (SIAM J. Imaging Sci., 2009)) have been proposed to address this challenging problem. However, surrounding this topic, there is still some space for improvement on two aspects: non-differentiability of total variation and low convergence performance. To improve the performance of the current algorithms on these two aspects, we propose a novel approach, called a preconditioned solver, by proposing a

gradient low approach with a special Sobolev inner product. Based on the proposed method, the convergence results are given, which show that the convergence condition in the proposed method is much more flexible than the condition in primal-dual algorithm proposed by Chambolle and Pock (J. Math. Imaging Vis., 2011). Numerical experiments are performed to validate the theoretical results, and show that the proposed algorithm needs less iterations to get good performance, compared with split Bregman and primal dual methods in image denoising, image reconstruction and image segmentation.

Cheng Tang,
Hong Kong Baptist University
22481184@life.hkbu.edu.hk

WG-IDENT: Weak Group Identification of PDEs with Varying Coefficients

Identifying partial differential equations (PDEs) from noisy spatiotemporal data is challenging, particularly when coefficients vary spatially. We present WG-IDENT, a weak-formulation, group-sparsity framework that employs B-spline representations and spectral analysis to mitigate noise effects and handle spatial variability. Test functions and unknown coefficients are expressed with optimally selected B-spline bases derived from the spectral analysis of the noisy data. To facilitate feature selection, we propose to integrate group sparse regression with a newly designed group feature trimming technique, called GF-trim, to eliminate unimportant features. Extensive and comparative ablation studies are conducted to validate our proposed method. The proposed method not only demonstrates greater robustness to high noise levels compared to state-of-the-art algorithms but also achieves superior performance while exhibiting reduced sensitivity to hyperparameter selection.

MS17 Scientific computing and machine learning

Organizers: Ruchi Guo (Sichuan University, ruchiguo@scu.edu.cn)
Fei Wang (Xi'an Jiaotong University, feiwang.xjtu@xjtu.edu.cn)

Yiqi Gu,
University of Electronic Science and Technology
yiqigu@uestc.edu.cn

Layer separation models with weighted auxiliary variables in deep learning

Abstract: We develop a new optimization framework for the least squares learning problem via fully connected neural networks or physics-informed neural networks. The gradient descent behaves inefficiently in deep learning because of the high non-convexity of loss functions and the vanishing gradient issue. Our work proposes layer separation models with self-adaptive weighted auxiliary variables. Specifically, we introduce auxiliary variables to separate the layers of the deep neural networks and construct self-adaptive weighted loss functions. We prove the consistency between the proposed weighted loss and the original mean squared loss. Numerical experiments are presented to verify the above theory and show the effectiveness and robustness of our models over gradient descent.

Zhengyu Huang,
Peking University
huangdz@bicmr.pku.edu.cn

Point Cloud Neural Operator for Parametric PDEs on Complex and Variable Geometries

Abstract: Surrogate models are critical for accelerating computationally expensive simulations in science and engineering, particularly for solving parametric partial differential equations (PDEs). Developing practical surrogate models poses significant challenges, particularly in handling geometrically complex and variable domains, which are often discretized as point clouds. In this work, we systematically investigate the formulation of neural operators—maps between infinite-dimensional function spaces—on

point clouds to better handle complex and variable geometries while mitigating discretization effects. We introduce the Point Cloud Neural Operator (PCNO), designed to efficiently approximate solution maps of parametric PDEs on such domains. We evaluate the performance of PCNO on a range of pedagogical PDE problems, focusing on aspects such as boundary layers, adaptively meshed point clouds, and variable domains with topological variations. Its practicality is further demonstrated through three-dimensional applications, such as predicting pressure loads on various vehicle types and simulating the inflation process of intricate parachute structures.

Hao Liu,
Hong Kong Baptist University,
haoliu@hkbu.edu.hk

Operator Learning and Neural Scaling Laws

Abstract: Deep neural networks have demonstrated a great success in many applications. For operator learning and large language model, neural scaling laws are observed in many works. Most of the observed laws are power laws, i.e., the testing error can be written as a power of number of parameters or the number of training samples. However, theoretical explanations of the scaling laws are largely missing. In this presentation, we focus on operator learning and analyze the approximation and generalization error of some popular network architectures. We provide a theoretical explanation of neural scaling laws, and show that if the data has low-dimensional structures, one can achieve power laws.

Junchi Yan,
Shanghai Jiao Tong University,
yanjunchi@sjtu.edu.cn

Generative models for combinatoial problems

Abstract: Recent studies have highlighted a key performance bottleneck in modeling Combinatorial Optimization (CO) as neural solution prediction

tasks. Neural networks, in attempting to minimize the average objective score across a distribution of historical problem instances, often deviate from the primary goal of CO, which is to find optimal solutions for each individual test instance. This calls for an effective search process for each problem instance, with the model providing supporting knowledge to guide the search. To address this, we propose a generative modeling approach that learns the distribution of high-quality solutions for each instance, aiming to capture the fundamental nature of the problem rather than just predicting a single solution point. We introduce the T2T (Training to Testing) framework, based on diffusion models, which first leverages generative modeling during training to estimate the high-quality solution distribution for each instance. During testing, a neural search process exploits the learned solution space through noise-addition and denoising iterations. Additionally, we propose an Optimization Consistency Model that accelerates solution finding by learning a consistency mapping to enable single-step or few-step generation, significantly improving solving speed. We also investigate the inference-time scaling dynamics of diffusion models for optimization problems and demonstrate that our proposed neural search process achieves superior performance, scaling better per computation than extending denoising steps. Building upon this, we design DiffSearch, a method that reallocates computational resources to higher-level iterative refinement cycles, rather than relying on over-parameterized single-round generation. Our method serves as a foundational framework adaptable to various combinatorial optimization problems, and experimental results on problems like TSP and MIS show significant performance improvements over existing learning-based approaches.

Linlin Zhong,
Southeast University,
linlin@seu.edu.cn

Operator learning-based low-temperature plasma simulation

Low-temperature plasma (LTP) systems are characterized by strong non-equilibrium, multi-scale, and multi-physics interactions, posing significant challenges for conventional numerical simulation methods in terms of computational efficiency and generalizability. In recent years, operator learning—a class of machine learning techniques designed to approximate infinite-dimensional mappings between function spaces—has emerged as a promising

128

approach for accelerating and generalizing scientific computing tasks. In this talk, I will demonstrate the application of operator learning to key components of low-temperature plasma modeling, including plasma fluid simulation, plasma kinetic simulation, plasma properties calculation, and electron-impact cross sections prediction. In the plasma fluid simulation, I will show an operator learning-based surrogate model for predicting transient multiphysics distribution of thermal plasmas generating during the opening process of circuit breakers. In the plasma kinetic simulation, I will show how to integrate proper orthogonal decomposition (POD) with deep operator network, i.e., PaRO-DeepONet, for accelerating Poisson solution in particle-in-cell simulations. In the plasma properties calculation, I will present an operator learning-based framework of Mixture of Expert (MoE), i.e., DeepPropNet, for predicting multi plasma properties, including thermodynamic properties, transport coefficients, and radiation coefficient. Lastly, I will show an operator learning-based method for predicting electron-impact doubly differential ionization cross sections, i.e., DeepCSNet. This talk will highlight the potential of operator learning as a foundational tool for the next generation of data-driven and physics-informed plasma simulation frameworks.

Bin Gao,
Chinese Academy of Science,
gaobin@lsec.cc.ac.cn

Low-rank optimization on matrix and tensor varieties

Imposing additional constraints on low-rank optimization has garnered growing interest recently. However, the geometry of coupled constraints restricts the well-developed low-rank structure and makes the problem non-smooth. In this paper, we propose a space-decoupling framework for optimization problems on bounded-rank matrices with orthogonally invariant constraints. The "space-decoupling" is reflected in several ways. Firstly, we show that the tangent cone of coupled constraints is the intersection of the tangent cones of each constraint. Secondly, we decouple the intertwined bounded-rank and orthogonally invariant constraints into two spaces, resulting in optimization on a smooth manifold. Thirdly, we claim that implementing Riemannian algorithms is painless as long as the geometry of additional

constraint is known a prior. In the end, we unveil the equivalence between the original problem and the reformulated problem. The numerical experiments validate the effectiveness and efficiency of the proposed framework.

Tao Xiong,
University of Science and Technology of China,
taoxiong@ustc.edu.cn

A DeepONet-based solver for multiscale kinetic equations

Abstract: Traditional numerical methods for kinetic equations often rely on numerical discretization of high-dimensional microscopic equations, leading to prohibitively computational costs that struggle to meet the demands of long-term efficient simulations. To address this challenge, we employ a macro-micro decomposition framework and propose a DeepONet-based solver incorporating operator learning for kinetic equations. This approach utilizes deep neural networks to directly learn the solution operator of microscopic equations, thereby avoiding cumbersome computations involving high-dimensional microscopic quantities. Meanwhile, the low-dimensional macroscopic variables are still updated using conventional conservative schemes, ensuring both high resolution of macroscopic quantities and accurate shock wave capture. Numerical experiments demonstrate that our method achieves promising performance with significantly reduced computational costs, offering a novel approach for solving high-dimensional kinetic equations.

Zhiwen Zhang,
The University of Hong Kong,
zhangzw@hku.hk

Neural Network Poisson–Boltzmann Electrostatics for Biomolecular Interactions

Abstract: We have developed a neural network approach to solving the dielectric-boundary Poisson–Boltzmann (PB) equation (PBE) and estimating the electrostatic free energy of charged molecules in an aqueous solvent.

This equation is the Euler–Lagrange equation of the classical PB electrostatic free-energy functional in the presence of a dielectric boundary. We construct a penalized dielectric-boundary PB functional to eliminate the constraint imposed by the boundary condition at the boundary of the computational region and demonstrate that such penalized functionals converge to the classical PB functional. We represent electrostatic potentials using fully connected feed-forward neural network functions with sigmoidal activation, employ the penalized functional and Monte Carlo integration method to construct a neural network loss function, and minimize it using a stochastic gradient-descent (SGD) method. Numerical results are presented to illustrate the convergence of the neural network simulations with varying learning rates, batch sizes, and network architectures. Moreover, the neural network PB method is applied to the calculation of the electrostatic free energy of solvation for single ions and the protein BphC, demonstrating that the new approach can handle both simple and complex geometries and predict the electrostatic energy qualitatively well.

Yuwen Li,
Zhejiang University,
liyuwen@zju.edu.cn,

Higher Order Approximation Rates for ReLU CNNs in Korobov Spaces

In this talk, we present some results about the Lp approximation error for higher order Korobov functions using deep CNNs with ReLU activation. For target functions having a mixed derivative of order m+1 in each direction, we improve classical approximation rate of 2nd order to (m+1)-th order in terms of the depth of CNNs. The key ingredients in our analysis include the Lp approximation error of sparse grid functions and representation of ReLU functions by high-order sparse grid basis.

Juncai He,
Tsinghua University
juncai.he@kaust.edu.sa

Multigrid-Structured Neural Operators: Theories, Algorithms, and
Applications

Abstract: In this talk, we will present recent results on applying multigrid structures to both neural networks and operators for problems in images and numerical PDEs. First, we will discuss some basic background on operator learning, including the problem setup, a uniform framework, and a general universal approximation result. Motivated by the general definition of neural operators, we propose MgNO, which utilizes multigrid structures to parameterize these linear operators between neurons, offering a new and concise architecture in operator learning. For the implementation issue of MgNO, we will illustrate MgNet as a unified framework for convolutional neural networks and multigrid methods. This approach provides both mathematical rigor and practical expressivity, with many interesting numerical properties and observations.

Huayi Wei,
School of Mathematics and Computational Science, Xiangtan
University
weihuayi@xtu.edu.cn

SOPTX: A High-Performance Multi-Backend Framework for Topology
Optimization

Abstract: Topology optimization is a powerful structural design tool widely applied in fields such as aerospace, automotive, and civil engineering. However, traditional methods are constrained in their widespread adoption and flexibility due to their tight integration with computational mechanics, as well as the significant demands they place on expertise and development effort. SOPTX is a high-performance topology optimization framework built on FEALPy. It achieves decoupling of analysis and optimization through a modular architecture, supports multiple computational backends (including NumPy, PyTorch, and JAX), and employs a non-intrusive design paradigm,

enabling efficient execution on both CPU and GPU platforms. Its core innovations include:

- A modular framework: Enhancing flexibility and ease of development;

- Cross-platform multi-backend support: Allowing seamless integration with various computational libraries;

- Efficient sensitivity analysis using automatic differentiation technology: Streamlining the optimization process;

- Fast matrix assembly techniques: Overcoming performance bottlenecks in finite element computations.

Through numerical experiments, SOPTX has demonstrated outstanding performance in terms of computational speed and memory efficiency, highlighting its immense potential for topology optimization research and engineering applications. Furthermore, SOPTX offers strong extensibility, with planned future support for additional topology optimization approaches (such as level set methods) and multi-physics problems. In particular, SOPTX provides a robust foundation for integrating AI algorithms and neural networks, enabling innovative applications such as data-driven topology optimization and intelligent search strategies. By leveraging machine learning models, SOPTX can accelerate the design process, while neural networks can be employed to predict optimal material distributions or enhance optimization algorithms. This integration of AI and neural networks will further elevate SOPTX's capabilities, making it a versatile tool for tackling complex engineering design challenges.

MS18 Fast Solvers for Numerical PDEs

Organizers: Shi Shu, Junxian Wang, Liuqiang Zhong

Speaker 1: Xingding Chen
School of Mathematics and Statistics, Beijing Technology and Business University
chenxd@th.btbu.edu.cn

Title: A preconditioning method with the Generalized-α time discretization for dynamic crack propagations based on XFEM

Abstract: In this talk, we consider the efficient simulations of dynamic crack propagations based on the Extended Finite Element Method (XFEM). For the time discretization, the Generalized-α method is adopted to instead of the commonly used Newmark method in engineering, and the non physical numerical oscillations can be reduced obviously in the Generalized-α method by choosing appropriate parameters. Moreover, in order to accelerate the convergence rate of the linear system arising from XFEM, a special crack-tip domain decomposition preconditioning method is developed, in which the computational domain is decomposed into regular subdomains and crack tip subdomains. To construct the Schwarz preconditioners, the subproblems are solved exactly in the crack tip subdomains and inexactly in the regular subdomains by an incomplete LU factorization. When cracks propagate, only the subdomains around the crack tips are updated, and all the other regular subdomains remain unchanged, which can save the computational cost significantly. The numerical experiments verify that the proposed preconditioning algorithm works well for the simulations of dynamic crack propagations.

Speaker 2: Chen Cui,
School of Mathematics and Computational Science, Xiangtan University
cuichensx@gmail.com

Title: A hybrid iterative neural solver based on spectral analysis for parametric PDEs

Recently, deep learning-based hybrid iterative methods (DL-HIM) have emerged as a promising approach for designing fast neural solvers for large-scale sparse linear systems. DL-HIM combine the smoothing effect of simple iterative methods with the spectral bias of neural networks, enabling them to effectively eliminate both high-frequency and low-frequency error components. However, their efficiency may degrade when simple iterative methods fail to provide effective smoothing, making it challenging for the neural network to capture all algebraically smooth error components. In this talk, we introduce a Fourier transform-based DL-HIM called the Fourier Neural Solver (FNS). FNS leverages spectral decomposition to guide the neural network in learning the error components that simple iterative methods struggle to eliminate in a comlementary manner. By learning in the frequency domain and adopting an end-to-end training strategy, FNS mitigates the spectral bias in neural operators. We demonstrate that FNS can be trained to achieve convergence rates that are independent of grid resolution and physical parameters across several classes of linear parametric PDEs. Finally, we extend FNS to general linear systems arising from unstructured grids by incorporating graph neural networks.

Speaker 3: Ruchi Guo,
School of Mathematics, Sichuan University
ruchiguo@scu.edu.cn

Title: Optimization and preconditioning: TPDv algorithms for nonlinear PDEs

Abstract: In physics and mathematics, a large class of PDE systems can be formulated as minimizing energy functionals subject to certain constraints. Lagrange multipliers are widely used for solving these problems, which however leads to minmax optimization problems, i.e., saddle point systems. The development of fast solvers for saddle point systems, especially the nonlinear ones, is particularly difficult in the sense that (i) one has to consider the preconditioning in two directions and (ii) the preconditioners have to evolve in iteration due to the nonlinearity. In this work, we introduce an efficient transformed primal-dual (TPD) algorithm to solve the aforementioned nonlinear saddle point problems. In this work, we introduce an efficient transformed

primal-dual (TPD) algorithm to solve the aforementioned nonlinear saddle point problems.

Speaker 4: Shihua Gong,
School of Science and Engineering, The Chinese University of
Hong Kong, Shenzhen
gongshihua@cuhk.edu.cn

Title: Power contractivity for RAS-Imp and RAS-PML for the
time-harmonic wave equations

Abstract: We consider two variants of restricted overlapping Schwarz methods for the time-harmonic wave equation. The first method, known as RAS-Imp, incorporates impedance boundary condition to formulate the local problems. The second method, RAS-PML, employs local perfectly matched layers (PML). These methods combine the local solutions additively with a partition of unity. We have shown that RAS-Imp has power contractivity for strip domain decompositions. More recently, we shown that RAS-PML has super-algebraic convergence with respective to wavenumber after a specified number of iterations. In this talk we review these results and then investigate their sharpness using numerical experiments. We also present some theoretical and numerical results of RAS-Imp for the time-harmonic Maxwell equation.

Speaker 5: Fei Wang,
School of Mathematics and Statistics, Xi'an Jiaotong University
feiwang.xjtu@xjtu.edu.cn

Overlapping Schwarz Preconditioners for Randomized Neural Networks with
Domain Decomposition

Randomized neural networks (RaNNs), characterized by fixed hidden layers after random initialization, offer a computationally efficient alternative to fully parameterized neural networks trained using stochastic gradient descent-type algorithms. In this talk, we integrate RaNNs with overlapping

Schwarz domain decomposition in two primary ways: firstly, to formulate the least-squares problem with localized basis functions, and secondly, to construct effective overlapping Schwarz preconditioners for solving the resulting linear systems. Specifically, neural networks are randomly initialized in each subdomain following a uniform distribution, and these localized solutions are combined through a partition of unity, providing a global approximation to the solution of the partial differential equation. Boundary conditions are imposed via a constraining operator, eliminating the necessity for penalty methods. Furthermore, we apply principal component analysis (PCA) within each subdomain to reduce the number of basis functions, thereby significantly improving the conditioning of the resulting linear system. By constructing additive Schwarz (AS) and restricted AS preconditioners, we efficiently solve the least-squares problems using iterative solvers such as the Conjugate Gradient (CG) and generalized minimal residual methods. Numerical experiments clearly demonstrate that the proposed methodology substantially reduces computational time, particularly for multi-scale and time-dependent PDE problems. Additionally, we present a three-dimensional numerical example illustrating the superior efficiency of employing the CG method combined with an AS preconditioner over direct methods like QR decomposition for solving the associated least-squares system.

Speaker 6: Ying Yang,
chool of Mathematics and Computational Science, Guilin
University of Electronic Technology
yangying@lsec.cc.ac.cn

Title: Machine Learning Accelerated Solution of PNP Equations with Applications to Ion Channels

Abstract: The Poisson-Nernst-Planck (PNP) equations are a set of nonlinear coupled partial differential equations, which are widely used to describe the transport of charged particles in biological ion channels, electrochemical systems and semiconductors, etc. The PNP equations in biological ion channels present challenges for numerical algorithms due to their highly irregular geometric interfaces, multiple singularities, and nonlinear coupling. Numerical methods, such as the finite element method, are often combined with the

Gummel iteration when solving the PNP equations. This iterative method is commonly used to decouple and linearize the PNP equations, but its efficiency is largely influenced by the relaxation parameter. The choice of the relaxation parameter is typically based on empirical selection, but this approach often fails to yield optimal values for practical problems, resulting in low efficiency. We apply two machine learning algorithms to predict the optimal parameters for the Gummel iteration, improving the efficiency of the iteration process. Specifically, we also apply these machine learning algorithms to solve practical PNP problems in various biological ion channels. Numerical experiments show that, compared to those selected by human experience, the parameters chosen by the machine learning algorithm are more stable and yield better results.

Speaker 7: Taishan Zeng,
chool of Mathematical Sciences, South China Normal University
zengtsh@m.scnu.edu.cn

Title: Sparse-regularized high-frequency enhanced neural network for solving high-frequency problems

Abstract: High-frequency problems frequently arise in various scientific and engineering applications. In this paper, we propose a high-frequency enhanced neural network (HFNN) to solve high-frequency partial differential equations. The basic idea of HFNN is to decompose the numerical solution into high-frequency and low-frequency components, and employ specific neural networks to handle these components separately by embedding high-frequency functions into the network. To further enhance the performance of the HFNN, we introduce a sparse-regularized high-frequency enhanced neural network (SR-HFNN) algorithm. The SR-HFNN algorithm employs a two-stage training strategy, where the first stage mainly learns to remove irrelevant frequency information through sparse regularization. By leveraging the power of deep neural networks and sparse learning, our proposed SR-HFNN algorithm demonstrates superior performance in solving high-frequency partial differential equations and inverse problems. The numerical results validate the fast convergence and high approximation accuracy of the SR-HFNN algorithm for high-frequency partial differential equations.

Speaker 8: Qingsong Zou,
School of Computer Science and Engineering, Sun Yat-sen
University
mcszqs@mail.sysu.edu.cn

Title: CFDONEval : A comprehensive evaluation of operator-learning
neural network models for computational fluid dynamics

Abstract: In this talk, we introduce CFDONEval, a comprehensive evaluation of 12 operator-learning-based neural network (ON) models to simulate 7 benchmark fluid dynamics problems. These problems cover a range of 2D scenarios, including Darcy flow, two-phase flow, Taylor-Green vortex, lid-driven cavity flow, tube flow, circular cylinder flow, and 3D periodic hill flow. For a rigorous evaluation, we establish 22 fluid dynamics datasets for these benchmark problems, 18 of which are newly generated using traditional numerical methods, such as the finite element method. Our evaluation tackles 5 key challenges: multiscale phenomena, convection dominance, long-term predictions, multiphase flows, and unstructured meshes over complex geometries. We assess computational accuracy, efficiency, and flow field visualization, offering valuable insights into the application of ON models in fluid dynamics research. Our findings show that attention-based models perform well in handling almost all challenges; models with a U-shaped structure excel in handling multiscale problems; and the NU-FNO model demonstrates the smallest relative error in L_2 norm when processing nonuniform grid data. The associated code and datasets will be released publicly.

MS19 Recent Advances in Analysis and Computation of Nonlocal and Fractional Models

Organizers: Zhi Zhou, Xiaobo Yin, Zhaopeng Hao, Kuang Huang

Zuoqiang Shi,
Tsinghua University
zqshi@tsinghua.edu.cn

Error Bound of Finite Element Method for Nonlocal Poisson Model with An Efficient Implementation

This talk presents an asymptotically compatible error estimate for the finite element method (FEM) applied to a nonlocal Poisson model. The analysis covers two scenarios: meshes with and without shape regularity. For shape-regular meshes, the error is bounded by $O(h^k + \delta)$, where h is the mesh size, δ is the nonlocal horizon, and k is the order of the FEM basis. Without shape regularity, the bound becomes $O(h^{k+1}/\delta + \delta)$. In addition, we present an efficient implementation of the finite element method of nonlocal model. For the nonlocal model with Gaussian kernel function, we can decouple the $2n$-dimensional integral to 2-dimensional integrals which reduce the computational cost tremendously. Numerical experiments verify the theoretical results and demonstrate the outstanding performance of the proposed numerical approach.

Xiaobo Yin,
Central China Normal University
yinxb@ccnu.edu.cn

Asymptotic error estimates for nonlocal problems with exact or approximated interaction neighborhoods

In this talk, we report our recent study on the asymptotic error analysis between the finite element solutions of nonlocal models with a bounded interaction neighborhood and the exact solution of the limiting local model. The limit corresponds to the case when the horizon parameter, the radius of the spherical nonlocal interaction neighborhood of the nonlocal model, and the

mesh size simultaneously approach zero. Two important cases are discussed: one involving the original nonlocal models and the other for nonlocal models with polygonal approximations of the nonlocal interaction neighborhood.

Shuonan Wu,
Peking University
snwu@math.pku.edu.cn

Local discontinuous Galerkin methods for the integral fractional Laplacian

We present the local discontinuous Galerkin (LDG) and minimal dissipation LDG (md-LDG) schemes for solving the integral fractional Laplacian equation. Using the Riesz potential, we reformulate the problem in a 3-field mixed form. By the error equation, we establish a priori error estimates for the LDG scheme on polygonal meshes. For triangular meshes, we prove a priori error estimates for both LDG and md-LDG schemes by utilizing continuous interpolation and special projection. Combining with the regularity theory of the problem, we demonstrate the convergence rates of these schemes on both quasi-uniform and graded meshes. Numerical experiments are provided to validate the effectiveness of our theoretical results.

Zhiping Mao,
Eastern Institute of Technology
zmao@eitech.edu.cn

A novel class of arbitrary high-order numerical schemes for fractional differential equations

It is well-known that designing efficient, high-order, and stable numerical schemes for time non-local or fractional differential equations faces three key challenges: non-locality, low solution regularity, and long-term simulation. Achieving this while minimizing storage costs is particularly difficult, especially when attempting to address all three issues simultaneously. In this

work, we propose a novel class of numerical schemes designed to simultaneously address the three key challenges associated with time fractional differential equations (TFDEs). To achieve this, we derive an equivalent integer-order extended parametric differential equation (EPDE) by dimensional expanding for the TFDE and establish its corresponding stability. Remarkably, for the resulting EPDE, we provide a rigorous analysis demonstrating that it exhibits high regularity with respect to the extended parameter dimension. This finding motivates us to apply a spectral method for discretizing the extended parametric space, enabling high accuracy. Consequently, we employ the Jacobi spectral collocation method combined with characteristic decomposition, resulting in M independent integer-order ordinary differential equations (ODEs), where M represents the number of nodes used for the spectral collocation method. Therefore, it is straightforward to apply any traditional numerical scheme for the resulting M independent integer ODEs. In the present work, we utilize the BDF-k ($k = 1, \ldots, 5$) formulas for the time discretization and conduct a rigorous stability analysis. Additionally, we provide an error estimate for the fully discretization scheme, demonstrating that the convergence order is $O(\Delta t^k + M^{-m})$, where Δt represents the time step size. Since M is fixed, we conclude that the computational cost and storage requirements of our proposed algorithm are essentially the same as those for ODEs, with a computational cost of $O(N)$ and a storage requirement of $O(1)$, where N is the total number of time step.

Yiqun Li,
Wuhan University
yiqunli@whu.edu.cn

The multiscale nonlocal-in-time Schrödinger bridge problem

We formulate the multiscale nonlocal-in-time Schrödinger bridge problem (SBP) constrained by a time-fractional Wasserstein gradient flow with the advective flux. A strongly coupled nonlinear system of a time-fractional equation and a time-fractional Hamilton-Jacobi equation is derived based on the first-order optimality condition. After changing of variables, we reformulate the nonlocal SBP as a related minimization problem constrained by a time-fractional transport equation. The corresponding cost function introduces an additional intricate term involving the time-fractional derivative

compared with its classical analogue, and this reformulation again yields a coupled nonlinear system equivalent to the original system. The widely used general-proximal primal-dual hybrid gradient (G-prox PDHG) algorithm is extended to solve the nonlocal SBP, and we apply a preconditioner induced by the discretization scheme of the time-fractional model to accelerate the convergence of the algorithm. Numerical experiments between Gaussian distributions are performed to investigate the performance of the nonlocal SBP, which demonstrate the reliability, efficiency, and effectiveness of our proposed algorithm and the multiscale feature of the nonlocal SBP.

Xuehong Cui,
Southeast University
230238475@seu.edu.cn

A Finite difference method for the relativistic Schrodinger operator:
algorithm, analysis and applications

In this work, we propose an efficient second-order accurate finite difference method for discretizing the multi-dimensional relativistic Schrodinger operator, based on an equivalent definition via Fourier transform. Using the approximation, we construct a simple and easy-to-implement finite difference scheme for solving elliptic equations involving the operator and provide a fast algorithm with quasi-linear complexity. We further prove the stability of the scheme and derive optimal error bounds for the solutions in the discrete Sobolev norm. We conduct several numerical simulations, including fractional Gaussian fields, Schrodinger equations, and nonlocal Allen-Cahn equations, to validate the accuracy and robustness of the scheme.

Changpin Li,
Shanghai University
lcp@shu.edu.cn

Analysis and computation for quenching solution to the time-space
fractional Kawarada problem

This report focuses on the existence, uniqueness, and quenching behavior of solution to the time-space fractional Kawarada problem, where the time

derivative is the Caputo-Hadamard derivative and the spatial derivative is the fractional Laplacian. Then the finite difference scheme is established for solving the quenching solution to the considered problem in one and two space dimensions. The numerical simulations show the effectiveness and feasibility of the theoretical analysis.

Changtao Sheng,
Shanghai University of Finance and Economics
ctsheng@mail.sufe.edu.cn

Efficient sparse Monte Carlo method for high dimensional semi-linear PDEs with jumps

In this talk, we present a sparse grid-based Monte Carlo method for solving high-dimensional semi-linear nonlocal diffusion equations with volume constraints. To overcome the curse of dimensionality and the dense systems introduced by nonlocal operators, we develop an implicit-explicit temporal discretization scheme based on a nonlinear Feynman-Kac representation. The use of sparse grid interpolation improves scalability and enables applications in high dimensions. We also design a tailored sampling strategy to handle hypersingular kernels accurately within the probabilistic framework. The proposed method inherits unconditional stability from the underlying stochastic representation and avoids restriction on temporal and spatial step sizes. A rigorous convergence analysis is provided, and numerical experiments with non-radial solutions in up to 100 dimensions confirm the method's accuracy and robustness.

Yufeng Nie,
Northwestern Polytechnical University
yfnie@nwpu.edu.cn

Stability and Error Analysis of Reduced-Order Methods Based on POD with Finite Element Solutions for Nonlocal Diffusion Problems

In this talk, we will introduce the formulation and theoretical analysis of the reduced-order numerical method constructed by proper orthogonal decomposition (POD) for nonlocal diffusion problems with a finite range of interactions. Due to the nonlocality, the corresponding discrete systems of nonlocal models have less sparsity than those for PDEs. Given the challenges of frequently handling large systems of linear equations with much lower sparsity, we establish a reduced-order model (ROM) for nonlocal diffusion problems to expedite the iterative solution process. The ROM is constructed using FE solutions in a very small time interval as snapshot data and has much fewer degrees of freedom than FEMs. In this contribution, we focus on discussing mathematical justifications for the existence, stability, and error estimates of the ROM method, which have not been considered in previous research for nonlocal models. Another important component of our work is that we systematically explore the effect of different parameters on the behavior of the POD algorithms. Numerical examples will be finally presented to validate the theoretical conclusions and to illustrate the efficiency of the proposed method.

Xiangcheng Zheng,
Shandong University
xzheng@sdu.edu.cn

Two methods addressing variable-exponent fractional initial and boundary value problems and Abel integral equation

Variable-exponent fractional models attract increasing attentions in various applications, while rigorous analysis is far from well developed. We provide general tools to address these models. Specifically, we first develop a convolution method to study the well-posedness, regularity, an inverse problem and numerical approximation for the sundiffusion of variable exponent. For models such as the variable-exponent two sided space-fractional boundary value problem (including the variable-exponent fractional Laplacian equation as a special case) and the distributed variable-exponent model, for which the convolution method does not apply, we develop a perturbation method to prove their well-posedness. The relation between the convolution method and the perturbation method is discussed, and we further apply the latter to prove the well-posedness of the variable-exponent Abel integral equation.

Daxin Nie,
Lanzhou University
ndx1993@163.com

Analysis and numerical approximation for space-dependent variable-order
fractional diffusion equation in the flowing media

We investigate a fully discrete scheme for a space-dependent variable-order fractional diffusion equation in the flowing media, which can be derived by introducing a velocity field to continuous time random walk model with waiting time obeying a spatially dependent power-law distribution. We provide regularity estimates for the solution under some regularity assumptions on the variable-order $\alpha(\mathbf{x})$ and the velocity field $\mathbf{v}$. A temporal semi-discrete scheme generated by the backward Euler convolution quadrature method is proposed, and an $O(\tau)$ convergence rate is obtained by some skillful error analyses. Then the fully discrete scheme is built by using finite element method to approximate the spatial operator, and an optimal spatial error estimate is obtained by introducing some discrete operators, i.e., the convergence order can well match the order of optimal spatial regularity of the solution. Finally, various numerical examples are presented to validate our theoretical results.

Maria Lopez-Fernandez,
University of Malaga
maria.lopezf@uma.es

Convolution Quadrature for the quasilinear subdiffusion equation

We construct a Convolution Quadrature (CQ) scheme for the quasilinear subdiffusion equation of order α and supply it with the fast and oblivious implementation. In particular, we find a condition for the CQ to be admissible and discretize the spatial part of the equation with the Finite Element Method. We prove stability and convergence of the scheme and find a bound on the error. Our estimates are globally optimal for all α and pointwise for $\alpha \geq 1/2$, in the sense that they reduce to the well-known results for the linear equation. For the semilinear case, our estimates are optimal both globally and locally. As a passing result, we also obtain a discrete Grönwall inequality

146

for the CQ, which is a crucial ingredient in our convergence proof based on the energy method. The paper is concluded with numerical examples verifying convergence and computational time reduction when using fast and oblivious quadrature.

Yuwen Li,
Zhejiang University
liyuwen@zju.edu.cn

A Rational Approximation Algorithm via the Empirical Interpolation Method

In this talk, I will present a rational approximation algorithm via the empirical interpolation method for interpolating a family of parametrized functions, leading to numerical algorithms for space-fractional differential equations, parameter-robust preconditioning, and evaluation of matrix functions. Compared to classical rational approximation algorithms, the proposed method is more efficient for approximating a large number of target functions. In addition, I will give a convergence estimate of the rational approximation algorithm using the metric entropy numbers.

Xiaochuan Tian,
University of California, San Diego
xctian@ucsd.edu

A Meshfree Framework for Nonlocal Models with Heterogeneous Localization

Motivated by recent advancements in nonlocal mechanical models like peridynamics, this work investigates nonlocal integral models with spatially varying horizons that vanish at domain boundaries. This work focuses on the strong form of such nonlocal models within a meshfree framework. Such nonlocal models with heterogeneous localization are also useful for local-nonlocal coupling. Depending on the ratio between the horizon and the discretization parameter, we employ different meshfree schemes. For larger ratios, where the model exhibits pronounced nonlocality, the midpoint rule is employed.

Conversely, for smaller ratios, as the model becomes more localized, the moving least squares method ensures accurate approximation. Numerical experiments are conducted to evaluate the behavior of these models under various conditions, including Dirichlet-type constraints and eigenfunction problems.

Nicola De Nitti,
Università di Pisa
nicola.denitti@unipi.it

Nonlocal regularizations for hyperbolic systems of conservation laws

We survey some recent developments in the study of the nonlocal-to-local singular limit problem for some classes of hyperbolic systems of conservation laws.

Jieqiong Zhang,
Northwest University
zhangjieqiong@nwu.edu.cn

Extended random batch method for short range nonlocal interactions with EAM potential

In this work, we investigate and validate the feasibility of the application of the random batch list method on the metallic system with the embedded atomic method (EAM) potential energy. The random batch idea is employed on the two summation parts of interactions in the EAM potential energy, in which the interaction for the nearest and second nearest neighboring atoms are directly calculated as the core region while small but random batches of neighboring atoms in the shell region are adopted to reduce the number of interaction pairs. Numerical examples on the characteristics of physical quantities including the lattice constant, radial distribution function and elastic constants have been performed to validate the applicability and effectiveness of the extended RBL method on the EAM metallic systems. It has been proved that this extended RBL method can be flexibly applied to the EAM metallic system to further speed up and scale up the molecular simulations.

Minghua Chen,
Lanzhou University
chenmh@lzu.edu.cn

Grönwall vector inequality for diagonally dominant systems arising from a class of time-dependent nonlocal problems

This work establishes a convergence framework for strictly or irreducibly diagonally dominant systems, which may be nonsymmetric and indefinite, arising from a class of linear/semilinear nonlocal PDEs. For steady-state nonlocal problems, the local truncation error $\mathcal{O}\left(h^{\mu_1}\right)$ and the global error $\mathcal{O}\left(h^{\mu_2}\right)$ exhibit a complex relationship (e.g., $\mu_1 = \mu_2, \mu_1 > \mu_2, \mu_1 < \mu_2$). For time-dependent nonlocal problems, the numerical analysis becomes particularly challenging, especially when $\mu_1 < 0 < \mu_2$, as the local truncation error exhibits divergent behavior at boundary layers. To address this gap, we first construct *discrete Mittag-Leffler kernels* to precisely capture and resolve the numerical solution. Furthermore, we prove novel *Grönwall-type vector inequalities* that enable rigorous error analysis for nonlocal evolution problems. Our central theoretical result demonstrates that the spatial convergence rate of the global error $\mathcal{O}\left(h^{\max\{\mu_1,\mu_2\}}\right)$ for PDEs is exactly the maximum of the local truncation error and the global error in associated steady-state equations.

MS20 Optimal control and financial mathematics

Organizers: Shuoqing Deng (HKUST), Xiaolu Tan (CUHK)

Lijun Bo
Xidian University and USTC, China
lijunbo@xidian.edu.cn

Extended mean field control problems with constraints: The generalized
Fritz-John conditions and Lagrangian method

This talk is concerned with the extended mean field control problems under general dynamic expectation constraints and/or dynamic pathwise state-control and law constraints. We aim to pioneer the establishment of the stochastic maximum principle (SMP) and the derivation of the backward SDE (BSDE) from the perspective of the constrained optimization using the method of Lagrangian multipliers. To this end, we first propose to embed the constrained extended mean-field control (C-MFC) problems into some abstract optimization problems with constraints on Banach spaces, for which we develop the generalized Fritz-John (FJ) optimality conditions. We then prove the stochastic maximum principle (SMP) for C-MFC problems by transforming the FJ type conditions into an equivalent stochastic first-order condition associated with a general type of constrained forward-backward SDEs (FBSDEs). Contrary to the existing literature, we treat the controlled Mckean-Vlasov SDE as an infinite-dimensional equality constraint such that the BSDE induced by the FJ first-order optimality condition can be interpreted as the generalized Lagrange multiplier to cope with the SDE constraint. Finally, we also present the SMP for stochastic control problems and MFG problems under similar types of constraints as consequences of our main result for C-MFC problems.

Ibrahim Ekren
University of Michigan, US
iekren@umich.edu

Uniform-in-Time Weak Propagation of Chaos for Consensus-Based Optimization

We show that the uniform-in-time weak propagation of chaos methodology of Delarue-Tse can be used to study consensus-based optimization algorithms. The methodology leads to quantitative bounds for the joint convergence to the large particle and large time limit. Based on joint work with Erhan Bayraktar and Hongyi Zhou.

Gaoyue Guo
CentraleSupélec, France
gaoyue.guo@centralesupelec.fr

On pairwise comparaison and the soccer model

Aldous and Kolesnik introduced the soccer model. They used it to give a new proof of Moon's theorem on the so-called generalised tournament matrices that appear for instance in the ranking models of sport competitions. We revisit the soccer model based on the martingale transport, thereby responding to an invitation from Aldous. By adopting a special choice of the parameters, we obtain the classical property of strong stochastic transitivity and thus a numerical scheme to construct generalised tournament matrices.

Saïd Hamadène
Le Mans Université
said.hamadene@univ-lemans.fr

The optimal switching problem with signed switching costs

In this talk we discuss the optimal multiple modes switching problem in finite horizon when the costs associated with the changes of regimes do not have a constant sign. The problem is solved by means of probabilistic

tools. The main assumption is the monotonicity of the switching costs. In the Markov setting, the associated HJB system of PDEs is also considered. We show the existence and uniqueness of the solution in viscosity sense. Switching problems get involved in energy markets, financial markets, cyber-security field, etc. This is a joint work with B.ElAsri and M.Souheil (Agadir University).

Simone Scotti
University of Pisa, Italy
simone.scotti@unipi.it

Fly to quality and walk back

This paper is concerned by an investment and consumption control problem for a risk averse investor in a financial market with one stock afflicted by self-exciting jumps, which can be observed in real world, eg after a bad announcement of the firm. We consider the case of proportional transaction costs and power utility function. The related value function will be formulated as the solution of a three-dimensional system of variational integro-differential inequalities. We show that our problem is equivalent to a bi-dimensional singular control problem, helping to show the uniqueness of the solution in viscosity sense. We conclude our work with à numerical approximation of the value function performed in order to provide sensitivity analysis and understand the evolution of the optimal investment policy in the space. In particular, we observe that after a negative jumps the optimal policy can be to sell the risky asset even in absence of short-selling opportunity. Our model shows then an endogenous fly-to-quality behaviour whose effect fades by an exponential recovery in the long run.

Hanxiao Wang
Shenzhen University, China
ehxwang@szu.edu.cn

Optimal Controls for Forward-Backward Stochastic Differential Equations:
Time-Inconsistency and Time-Consistent Solutions

This talk is concerned with an optimal control problem for a forward-backward stochastic differential equation (FBSDE, for short) with a recursive cost functional determined by a backward stochastic Volterra integral equation (BSVIE, for short). It is found that such an optimal control problem is time-inconsistent in general, even if the cost functional is reduced to a classical Bolza type one as in Peng (AMO 1993), Lim-Zhou (SICON 2001), and Yong (SICON 2010). Therefore, instead of finding a global optimal control (which is time-inconsistent), we will look for a time-consistent and locally optimal equilibrium strategy, which can be constructed via the solution of an associated equilibrium Hamilton-Jacobi-Bellman (HJB, for short) equation. A verification theorem for the local optimality of the equilibrium strategy is proved by means of the generalized Feynman-Kac formula for BSVIEs and some stability estimates of the representation parabolic partial differential equations (PDEs, for short). Under certain conditions, it is proved that the equilibrium HJB equation, which is a nonlocal PDE, admits a unique classical solution. As special cases, a linear-quadratic problem is considered, in which the solvability of a non-local and non-symmetric matrix-valued Riccati equation is established. As applications, a social planner problem with heterogeneous Epstein-Zin utilities is briefly mentioned, by which we show that the Epstein-Zin utility is much more effective than the power utility in this model.

Jiaqiang Wen
SusTech, China
wenjq@sustech.edu.cn

Mean-field BSDEs with quadratic growth and applications

In this talk, I will present some of our recent results on general mean-field backward stochastic differential equations with quadratic growth. This includes results on existence, uniqueness, and comparison theorems, as well as applications of the stochastic maximum principle, the nonlinear Feynman-Kac formula, and the convergence and convergence rates of the related particle systems.

Lihu Xu
University of Macau, Macau SAR
lihuxu@um.edu.mo

Stable CLT in the total variation distance

Under certain general conditions, we prove that the stable central limit theorem holds in total variation distance and get its optimal convergence rate for all $\alpha \in (0, 2)$. Our method is by two measure decompositions, one-step estimates, and a very delicate induction with respect to α. One measure decomposition is light tailed, while the other one is heavy tailed and indispensable for lifting convergence rate for small α. The proof is elementary and composed of ingredients at the postgraduate level.

Student Chapters

Organizers: Xingguang Jin (CUHK)

Sesssion 1

Kota Takeda
Nagoya University

Error analysis of the ensemble Kalman filter for chaotic dynamical systems with covariance inflation techniques

In this talk, we focus on the sequential state estimation problems for a class of chaotic dynamical systems on Hilbert spaces, including the two-dimensional Navier–Stokes equations and the Lorenz 63 and 96 models. Data assimilation combines numerical models with observational data to estimate the system state, representing the estimate as a probability distribution. For nonlinear dynamical systems, the ensemble Kalman filter (EnKF) is commonly employed to approximate the mean and covariance of this distribution, thereby capturing the uncertainty in the state estimate. In practice, ad-hoc numerical techniques known as covariance inflation are applied to stabilize the EnKF, despite a lack of rigorous theoretical justification. We analyze the state estimation error when the EnKF is applied to such chaotic dynamical systems, with particular attention to the role of covariance inflation in ensuring the accuracy.

Yueqi Wang
The University of Hong Kong

Numerical homogenization for time-harmonic Maxwell equations in heterogeneous media with large wavenumber

We propose a new numerical homogenization method based upon the edge multiscale method for time-harmonic Maxwell equations in heterogeneous media with large wavenumber. Numerical methods for time-harmonic Maxwell equations in homogeneous media with large wavenumber is very challenging due to the so-called pollution effect: the mesh size should be

156

much smaller than the reciprocal of the wavenumber to obtain a solution with certain accuracy. It is much more challenging for the case with heterogeneous media that occurrs often in the practical applications, such as the simulation of metamaterial, since one has to resolve the heterogeneity for a reasonable numerical solution. We devise a novel approach that do not resolve the heterogeneity in the coefficient and has a mesh size linearly depends on the reciprocal of the wavenumber, which has a first order convergence rate. Extensive numerical tests are provided to verify our theoretical findings.

Zexian Li
The Hong Kong Polytechnic University

Optimal Quantum Gate Cost for Block-Encoding Classical Matrices

The optimal cost of encoding classical matrices into quantum gates can be characterized in two ways: minimal circuit depth and minimal circuit size. This presentation examines two key scenarios: 1. The conditions under which encoding a general matrix achieves minimal circuit size; 2. The conditions under which encoding a sparse matrix achieves minimal circuit depth.

Sesssion 2

Chenhao Lu
City University of Hong Kong

On the Eigenvalue Rigidity of the Jacobi Unitary Ensembles

This project aims to establish the eigenvalue rigidity of Jacobi unitary ensembles. We want to find an optimal bound for the fluctuations of eigenvalues away from their limiting values. Different from the Gaussian unitary ensemble, hard edges appear in the Jacobi case, hence the eigenvalues are expected to concentrate near the edges. The main idea of our proof is to combine the extreme value theory of log-correlated Gaussian field, especially the fractal properties of the Gaussian multiplicative chaos measure, together with asymptotic analysis of the Hankel determinants with Fisher-Hartwig

singularities, where Riemann-Hilbert approach is adopted. Some estimates of the exponential moments of an asymptotically Gaussian process are also obtained.

Xingguang Jin
The Chinese University of Hong Kong

Efficient numerical method for the Schrödinger equation with high-contrast potential

We developed constraint energy minimization generalized multiscale finite element method (CEM-GMsFEM) in the framework of Crank-Nicolson (CN) discretisation in time for Schrödinger equations with multiscale potential functions. The localized multiscale basis functions are constructed by addressing the spectral problem and a constrained energy minimization problem related to the Hamiltonian norm. A first-order convergence in the energy norm and second-order convergence in the L^2 norm for our numerical scheme are shown, with a relation between the oversampling number in the CEM-GMsFEM method, the spatial mesh size and the semiclassical parameter provided. Several numerical examples, including 1D and 2D in space, with high-contrast potential, are conducted to demonstrate the efficiency and accuracy of our proposed scheme.

Qingle Lin
The Hong Kong Polytechnic University

Optimizing Coarse Propagators in Parareal Algorithms

The parareal algorithm represents an important class of parallel-in-time algorithms for solving evolution equations and has been widely applied in practice. To achieve effective speedup, the choice of the coarse propagator in the algorithm is vital. In this work, we investigate the use of optimized coarse propagators. Building upon the error estimation framework, we present a systematic procedure for constructing coarse propagators that enjoy desirable stability and consistent order. Additionally, we provide preliminary

mathematical guarantees for the resulting parareal algorithm. Numerical experiments on a variety of settings, e.g., linear diffusion model, Allen-Cahn model, and viscous Burgers model, show that the optimizing procedure can significantly improve parallel efficiency when compared with the more ad hoc choice of some conventional and widely used coarse propagators.

Sesssion 3

Zhenyi Zhu
The Chinese University of Hong Kong

Deep Learning for Solving PDEs

We explore innovative deep learning methods to solve complex partial differential equations (PDEs), including the semiconductor Boltzmann equation, time-dependent PDEs, and the semiclassical Schrödinger equation's moment system. Our approaches—Asymptotic-Preserving Neural Networks (APNNs), PhysicsSolver, and a two-stage neural network—address multi-scale challenges, temporal extrapolation, and multi-phase closures. APNNs ensure scale uniformity, PhysicsSolver merges physical insights with predictive power, and the two-stage method learns moment relationships to close systems. Supported by convergence analysis and validated through numerical tests, these methods demonstrate high accuracy and efficiency, even with sparse data, advancing deep learning's role in PDE solutions.

Xiao MENG
Hong Kong Baptist University

Analysis of a Diffusive SIR Model on Metric Graph and Sub-domains

In this work, we analyze a diffusive SIR model formulated on a coupled structure consisting of metric graphs and subdomains. A weak formulation is developed to describe the dynamics within the subdomains, along the edges of the graph, and at the vertices where the two structures interact. The well-posedness of the system is established, including the existence and uniqueness. Furthermore, the adjoint system is derived, and the associated

optimality conditions are obtained, leading to a coupled system of state and adjoint equations. These results provide a mathematical framework for the analysis of diffusive SIR models on a hybrid structure, with potential applications to modeling and managing the spatial spread of epidemics.

Yixuan Zhang
The Hong Kong Polytechnic University

A Smoothing Implicit Gradient Algorithm for Optimization with Parametric Variational Inequality Constraints on a Moving Polyhedron

This work introduces a Smoothing Implicit Gradient Algorithm with Inexactness (SIGAI) to address optimization problems constrained by Parametric Variational Inequalities (PVI) defined on a moving polyhedron. Unlike prior works limited to fixed feasible sets, SIGAI handles moving constraints where the feasible region evolves with parameters. Key innovations of the proposed SIGAI framework include: (i) smoothing approximation of the projection operator with vanishing smoothing parameters; (ii) inexact sub-problem solutions requiring only finite iterations per sub-problem; and (iii) convergence guarantees to stationary points and convergence rate characterization. Numerical experiments validate the algorithm's convergence and efficiency, with applications to real-world portfolio management problems.

Tsz Ching Chow
The Chinese University of Hong Kong

Inertial Proximal Difference-of-Convex Algorithm with Convergent Bregman Plug-and-Play for Nonconvex Imaging

Imaging tasks are typically tackled using a structured optimization framework. We delve into a class of algorithms for difference-of-convex (DC) structured optimization, focusing on minimizing a DC function and possibly a nonconvex function. Existing DC algorithms (DCA) often fail to handle nonconvex functions or exhibit slow convergence rates effectively. We propose a novel inertial proximal DC algorithm in Bregman geometry, named

iBPDCA, designed to address nonconvex terms and enhance convergence speed through inertial techniques. We provide a detailed theoretical analysis, establishing both subsequential and global convergence of iBPDCA via the Kurdyka-Łojasiewicz property. Additionally, we introduce a Plug-and-Play variant, PnP-iBPDCA, which employs a deep neural network-based prior for greater flexibility and robustness while ensuring theoretical convergence. We also establish that the Gaussian gradient step denoiser used in our method is equivalent to evaluating the Bregman proximal operator for an implicitly weakly convex function. We extensively validate our method on Rician noise and phase retrieval and demonstrate state-of-the-art performance.

Sesssion 4

Yuchen Huang
The Chinese University of Hong Kong

Boojum type singularities of weak anchoring liquid crystals around a particle

We study the one constant limit in the Landau-de Gennes theory where the generalized Rapini-Papoular surface energy density is imposed in the particle surface, and the far-field condition is imposed in the infinity. Under the axial ansatz, we show that singularities of the director field will occur as the boojum type on the antipodes when the anchoring strength is sufficiently large.

Tsz Lok Ip
The Chinese University of Hong Kong

Quasi-Conformal Convolution: A Learnable Convolution for Deep Learning on Riemann Surfaces

Deep learning on non-Euclidean domains is important for analyzing complex geometric data that lacks common coordinate systems and familiar Euclidean properties. A central challenge in this field is to define convolution on domains, which inherently possess irregular and non-Euclidean structures. In

this work, we introduce Quasi-conformal Convolution (QCC), a novel framework for defining convolution on Riemann surfaces using quasi-conformal theories. Each QCC operator is linked to a specific quasi-conformal mapping, enabling the adjustment of the convolution operation through manipulation of this mapping. By utilizing trainable estimator modules that produce Quasi-conformal mappings, QCC facilitates adaptive and learnable convolution operators that can be dynamically adjusted according to the underlying data structured on Riemann surfaces. QCC unifies a broad range of spatially defined convolutions, facilitating the learning of tailored convolution operators on each underlying surface optimized for specific tasks. Building on this foundation, we develop the Quasi-Conformal Convolutional Neural Network (QCCNN) to address a variety of tasks related to geometric data. We validate the efficacy of QCCNN through the classification of images defined on curvilinear Riemann surfaces, demonstrating superior performance in this context. Additionally, we explore its potential in medical applications, including craniofacial analysis using 3D facial data and lesion segmentation on 3D human faces, achieving enhanced accuracy and reliability.

Trung Hieu Giang
City University of Hong Kong

Existence and uniqueness results for a nonlinear shell model

A nonlinear shell model is considered in this talk. This is a nonlinear variant of the Budiansky-Sanders linear shell model. Under some suitable assumptions on the magnitude of the applied force, we will prove the existence of a minimizer for this shell model. In addition, we will also show that our existence result can be applied to all kinds of geometries of the middle surface of the shell. We will also show that the minimiser found in this fashion is unique, provided the applied forces are small enough. Our result hence extends the one given by Destuynder in 1980s.

Zhen Hao
The Chinese University of Hong Kong

Asymptotic-Preserving Schemes for Boltzmann Mixture Models with
Disparate Masses

Simulating gas mixtures with particles of vastly different masses is computationally challenging due to the disparity in their thermal velocities. In this talk, we introduce an asymptotic-preserving numerical scheme for the Boltzmann mixture model that efficiently handles large mass ratios. By employing asymptotic expansions for the collision operators and accounting for the multiple time scales in the relaxation process, our method captures the essential dynamics, including the epochal relaxation phenomenon. Numerical results validate the scheme's effectiveness and asymptotic properties, offering a powerful tool for studying multi-scale gas mixture systems.