HKUST Scientific Computation Concentration Workshop 2025

Scientific Computation and AI for Science

Date: 25 October 2025, Saturday, 14:00-18:00

Venue: *Chen Kuan Cheng Forum Lecture Theater H (LTH), HKUST*

Invited Speakers

Prof Shensheng CHEN, Department of Chemical and Biological Engineering, HKUST
Prof Jack CHENG, Department of Civil and Environmental Engineering, HKUST
Prof Zhongkang HAN, School of Materials Science and Engineering, Zhejiang University
Prof Yanglong LU, Department of Mechanical and Aerospace Engineering, HKUST
Prof Zhichao PENG, Department of Mathematics, HKUST
Prof Jidong ZHAO, Department of Civil and Environmental Engineering, HKUST

Organized by Committee of Scientific Computation Concentration, HKUST

http://www.csc.ust.hk/scc/

All are welcome!

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Chen Kuan Cheng Forum Lecture Theater H (LTH), HKUST

Workshop Organizing Committee Chairs

Prof Yang XIANG, Department of Mathematics
Prof Jidong ZHAO, Department of Civil and Environmental Engineering

Committee of Scientific Computation Concentration/Workshop Organizers

Prof Yang XIANG, Department of Mathematics, Chair of Scientific Computation Concentration
Prof Haibin SU, Department of Chemistry
Prof Jiguang WANG, Department of Chemical and Biological Engineering, Division of Life Science
Prof Kun XU, Department of Mathematics
Prof Can YANG, Department of Mathematics
Prof Ding PAN, Department of Physics
Prof Ke YI, Department of Computer Science and Engineering
Prof Jidong ZHAO, Department of Civil and Environmental Engineering
Prof Weichuan YU, Department of Electronic and Computer Engineering
Prof Zhigang LI, Department of Mechanical and Aerospace Engineering
Prof Lin FU, Department of Mechanical and Aerospace Engineering

Workshop Secretariat

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Workshop Program

14:00 – 14:10	Opening speech by Prof. Yang XIANG	
14:10 – 14:40	Prof. Jidong ZHAO CIVIL	Computational Challenges in Building a Predictive Digital Twin Coast for Hong Kong
14:40 – 15:10	Prof. Jack CHENG CIVIL	Intelligent Synergy: Digital Twin, AI, and Robotics for Next-Gen Sustainable Smart Infrastructure and Construction
15:10 – 15:40	Prof. Zhongkang HAN Zhejiang University	Lattice Oxygen Migration via Cooperative Revolution
15:40 – 16:10	*Coffee break*	
16:10 – 16:40	Prof. Shensheng CHEN CBE	Anomalous Guest Polymer Interactions within Highly Charged Biocondensate Coacervates
16:40 – 17:10	Prof. Yanglong LU MAE	Physics-informed machine learning for inverse problems in engineering applications
17:10 – 17:40	Prof. Zhichao PENG MATH	On Reduced Order Model Enhanced Preconditioners for Radiative Transfer Equation
17:40 – 18:00	Open discussion	
18:00 – 20:00	*Dinner* (by invitation)	

Computational Challenges in Building a Predictive Digital Twin Coast for Hong Kong

Jidong ZHAO

Department of Civil and Environmental Engineering,
The Hong Kong University of Science and Technology

Abstract:
This presentation introduces the ongoing effort for developing a predictive digital twin for Hong Kong's coastline, designed to enhance preparedness for severe weather events like super typhoons and storm surges. As a dynamic virtual replica of the physical coast, the digital twin is expected to continuously updated with real-time data, enabling predictive analytics to inform coastal resilience, risk management, and hazard mitigation. A central feature is the bidirectional interaction between the physical and virtual systems. We address the key computational challenges in building this twin, focusing on the mathematical and algorithmic frameworks required to unify data-driven and physics-based models across multiple scales. These challenges encompass: (1) Developing effective coupling techniques to combine data-driven models with mechanistic, physics-based simulations, ensuring seamless information flow. (2) Enabling the rigorous integration of diverse subsystems that constitute the complex coastal-city-ocean environment. (3) Inverse Problem Solving for calibrating model parameters and inferring hidden states from observed system outputs. (4) Scalable data assimilation methods to continuously integrate real-time observations with numerical models. (5) Leveraging AI & Machine Learning techniques such as online learning, active learning and transfer learning for dynamic model refinement using streaming data. (6) Establishing rigorus methdologies for Verification, Validation, and Uncertainty Quantification (VVUQ) to ensure model reliability and quantify predictive confidence.

Intelligent Synergy: Digital Twin, AI, and Robotics for Next-Gen Sustainable Smart Infrastructure and Construction

Jack Cheng

Department of Civil and Environmental Engineering,
The Hong Kong University of Science and Technology

Abstract:
Digital twins create real-time digital replicas of physical assets, enhancing urban planning and infrastructure management. Artificial intelligence optimizes data analysis and decision-making processes, making city management more efficient and responsive. Meanwhile, drones facilitate low-altitude operations, revolutionizing surveying, monitoring, and logistics, whereas robotics support autonomous operations, inspection in challenging environment, and repetitive tasks.

This seminar will explore the transformative roles of digital twins, artificial intelligence (AI), and the drones/robotics in advancing smart construction and smart city initiatives. Topics including low carbon sustainable building design, smart site safety and city resilience monitoring, low-cost high-resolution 3D reconstruction, and automated drone-based inspections using cutting-edge solutions will be discussed, illustrated with examples. Potential challenges will also be presented.

Lattice Oxygen Migration via Cooperative Revolution

Zhongkang HAN

School of Materials Science and Engineering,
Zhejiang University

Abstract:
Lattice oxygen migration in solid oxides is a fundamental phenomenon in physics, chemistry, and materials science. It is well established that lattice oxygen migration is usually governed by two mechanisms: interstitial- and vacancy-driven migration. However, experimental lattice oxygen mobilities in many cases are higher than those predicted by the conventional mechanisms. Whether an alternative migration mechanism exists remains an open question. By integrating a global structural search algorithm, a machine learning atomic potential, and in situ scanning transmission electron microscopy (STEM) combined with integrated differential phase contrast (iDPC) imaging, we have uncovered a cooperative revolution mechanism (CRM) for lattice oxygen migration throughout the reconstructed CeO2 (100) surface. In this mechanism, oxygen migration around cerium atoms is driven by dynamic changes in the coordination number of surface oxygen atoms coupled to vertical vibrations of cerium atoms. Remarkably, this CRM is independent of oxygen vacancies or interstitial defects and results in an oxygen migration rate that is at least ten times faster than vacancy-driven or interstitial-driven mechanisms at 900 K. Moreover, CRM-driven lattice oxygen migration is also observed in other CeO2 (100) reconstructions as well as on the pristine Ce2O3 (100) surface. These results advance our understanding of lattice oxygen migration and provide new insights into the fundamental dynamics of surface and interface phenomena associated with ultrafast lattice oxygen migration.

Anomalous Guest Polymer Interactions within Highly Charged Biocondensate Coacervates

Shensheng CHEN

Department of Chemical and Biological Engineering,
The Hong Kong University of Science and Technology

Abstract:
Biocondensate coacervates, macromolecular liquids arising from liquid-liquid phase separation (LLPS) of charged biopolymers in aqueous environments, have transformed our understanding of intracellular functions and inspired cutting-edge biotechnologies. A key characteristic of typical coacervates is their polymer-rich and highly charged environment, which enables them to selectively encapsulate guest molecules and host biochemical reactions. Consequently, the functionalities and applications of coacervates are significantly influenced by the dispersion and aggregation states of guest molecules.

Intriguingly, guest macromolecules exhibit a strong tendency to aggregate within coacervates even in the absence of apparent chemical incompatibility, indicating a universal aggregation mechanism at play in these environments. Using extensive MD simulations, we identify electrostatic depletion — a strong force arising from electrostatic correlations within the host polyelectrolyte network that drives guest aggregations. Due to electrostatic depletion, neutral polymers, low-charge-density polyelectrolytes, and intrinsically disordered proteins (IDPs) with random charge sequences exhibit effective attractions in coacervates, in stark contrast to their behavior in dilute solutions.

Unlike the traditional depletion effect that requires mismatched length scale and morphology, electrostatic depletion is relevant in fluid systems where solute and solvent are both polymers with comparable size. Our discovery bridges a critical knowledge gap in the molecular physics of densely charged, crowded liquids and holds significant implications for the design of synthetic protocells and advanced drug delivery systems.

Physics-informed machine learning for inverse problems in engineering applications

Yanglong LU

Department of Mechanical and Aerospace Engineering,
The Hong Kong University of Science and Technology

Abstract:
Machine learning (ML) techniques are essential for addressing inverse problems in various engineering applications, as they can uncover hidden insights and establish complex relationships by recognizing patterns in data. However, the inherent "black-box" nature of ML poses significant challenges in understanding the mechanisms and outcomes of these models. Additionally, the reliability of ML predictions is heavily reliant on the quantity and quality of training data. To tackle these challenges, a new research field known as physics-informed machine learning (PIML), or scientific machine learning, has emerged. PIML integrates physical and domain knowledge into ML models to guide the training process, resulting in models that are both more interpretable and reliable. PIML techniques can be categorized into three main types: hybrid models, physical loss-based models, and physics-embedded architectures. Each category is further divided based on different integration methods and ML models. In this presentation, I will introduce several PIML architectures developed by our group, including Physics-based Compressive Sensing, Physics-constrained Dictionary Learning, Physics-Informed Fully Convolutional Networks, and Finite Volume Physics-Informed U-Net, all aimed at solving inverse problems with sparse data. Additionally, I will present case studies for each model to illustrate their applications.

On Reduced Order Model Enhanced Preconditioners for Radiative Transfer Equation

Zhichao PENG

Department of Mathematics,
The Hong Kong University of Science and Technology

Abstract:
Radiative transfer equation (RTE) is a kinetic equation modeling particles interacting with a background medium. It has a wide range of applications including medical imaging, nuclear engineering and astrophysics. Multi-query applications, such as uncertainty quantification, inverse problem, sensitivity analysis and design optimization, require solving RTE repeatedly for various parameters, e.g. material properties. Due to its high dimensional and multiscale nature, efficient iterative solvers for RTE are highly desired. Classical diffusion synthetic acceleration (DSA) uses the diffusion limit of RTE as a preconditioner. However, when the scattering effect is not sufficiently strong, RTE may not be well-approximated by its diffusion limit. Additionally, DSA does not leverage low-rank structures of the solution manifold in the parameter-domain.

To address these limitations, we have developed a data-driven reduced order model (ROM)-enhanced preconditioner for parametric RTE. ROM is able to exploit low-rank structures across parameters, and it also allows us to start from the original kinetic description. Intuitively, in our preconditioner, ROM corrects low frequency errors, while classical DSA damps high frequency errors. We further improve the efficiency and robustness of ROM-enhanced preconditioner by accounting for the preconditioner dependent trajectory of residuals during iterations. We also extend this approach to non-parametric time-dependent RTE by building a ROM on-the-fly to leverage low-rank structures across time.