

A composite image featuring a server room on the left, a night view of the HKUST building with a red sculpture in the center, and a colorful galaxy on the right. The text "Scientific Computation Concentration" is overlaid in yellow at the top. The HKUST logo is visible on the right side of the building.

Scientific Computation Concentration

HKUST Scientific Computation Concentration Workshop 2024 **Scientific Computation and AI for Science**

Date: 4 May 2024, Saturday, 14:00-18:00

Venue: *Leung Yat Sing Lecture Theater (LTF), HKUST*

Invited Speakers

Prof Xian CHEN, Department of Mechanical and Aerospace Engineering, HKUST

Prof Hanyu GAO, Department of Chemical and Biological Engineering, HKUST

Prof Xiaolong MA, Department of Materials Science and Engineering, City University of Hong Kong

Prof Wei SU, Division of Emerging Interdisciplinary Areas & Department of Mathematics, HKUST

Prof Can YANG, Department of Mathematics, HKUST

Prof Jize ZHANG, Department of Civil and Environmental Engineering, HKUST

Organized by Committee of Scientific Computation Concentration, HKUST

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

All are welcome!

HKUST Scientific Computation Concentration Workshop 2024

Scientific Computation and AI for Science

4 May 2024, Saturday, 14:00-18:00

Leung Yat Sing Lecture Theater (LTF), HKUST

Workshop Organizers

Prof Haibin SU, Department of Chemistry

Prof Ding PAN, Department of Physics

Prof Yang XIANG, Department of Mathematics

Prof Kun XU, Department of Mathematics

Prof Jidong ZHAO, Department of Civil and Environmental Engineering

Committee of the Scientific Computation Concentration

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. Can Yang MATH	AI for science: examples from spatial transcriptomics data
14:40 – 15:10	Prof. Hanyu Gao CBE	Deep learning and large language models for chemical information extraction
15:10 – 15:40	Prof. Jize Zhang CIVIL	Engineering synthetic tropical cyclones and storm surges for safer coastal communities
15:40 – 16:10	<i>Coffee break</i>	
16:10 – 16:40	Prof. Xian Chen MAE	Two tier compatibility conditions for phase transforming polycrystals
16:40 – 17:10	Prof. Wei Su EMIA & MATH	Multiscale modelling of non-equilibrium transport phenomena
17:10 – 17:50	Prof. Xiaolong Ma CityU	Quantifying intragranular and interfacial plasticity contribution in nanolaminates
17:50 – 18:00	Open discussion	
18:00 – 20:00	<i>Dinner</i> (by invitation)	

AI for science: examples from spatial transcriptomics data

Can YANG

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

Abstract:

The rapid emergence of spatial transcriptomics (ST) technologies is revolutionizing our understanding of tissue spatial architecture and biology. Although current ST methods, whether based on next-generation sequencing (seq-based approaches) or fluorescence in situ hybridization (image-based approaches), offer valuable insights, they face limitations either in cellular resolution or transcriptome-wide profiling. To address these limitations, we present SpatialScope, a unified approach integrating scRNA-seq reference data and ST data using deep generative models. With innovation in model and algorithm designs, SpatialScope not only enhances seq-based ST data to achieve single-cell resolution, but also accurately infers transcriptome-wide expression levels for image-based ST data. We demonstrate SpatialScope's utility through simulation studies and real data analysis from both seq-based and image-based ST approaches. SpatialScope provides spatial characterization of tissue structures at transcriptome-wide single-cell resolution, facilitating downstream analysis, including detecting cellular communication through ligand-receptor interactions, localizing cellular subtypes, and identifying spatially differentially expressed genes. This is a joint work with Xiaomeng Wan, Jiashun Xiao, Cindy Sing Ting Tam, Mingxuan Cai, Ryohichi Sugimura, Yang Wang, Xiang Wan, Zhixiang Lin, Angela Ruohao Wu, Yan Yan, Jia Zhao, and Gefei Wang.

Deep Learning and Large Language Models for Chemical Information Extraction

Hanyu GAO

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

Abstract:

Artificial intelligence has been transforming the way of thinking in many scientific domains. In organic chemistry, machine learning models have been developed for molecular property prediction, reaction outcome and condition prediction, as well as synthetic route design. While initial success has been encouraging, further development of AI in chemistry is largely limited by the quantity and quality of datasets. In order to apply machine learning methods in specific domains, a reasonable amount of data needs to be extracted from the chemical literature, which is mostly a manual process that is time consuming and costly. Researchers are in need of tools that can accelerate or even automate this process.

In this work, we developed computational tools for automatic chemical information extraction from the literature. We focused on two types of prevalent chemical information – molecules and reactions. The goal was to convert images of molecules and reactions into cheminformatics representations (e.g. SMILES). For molecular image recognition, we used advanced models in computer vision that can both attend to local patterns and understand the global relationship. For reaction image recognition, we used object detection models combined with large language models to identify the roles of different molecular or textual entities in the image. Data augmentation strategies were designed for both models to represent complexity in real chemical images as much as possible. Results showed that our model outperforms the state-of-the-art methods and can accurately extract chemical information from chemical images of various types.

Engineering synthetic tropical cyclones and storm surges for safer coastal communities

Jize ZHANG

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

Abstract:

Tropical cyclones (TCs) and the resulting storm surges pose significant threats to coastal communities and infrastructure reliability. In this talk, we present two novel AI-driven approaches that leverage historical data and physics-based principles to advance TC risk analysis and storm surge forecasting, ultimately contributing to improved coastal resilience.

Firstly, we introduce a data-driven framework that discovers parsimonious, interpretable, and effective governing equations for TC track and intensity evolution using the Sparse Identification of Nonlinear Dynamics (SINDy). By treating TC evolutions as dynamical systems and adaptively learning from historical and environmental data, our models outperform alternative physics-based models in capturing key TC characteristics. These advancements directly inform the design, maintenance, and adaptation strategies for coastal infrastructure.

Secondly, we propose the Causal-inference based Spatio-Temporal Graph Neural Network (CSTGNN) for rapid and precise storm surge forecasting. CSTGNN integrates graph neural networks and gated recurrent units to capture spatial and temporal dependencies across multiple observation stations, addressing the challenges of data scarcity and real-world complexity. Employing the Liang–Kleeman information flow theory for establishing a causal-inference based graph edge scheme, CSTGNN accounts for the effect of complex coastline topography. CSTGNN outperforms competitive baselines across various metrics and lead times, affirming its competence in storm surge forecasting.

These AI-driven approaches showcase the immense potential of harnessing data-driven techniques and physics-based principles for advancing TC risk analysis and storm surge prediction, ultimately contributing to enhanced coastal infrastructure reliability and resilience.

Two tier compatibility conditions for phase transforming polycrystals

Xian CHEN

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

Abstract:

For micro and nano-devices used for biomedical applications, e.g. neural stents and heart valves, both crystallographic compatibility and grain boundary engineering play profound role in their functionalities. But these two mechanisms are not well synergized. Here we theorize a two-tier compatibility criterion to optimize the textures across the grain boundary, to enhance the mechanical reversibility of transforming polycrystals under stress-induced phase transformation. In this talk, we will present an experimental demonstration that a micropillar fabricated at the grain boundary achieves a remarkable transformability under the demanding driving stress (~600MPa) over 10,000 nanomechanical cycles without fulfilling the crystallographic compatibility condition by lattice parameters. The experiment provides an important insight to the design of low fatigue materials by considering the orientation dependent compatibility between grains. By modern nanotechnologies, it is possible to fabricate bi-crystal, tri-crystal and/or quart-crystal nano structures with designed textures, which underlies a new method for the smart materials and structures design.

1. M. Karami, Z. Zhu, Z. Zeng, N. Tamura, Y. Yang and X. Chen, Two-tier compatibility of Superelastic Bi-crystal Micropillar at Grain Boundary, *Nano Letters* 20, 11(2020) 8332.
2. M. Karami, K. Chu, Z. Zhu, Z. Wang, Q. P. Sun, M. Huang and X. Chen, Orientation-dependent superelasticity and fatigue of CuAlMn alloy under in situ micromechanical tensile characterization, *J. Mech. Phys. Solids*, 104787 (2022).

Multiscale Modelling of Non-Equilibrium Transport Phenomena

Wei SU

*Division of Emerging Interdisciplinary Areas & Department of Mathematics,
The Hong Kong University of Science and Technology*

Abstract:

By simultaneously considering models at different scales, multiscale modelling offers an approach to describing mass and heat transport problems, in which the multiscale character is the dominant issue, and the traditional physical laws lose their validity; for instance, gas flows in porous media and heat dissipation in semiconductor materials at nano-/micro-scales. In this talk, I will introduce my works on the multiscale modelling of non-equilibrium gas and phonon transport, which are based on a hybrid of macroscopic equations, which resolve field variables in terms of macroscopic quantities, and Boltzmann kinetic equations that describe the variation of distribution functions of mass or energy carriers. Combined with advanced numerical techniques, the developed schemes can accurately and efficiently simulate multiscale transport phenomena, including gas flows of single components and/or internal energy relaxations, gas mixture flows, and non-Fourier heat conduction. Theoretical analysis and numerical tests will be provided to show the performance of the schemes.

Quantifying intragranular and interfacial plasticity contribution in nanolaminates

Xiaolong MA

*Department of Materials Science and Engineering,
City University of Hong Kong*

Abstract:

Disentangling the intragranular and interfacial plasticity contribution to the overall strain accommodation is crucial to understanding the microstructural evolution and mass transport upon deformation in materials with the nanoscale feature size. In this presentation, we devised an experimental approach to tackle the issue by introducing shear strain gradients into Cu/Nb nanolaminates of different layer thicknesses with the shear perpendicular to the laminate interfaces. Measuring the strain gradient and the resultant lattice disorientation enables a quantitative understanding of the intragranular and interfacial dislocation storage and hence plasticity contribution. We found that intragranular dislocation slip governs the deformation in the 300 nm-layer laminate entirely and, unexpectedly, contributes ~to 80% of the total plasticity in the 30 nm-layer laminate. The experimental method is expected applicable for studying other nanostructured materials.