Scientific Computation Concentration Workshop

April 29th, 2023

Lecture Theater H

The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

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

Workshop Organizers

Prof Lin Fu	Department of Mechanical and Aerospace Engineering
Prof Jiguang Wang	Department of Chemical and Biological Engineering, Division of Life Science
Prof Jidong Zhao	Department of Civil and Environmental Engineering
Prof Ding Pan	Department of Physics
Prof Zhigang Li	Department of Mechanical and Aerospace Engineering
Prof Yang Xiang	Department of Mathematics

Committee of the Scientific Computation Concentration

Prof Yang Xiang	Department of Mathematics
Prof Kun Xu	Department of Mathematics
Prof Can Yang	Department of Mathematics
Prof Jidong Zhao	Department of Civil and Environmental Engineering
Prof Weichuan Yu	Department of Electronic and Computer Engineering
Prof Ke Yi	Department of Computer Science and Engineering
Prof Ding Pan	Department of Physics
Prof Jiguang Wang	Department of Chemical and Biological Engineering, Division of Life Science
Prof Lin Fu	Department of Mechanical and Aerospace Engineering
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Workshop Secretariat

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Workshop Program

April 29th, 2023

Session 1
Chair: Professor Zhigang Li and Yanguang Zhou

09:00 – 09:5	Opening speech by Prof. Yang Xiang
09:05 – 09:45	Invited Talk: Nanoengineering for Advanced Materials & Structures with Applications in Water Harvesting and Heat Dissipation Prof. Yanguang Zhou, Mechanical and Aerospace Engineering
09:45 – 10:25	Invited Talk: Computational study of soft matter physics Prof. Rui Zhang, Physics
10:25 – 10:40	**Coffee break**
10:40 – 11:20	Invited Talk: Recent progress in modelling the incompressible and compressible wall-bounded turbulence Prof. Lin Fu, Mechanical and Aerospace Engineering
11:20 – 12:00	Invited Talk: Computational Investigation of Sequence and Properties in Polymer Materials Prof. Hanyu Gao, Chemical and Biological Engineering
12:00 – 14:00	**Lunch**

Session 2
Chair: Professor Lin Fu

14:00 – 14:40	Invited Talk: Planning ahead is all you need Prof. Zhe Wang, Civil and Environmental Engineering
14:40 – 15:20	Invited Talk: Entanglement renormalization and quantum many-body states Prof. Adrian Po, Physics
15:20 – 15:50	**Coffee break**
15:50 – 16:30	Invited Talk: On the low-frequency unsteadiness in shock-wave/turbulent boundary-layer interactions Prof. Jiaao Hao, Department of Aeronautical and Aviation Engineering, The Hong Kong Polytechnic University
16:30 – 17:10	Invited Talk: Nonlinear Dynamics and Design Principles of Biology Prof. Yi Liao, Life Science
17:10 – 17:30	Open discussion
17:30 – 20:00	**Dinner**

Nanoengineering for Advanced Materials & Structures with Applications in Water Harvesting and Heat Dissipation

Yanguang Zhou
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Abstract:
When the scale of materials goes down to a tiny scale, i.e., nanometer scale which is a billionth of a meter, the physical and chemical properties of the materials become quite unusual due to the quantum and size effects. As a result, nanotechnologies have often served as tools for design of highly functional engineered materials & structures with potential applications in health, energy and manufacturing. In this seminar, I will discuss a number of nanoengineering examples showcasing our recent materials and technologies innovations including optimizing the boiling heat transfer via surface functionalization for water harvesting, enhancing the interfacial thermal transport via the water adsorption in metal-organic frameworks (MOFs), and understanding the thermal transport behavior of vibrations in glasses at low temperatures.

Biography:
Dr. Yanguang Zhou received his Ph.D. degree with "Ausgezeichnet" in the Mechanical Engineering Department at RWTH-Aachen University. He worked as a postdoc research associate and an assistant visiting project scientist at the University of California, Los Angeles (UCLA) before joining Hong Kong University of Science and Technology (HKUST) as an assistant professor. Dr. Zhou's group at HKUST designs advanced materials & structures, i.e., thermoelectric materials, magnetic materials and nanocomposites, via using nanotechnologies (both experimental and theoretical methods), with applications in water harvesting and thermal management. His research has been published in Nature Communications, Nano Letters, Advanced Functional Materials, International Journal of Heat and Mass Transfer and Physical Review B. Dr. Zhou is a receipt of AICES Fellowship, Chinese Government Award for Outstanding Self-financed Students Abroad, Borchers-Plakette at RWTH-Aachen University, National Young Talent Project of China and Hong Kong SciTech Pioneers Award.

Computational study of soft matter physics

Rui Zhang
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Abstract:
Complex fluids are ubiquitous. Examples include bio fluids, toothpastes, liquid crystals and etc. Simulations of complex fluids are important for understanding their structural and dynamical properties, and can be helpful for designing new materials. In this talk, I will introduce several computational methods that are widely used to model complex fluids. I will also discuss interesting phenomena associated with driven and active complex fluids. Through these we demonstrate the power of high performance computation in complex fluids research.

Biography:
Prof. ZHANG, Rui obtained a BS degree in physics in 2007 from the Department of Physics at Fudan University, China. Before he joined the Department of Physics at HKUST in 2020 as a PI, he worked with Liew Family Professor Juan J. de Pablo, a member of the National Academy of Engineering, at the Pritzker School of Molecular Engineering, the University of Chicago in the United States, where he collaborated with Horace B. Horton Professor Margaret Gardel's group on actin filaments, an important type of biopolymers. Prior to his postdoc experience at the University of Chicago, he did his PhD with Prof. Joel Koplik on nano fluids simulations from 2009 to 2013 at the Benjamin Levich Institute and the Department of Physics at the City College, a senior flagship college in the City University of New York system. During his PhD, he also collaborated with Prof. Taehun Lee's group on droplet impact simulations.

Prof. Zhang has a broad interest in Computational Soft Matter Physics, with a focus on biologically relevant systems, such as biopolymers and bacteria suspensions. The overarching goal of his research group is to understand emerging phenomena in nature and borrow the wisdom to design biomimetic materials to help tackle human's grand challenges in energy, health, and environments. Specifically, his group strives to develop theoretical frameworks and multiscale simulation tools, including molecular dynamics and computational fluid dynamics, to understand the complex dynamical phenomena in a wide range of soft matter and biophysical systems. His group is closely working with world-leading experimentalists to test model predictions, interpret new observations, and further design synthetic materials for practical applications. His current research interests include active matter, liquid crystals, multiphase and porous materials, and mechanical metamaterials. He is also interested in applying machine learning for certain materials design problems.

Recent progress in modelling the incompressible and compressible wall-bounded turbulence

Lin Fu[1, 2]

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Abstract:
In this talk, we will focus on the physics and modelling of the incompressible and compressible wall-bounded turbulence. Firstly, for incompressible wall turbulence, we develop a new methodology to assess the streamwise inclination angles (SIAs) of the wall-attached eddies populating the logarithmic region with a given wall-normal height. The present results show, for the first time, that the SIAs of attached eddies are Reynolds-number dependent in low and medium Reynolds numbers and tend to saturate at 45o as the Reynolds number increases. These findings clarify the long-term debate and perfect the picture of the attached-eddy model. Secondly, we will present our recent efforts in modelling the compressible wall-bounded turbulence. The extension of incompressible wall model to high-speed flows is accommodated by proposing a novel transformation, which maps the mean velocity profiles of compressible wall turbulence to the incompressible law of the wall. The performance of the transformation is verified for compressible wall-bounded flows with edge Mach numbers ranging from 0 to 15 and friction Reynolds numbers ranging from 200 to 2000. (Ref. PNAS 2021, JFM 2021, JFM 2022, etc.).

Biography:
Prof. Lin Fu is an Assistant professor in the Department of Mathematics and the Department of Mechanical and Aerospace Engineering at The Hong Kong University of Science and Technology (HKUST). Before he joined HKUST, he was a postdoctoral fellow working with Prof. Parviz Moin at Center for Turbulence Research (CTR), Stanford University, for more than 3 years. And he also did postdoctoral research with Prof. Nikolaus Adams at Technical University of Munich, where he obtained his Ph.D. degree with a grade of Summa Cum Laude (passed with the highest distinction). His research is funded by the Research Grants Council (RGC) of Hong Kong with the recognition of Early Career Award. He has published more than 50 journal papers on PNAS, JFM, PRF, JCP, CMAME, etc.

Computational Investigation of Sequence and Properties in Polymer Materials

Hanyu Gao

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Abstract:
Polymers are important materials that make the modern life possible. Both synthetic and natural polymers have various domestic and industrial applications. One key factor that makes polymers unique is the infinite diversity in molecular sequences, including the length of polymer chains and the arrangement of the repeating units. Being able to understand and hence control and design polymer sequences for desired properties is therefore crucial to fully exploit the potential of polymer materials, yet it is insufficient to rely on experimental approaches alone, since the design space is too large.

In this work, we present some computational approaches for designing polymer sequences and elucidating their relationships with properties. For synthetic polymers, we use kinetic Monte Carlo to simulate the construction of polymer chains in polymerization reactions, and molecular dynamic simulations to explore the relationship between sequence and macroscopic polymers. For natural polymers, we use machine learning to predict topological properties based on protein sequences, and apply the model to search for building blocks for topological protein materials.

Biography:
Hanyu Gao is an assistant professor at the Hong Kong University of Science and Technology. Hanyu obtained his Bachelor's degree in chemical engineering from Tsinghua University in 2012, where he was Magna Cum Laude. He then completed his Ph. D. in the Department of Chemical and Biological Engineering at Northwestern University with Prof. Linda Broadbelt. After that he worked as a postdoctoral associate at MIT in Prof. Klavs Jensen's group from 2017 to 2020. Hanyu's research interest lies in using modeling techniques, including simulation, optimization and machine learning, to solve chemical engineering problems ranging from polymer reaction engineering to organic synthesis design.

Planning ahead is all you need

Zhe Wang

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Abstract:
With higher renewable penetration, demand side management becomes increasingly important to help maintain the real-balance between supply and demand, and to help the grid absorb more renewable generations. Buildings are a major electricity end-user, which has large potential for demand response. However, the current rule-based control cannot unlock the demand response potential of buildings. In this talk, we will introduce how model predictive control can facilitate more efficient dynamic energy management, and help building respond to the grid signal in a more effective way. We will prove that battery management can be formulated as a convex optimization problem. We will also demonstrate that model predictive control is robust to model and prediction uncertainty. To achieve our carbon neutrality goal, a new building control paradigm, i.e. model predictive control rather than rule based control, is needed.

Biography:
Zhe (Walter) is an Assistant Professor working with the Department of Civil and Environmental Engineering at HKUST. His current research is about human-building interaction, and building energy system control. Prior to joining HKUST, he was a Project Scientist in Lawrence Berkeley National Laboratory working on smart building control. Zhe has published 73 articles in SCI journals, 23 as first author, 8 as corresponding author, 6 as the co-first author. He has first authored 1 ESI highly cited paper and 2 Applied Energy highly cited papers. Zhe was invited to give a speech on the Seventh-Round High-level Consultation on U.S.-China People to People Exchange, chaired by U.S. Secretary of States John Kerry and Chinese Vice-Premier Yandong Liu, as the only representative of Chinese young scholar. Recently, Zhe has won the first prize in the 2022 Global AI Challenge for Building E&M Facilities hosted by Hong Kong EMSD.

Entanglement renormalization and quantum many-body states

Adrian Hoi Chun PO

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Abstract:
In principle, the resources required to describe a quantum many-body states increase exponentially with the size of the system. This exponential growth makes it impractical to describe a quantum many-body state in an exact manner beyond around 20 qubits. Yet, a physical states, say the ground state of a local Hamiltonian, is expected to be much more structured and therefore might be describable using much less resources. Tensor network states represent one class of quantum many-body states which can be described and simulated efficiently on a classical computer. In this talk, we explore how we could extend the capability of the tensor-network ansatz by combining them with the entanglement renormalization of a Gaussian reference state.

Biography:
Dr. Hoi Chun (Adrian) Po is a condensed matter theorist and he is broadly interested in the study of collective phenomena arising from a large number of quantum particles. Some of his research foci include the interplay between symmetries and topology in quantum materials, the intersection between quantum information and condensed matter theories, as well as out-of-equilibrium quantum dynamics.
Dr. Po grew up in Hong Kong and obtained his bachelor's degree from the Chinese University of Hong Kong in 2013. He began his doctoral studies at the University of California, Berkeley, but transferred to Harvard University in 2016 together with the move of his thesis advisor, Prof. Ashvin Vishwanath. After obtaining his PhD from Harvard in 2018, he moved to MIT as a Pappalardo Postdoctoral Fellow. He returned to Hong Kong and joined HKUST as an assistant professor in 2021.

On the low-frequency unsteadiness in shock-wave/turbulent boundary-layer interactions

Jiaao Hao

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Abstract:
The shock wave/turbulent boundary layer interaction over a compression corner is studied using global stability analysis (GSA) and resolvent analysis based on a separation of scales between the low-frequency, large-scale motions and the turbulent fluctuations. The GSA identifies a leading stationary mode, which becomes globally unstable as the ramp angle is beyond a critical value. For globally stable flows, the resolvent analysis captures two-dimensional and three-dimensional local maxima in optimal gain, both of which are due to modal resonance between the forcing and the leading global mode. Notably, the frequency-premultiplied optimal gain associated with two-dimensional disturbances peaks at a low frequency. For different interaction strengths, the peak frequencies collapse onto a universal value of 0.015 when nondimensionalized using the length of the separation region and the freestream velocity. A numerical simulation perturbed with the corresponding optimal forcing reveals that the response is in the form of large-scale shock motion.

Biography:
Dr. Jiaao Hao is an Assistant Professor in the Department of Aeronautical and Aviation Engineering, the Hong Kong Polytechnic University. He received his PhD in Fluid Mechanics and BEng in Aircraft Design and Engineering from Beihang University in 2018 and 2013, respectively. His research interests include hypersonic aerodynamics, aerothermodynamics, computational fluid dynamics, and flow stability.

Nonlinear Dynamics and Design Principles of Biology

Yi Liao

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Abstract:
Nonlinearity is ubiquitous in biology and a critical factor contributing to the complexities of living systems. In this talk, I will explore several nonlinear phenomena in biology, ranging from the dynamics of biochemical networks to the behaviors of cell populations. I will delve into the ways in which nonlinear interactions can give rise to unexpected emergent properties, such as oscillations, stochastic fluctuations and pattern formations that can profoundly shape the behaviors and functions of living organisms. Together, the examples presented here highlight how quantitative theories and methods can be integrated with traditional wet lab experiments to uncover fundamental principles that are generally applicable in biology.

Biography:
Dr. Liao received his Ph.D. from the University of Michigan where he worked with Prof. Julie S. Biteen on single-molecule dynamics in bacterial cells. After completing his Ph.D., he joined the lab of Prof. Michael J. Rust at the University of Chicago as a postdoctoral scholar to study biological oscillators and self-organizing processes in bacteria. His research has emphasized that even relatively simple biochemical networks can give rise to complex spatiotemporal phenomena and sophisticated stress-adaptation strategies in bacteria. He started his independent career at HKUST in 2023, where his lab continues to investigate the relationship between gene regulatory networks and emergent properties in bacteria using experimental and computational approaches.