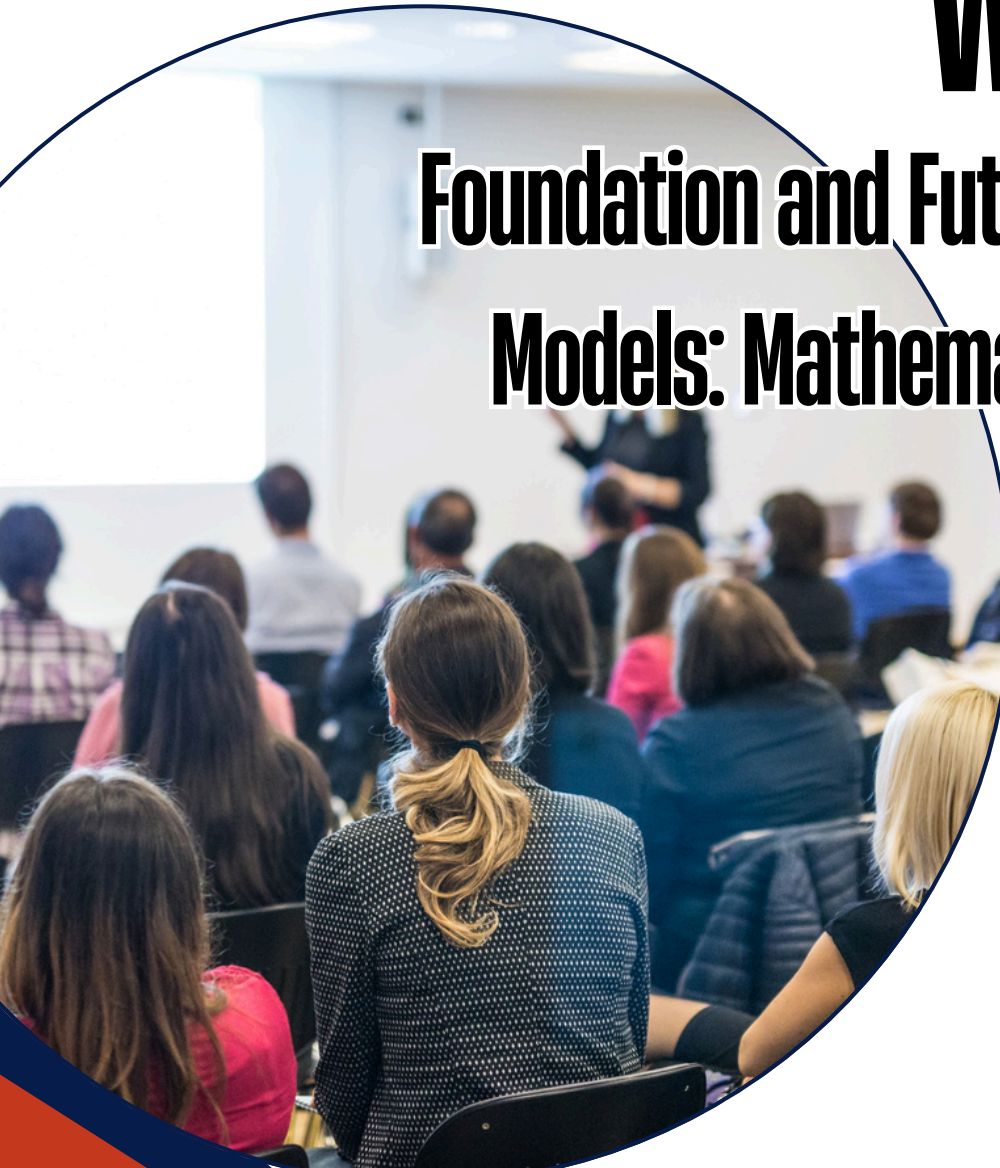




Liu Bie Ju Centre for
Mathematical Sciences

香港城市大學
City University of Hong Kong

28 - 30 July 2025

A circular inset image showing the back view of an audience seated in a lecture hall, looking towards a presentation screen. The text is overlaid on the right side of this image.

Workshop: Foundation and Future of Generative Models: Mathematics, Algorithms, and Applications

**Workshop on Foundation and Future of Generative Models: Mathematics,
Algorithms, and Applications**

City University of Hong Kong

28-30 July 2025, City University of Hong Kong

Program and Abstracts

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Welcome Message

We are delighted to welcome you to Workshop on Foundation and Future of Generative Models: Mathematics, Algorithms, and Applications. This workshop is designed to explore the foundations, advancements, and future directions of generative AI, fostering collaboration across diverse fields.

Workshop Highlights

- Techniques: Normalizing flows, score-based diffusion models, and beyond.
- Foundations: Dynamical systems, probability flow, optimal transport, and more.
- Mathematical Understanding: Model development and training algorithms.
- Applications: Sampling problems, inverse problems, AI for science, and design space exploration.

Through tutorial lectures, presentations, and discussions, we aim to:

- Deepen the theoretical and practical understanding of generative models.
- Examine their capabilities and limitations from mathematical and scientific perspectives.
- Encourage cross-disciplinary collaboration and inspire junior researchers.

We hope this workshop serves as a vibrant platform for exchanging ideas, sparking innovation, and building lasting connections. Your participation is invaluable in shaping this exciting field's future.

Thank you for joining us!

General Information

Organizing Committee

Neil Kumar CHADA, City University of Hong Kong, Hong Kong

Xiang ZHOU, City University of Hong Kong, Hong Kong

Workshop Coordinators

Secretary

Nina CHAN

Liu Bie Ju Centre for Mathematical Sciences, City University of Hong Kong

Website: <https://www.cityu.edu.hk/rcms/wgm2025/index.html>

Workshop Venue

Mr & Mrs David TF Chow Lecture Theatre (LT-4), 4/F, Yellow Zone, Yeung Kin Man Academic Building, CityU

Mr & Mrs David TF Chow Lecture Theatre (LT-4) is equipped with a desktop computer, a cable for connecting to laptop, an overhead projector and white boards.

Poster Venue

Y4502, 4/F, Yellow Zone, Yeung Kin Man Academic Building, CityU

Social Events

Welcome Lunch (by Invitation Only)

Date: 28 July 2025 (Mon)

Time: 12:10 pm - 2:00 pm

Venue: City Chinese Restaurant

8/F, Bank of China (Hong Kong) Complex, City University of Hong Kong

Banquet (by Invitation Only)

Date: 29 July 2025 (Tue)

Time: 6:30 pm

Venue: City Chinese Restaurant

8/F, Bank of China (Hong Kong) Complex, City University of Hong Kong

Other Information

Name Badges

All attendees are requested to wear their name badge. Workshop Secretary and Workshop Assistants are ready to assist you if needed.

Banking Service

Opening hours: 09:00–17:00 (Monday–Friday)

Location: 3/F Yeung Kin Man Academic Building (next to Run Run Shaw Library)



Services including foreign currency and traveler's cheque exchange are provided at Hang Seng bank.

Message Board

Message boards are located outside LT-4. The latest information of the workshop and messages for attendees will be posted on these boards.

Computer & Internet Services

Networked computers are available at Mathematical Laboratory during the workshop period:

Date: 28-30 July 2025

Time: 09:30-12:30, 13:45-17:30

Location: P5708, 5/F Yeung Kin Man Academic Building (near Lift 1)

Please contact our colleague to unlock the door of the computer lab for you.

Wireless internet access through your own mobile device within CityU campus is also available.

Login name and password can be found at the inner side of your name badge.

Dining

Several canteens are available at the campus and over 30 restaurants can be found at the adjacent shopping mall Festival Walk.

CityU Campus

AC2 Canteen



Location: 3/F, Li Dak Sum Yip Yio Chin Academic Building

Opening hours: 07:30–21:00 (Monday–Sunday)

Menu: Fast food

City Chinese Restaurant



Location: 8/F, Bank of China (Hong Kong) Complex

Opening hours: 11:00–15:50 & 17:30–21:30 (Monday–Friday)

09:00–15:50 & 17:30–21:30 (Saturday, Sunday and public holidays)

Menu: Chinese menu with full selection

Faculty Lounge



Location: 9/F, Bank of China (Hong Kong) Complex

Opening hours: 11:00–22:30 (Monday–Sunday)

Menu: Western menu

AC3 Bistro



Location: 7/F, Lau Ming Wai Academic Building

Opening hours: 07:30–21:00 (Monday–Saturday)

Closed on Sunday and public holidays

Menu: Western food

AC3 Café



Location: 3/F, Lau Ming Wai Academic Building
Opening hours: 07:30–21:00 (Monday–Friday)
09:00–19:00 (Saturday and Sunday)
Closed on public holidays
Menu: Sandwich, salad, snacks and drinks

Lodge Bistro



Location: G/F, Academic Exchange Building
Opening hours: 07:30–20:30 (Monday–Sunday)
Menu: Western food

5380 Cafe (Kebab Station)



Location: 5/F, Bank of China (Hong Kong) Complex
Opening hours: 10:00–20:00 (Monday–Saturday)
Closed on Sunday and public holidays
Menu: Hot halal food and kebab

Coffee Cart

Location: Purple Zone, 4/F, Yeung Kin Man Academic Building
Opening hours: 08:00–20:00 (Monday–Friday)
08:00–17:00 (Saturday)
Closed on Sundays and public holidays
Service: Snacks, drinks and stationeries

Homey Kitchen

Location: Student Residence Multi-function Hall B
Opening hours: 9:30 – 15:15 & 15:45 – 19:30 (Monday – Friday)
11:00 – 16:00 (Saturday)
Closed on Sundays and public holidays
Service: Snacks, drinks and stationeries

Festival Walk (shopping mall)

With an extensive selection of restaurants and menus, this adjacent shopping mall provides more choices for dining.

Useful Telephone Numbers

CityU Campus

| | |
|------------------|----------------|
| LBJ Centre: | +852 3442 6570 |
| Health Centre: | +852 3442 6066 |
| Security Office: | +852 3442 8888 |

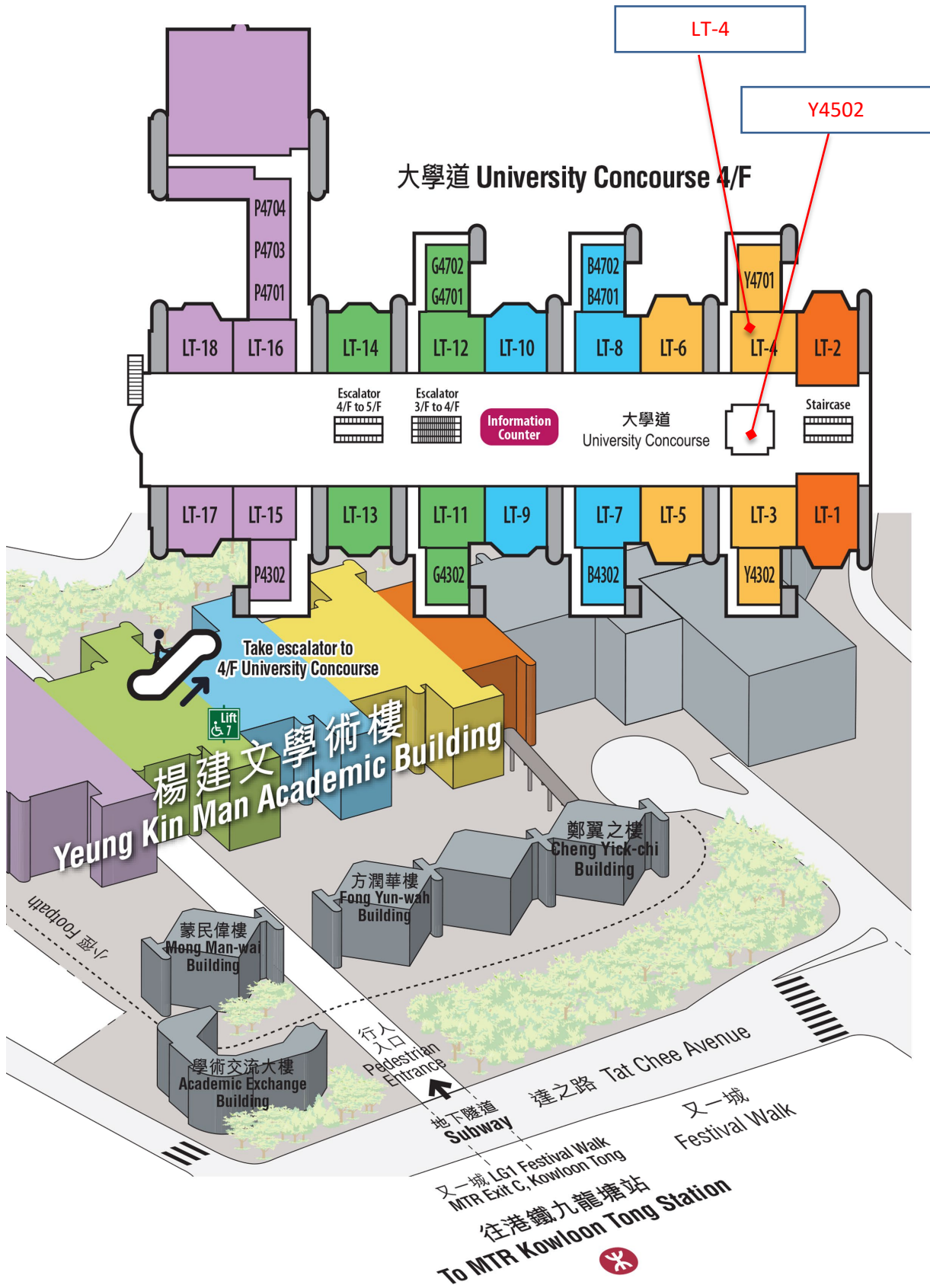
Hotels

| | |
|----------------|-----------------|
| CityUHK Lodge: | + 852 2622 6291 |
|----------------|-----------------|

MISC

| | |
|-------------------------|----------------|
| Immigration Department: | +852 2824 6111 |
| Hong Kong Police: | 999 |

CityU Location Plan



Program at a Glance

| <u>Time</u> | <u>28 July 2025, Monday</u> |
|---------------|---|
| 8:30 – 8:50 | Registration |
| 8:50 – 9:00 | Opening Ceremony |
| 9:00 - 9:50 | Tutorials I: LEE Juho (Part 1) |
| 10:00 - 10:50 | Tutorials I: LEE Juho (Part 2) |
| 10:50 - 11:20 | Coffee Break |
| 11:20 - 12:10 | Tutorials II: JIAO Yuling (Part 1) |
| 12:10 – 14:00 | Welcome Lunch (by Invitation Only) City Chinese Restaurant 8/F, Bank of China (Hong Kong) Complex, City University of Hong Kong |
| 14:00 – 14:50 | Tutorials II: JIAO Yuling (Part 2) |
| 15:00 – 15:50 | Tutorials III: WANG Lei (Part 1) |
| 16:00 – 16:50 | Tutorials III: WANG Lei (Part 2) |
| 16:50 – 17:20 | Coffee Break |
| 16:50 – 17:50 | Poster Session Y4502, 4/F, Yellow Zone, Yeung Kin Man Academic Building, CityU Campus |

Program at a Glance

| <u>Time</u> | <u>29 July 2025, Tuesday</u> |
|----------------------|---|
| 8:30 – 9:00 | Registration |
| 9:00 - 9:50 | William Benter Distinguished Lecture: XIA Zhihong Jeff |
| 9:50 – 10:10 | Coffee Break |
| | Poster Session Y4502, 4/F, Yellow Zone, Yeung Kin Man Academic Building, CityU Campus |
| 10:10 – 10:40 | Invited Talk 1: CAO Yu |
| 10:40 - 11:10 | Invited Talk 2: GAO Xuefeng |
| 11:10 - 11:40 | Invited Talk 3: ZHU Tong |
| 11:40 – 12:10 | Invited Talk 4: CHEN Jingrun |
| 12:10 – 14:00 | Lunch Break |
| 14:00 – 14:30 | Invited Talk 5: ZHANG Xiaoqun |
| 14:30 – 15:00 | Invited Talk 6: ZHANG Zhiwen |
| 15:00 - 15:30 | Invited Talk 7: LIU Zhaoqiang |
| 15:30 - 16:00 | Invited Talk 8: TANG Rong |
| 16:00 - 16:30 | Coffee Break |
| | Poster Session Y4502, 4/F, Yellow Zone, Yeung Kin Man Academic Building, CityU Campus |
| 16:30 – 17:00 | Invited Talk 9: WANG Yuguang |
| 17:00 – 17:30 | Invited Talk 10: ZHOU Peijie |
| 17:30 - 18:00 | Invited Talk 11: ZOU Difan |
| 18:30 | Banquet (by Invitation Only) City Chinese Restaurant 8/F, Bank of China (Hong Kong) Complex, City University of Hong Kong |

Program at a Glance

| <u>Time</u> | <u>30 July 2025, Wednesday</u> |
|---------------|--|
| 8:30 – 9:00 | Registration |
| 9:00 - 9:50 | Distinguished Lecture: HUANG Jian |
| 9:50 – 10:10 | Coffee Break |
| | Poster Session Y4502, 4/F, Yellow Zone, Yeung Kin Man Academic Building, CityU Campus |
| 10:10 – 10:40 | Invited Talk 12: ZHOU Kai |
| 10:40 - 11:10 | Invited Talk 13: HOU Junhui |
| 11:10 - 11:40 | Invited Talk 14: ZENG Jia |
| 11:40 – 12:10 | Invited Talk 15: LI Gen |
| 12:10 – 14:00 | Lunch Break |
| 14:00 – 14:30 | Invited Talk 16: GAO Weiguo |
| 14:30 – 15:00 | Invited Talk 17: WANG Zhongjian |
| 15:00 - 15:30 | Invited Talk 18: WEI Chaozhen |
| 15:30 - 16:00 | Invited Talk 19: YUAN Yancheng |
| 16:00 - 16:30 | Coffee Break |
| | Poster Session Y4502, 4/F, Yellow Zone, Yeung Kin Man Academic Building, CityU Campus |
| 16:30 – 17:00 | Invited Talk 20: HUANG Yuanfei |
| 17:00 – 17:30 | Invited Talk 21: MOU Chenchen |
| 17:30 - 18:00 | Invited Talk 22: QI Shuren |

**Workshop on Foundation and Future of Generative Models:
Mathematics, Algorithms, and Applications
Day 1, 28 July 2025, Monday**

| HK Time | | Venue |
|-------------------------------------|--|-------------------------|
| 8:30 – 8:50 | Registration opens | LT-4 |
| 8:50 – 9:00 | Opening Ceremony Photo Session | LT-4 |
| 9:00 - 9:50 & 10:00 - 10:50 | Tutorials I: Generative Modeling with Diffusion Models <i>Prof. Juho Lee, Kim Jaechul Graduate School of AI, KAIST, South Korea</i> | LT-4 |
| 10:50 - 11:20 | Coffee Break | |
| 11:20 - 12:10 | Tutorials II: Theory for deep generative learning <i>Prof. Yuling Jiao, Department of Artificial Intelligence, Wuhan University</i> | LT-4 |
| 12:10 – 14:00 | Welcome Lunch (by Invitation Only) | City Chinese Restaurant |
| 14:00 – 14:50 | Tutorials II: Theory for deep generative learning <i>Prof. Yuling Jiao, Department of Artificial Intelligence, Wuhan University</i> | LT-4 |
| 15:00 – 15:50 & 16:00 – 16:50 | Tutorials III: A Physicist's Perspective on Generative Models <i>Prof. Lei Wang, Institute of Physics, Chinese Academy of Sciences</i> | LT-4 |
| 16:50 – 17:20 | Coffee Break | |
| 16:50 – 17:50 | Poster Session | Y4502 |

**Workshop on Foundation and Future of Generative Models:
Mathematics, Algorithms, and Applications
Day 2, 29 July 2025, Tuesday**

| HK Time | | Venue |
|---------------|--|-------------------------|
| 8:30 – 9:00 | Registration opens | LT-4 |
| 9:00 - 9:50 | William Benter Distinguished Lecture: Efficient Machine Learning Algorithms Inspired by Pure Math <i>Prof. Zhihong Jeff Xia, Great Bay University, Northwestern University</i> | LT-4 |
| 9:50 – 10:10 | Coffee Break & Poster Session | Y4502 |
| 10:10 – 10:40 | Exploring the Crossroads of Machine Learning and Quantum Dynamics <i>Prof. Yu Cao, Shanghai Jiao Tong University</i> | LT-4 |
| 10:40 - 11:10 | Reward-Directed Score-Based Diffusion Models via q-Learning <i>Prof. Xuefeng Gao, Chinese University of Hong Kong</i> | LT-4 |
| 11:10 - 11:40 | General reactive machine learning potentials for CHON elements <i>Prof. Tong Zhu, East China Normal University</i> | |
| 11:40 – 12:10 | Consensus-based optimization methods with adaptive momentum estimation <i>Prof. Jingrun Chen, University of Science and Technology of China</i> | |
| 12:10 – 14:00 | Lunch Break | |
| 14:00 – 14:30 | Flow based generative models for medical image synthesis <i>Prof. Xiaoqun Zhang, Shanghai Jiao Tong University</i> | LT-4 |
| 14:30 – 15:00 | A Bidirectional DeepParticle Method for Efficiently Solving Low-dimensional Transport Map Problems <i>Prof. Zhiwen Zhang, The University of Hong Kong</i> | LT-4 |
| 15:00 - 15:30 | Recent Advances in Solving Imaging Inverse Problems using Diffusion Models <i>Prof. Zhaoqiang Liu, University of Electronic Science and Technology of China</i> | LT-4 |
| 15:30 - 16:00 | Minimax Optimal Rates for Distribution Regression <i>Prof. Rong Tang, Hong Kong University of Science and Technology</i> | |
| 16:00 - 16:30 | Coffee Break & Poster Session | Y4502 |
| 16:30 – 17:00 | Multimodal LLM for Protein Design <i>Prof. Yuguang Wang, Shanghai Jiao Tong University</i> | LT-4 |
| 17:00 – 17:30 | Towards AI Virtual Cell Through Dynamical Generative Modeling of Single-cell Omics Data <i>Prof. Peijie Zhou, Peking University, China</i> | LT-4 |
| 17:30 - 18:00 | Towards understanding the representation learning of diffusion models <i>Prof. Difan Zou, The University of Hong Kong</i> | LT-4 |
| 18:30 | Banquet (by Invitation Only) | City Chinese Restaurant |

**Workshop on Foundation and Future of Generative Models:
Mathematics, Algorithms, and Applications
Day 3, 30 July 2025, Wednesday**

| HK Time | | Venue |
|---------------|---|-------|
| 8:30 – 9:00 | Registration opens | LT-4 |
| 9:00 - 9:50 | Distinguished Lecture: Large Model-Powered Statistical Analysis <i>Prof. Jian Huang, The Hong Kong Polytechnic University</i> | LT-4 |
| 9:50 – 10:10 | Coffee Break & Poster Session | Y4502 |
| 10:10 – 10:40 | QCD matter exploration meets Generative AI <i>Prof. Kai Zhou, The Chinese University of Hong Kong (Shenzhen)</i> | LT-4 |
| 10:40 - 11:10 | Advancing Spatial Intelligence from 3D/4D Representation and Learning Process <i>Prof. Junhui Hou, City University of Hong Kong</i> | LT-4 |
| 11:10 - 11:40 | Physical AI Roadmap <i>Dr. Jia Zeng, Huawei, China</i> | |
| 11:40 – 12:10 | Faster Convergence and Acceleration for Diffusion-Based Generative Models <i>Prof. Gen Li, The Chinese University of Hong Kong</i> | |
| 12:10 – 14:00 | Lunch Break | |
| 14:00 – 14:30 | Evolution of Discriminator and Generator Gradients in GAN Training: From Fitting to Collapse <i>Prof. Weiguo Gao, Fudan University</i> | LT-4 |
| 14:30 – 15:00 | Wasserstein Bounds for generative diffusion models with Gaussian tail targets <i>Prof. Zhongjian Wan, Nanyang Technological University</i> | LT-4 |
| 15:00 - 15:30 | Primal dual splitting methods for minimizing movement schemes with general nonlinear mobility transport distances <i>Prof. Chaozhen Wei, University of Electronic Science and Technology of China</i> | LT-4 |
| 15:30 - 16:00 | HOT: An efficient Halpern accelerating algorithm for optimal transport problems <i>Prof. Yancheng Yuan, Hong Kong Polytechnic University</i> | |
| 16:00 - 16:30 | Coffee Break & Poster Session | Y4502 |
| 16:30 – 17:00 | Balancing Diffusion and Lévy-Based Generative Modeling: A Hybrid Lévy-Diffusion Generative Model <i>Prof. Yuanfei Huang, City University of Hong Kong</i> | LT-4 |
| 17:00 – 17:30 | On Well-posedness of Mean Field Game Master Equations: A Unified Approach <i>Prof. Chenchen Mou, City University of Hong Kong</i> | LT-4 |
| 17:30 - 18:00 | Rethink Deep Learning with Invariance in Data Representation <i>Dr. Shuren Qi, The Chinese University of Hong Kong</i> | LT-4 |

Abstracts

**Workshop: Foundation and Future of Generative
Models: Mathematics, Algorithms, and Applications
2025**

28 July - 30 July, 2025
City University of Hong Kong

Co-organized by
Liu Bie Ju Centre for Mathematical Sciences
Department of Mathematics

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| 3 | Invited Talks | 23 |

1 Plenary Talks

Efficient Machine Learning Algorithms Inspired by Pure Math

ZHIHONG JEFF XIA

Great Bay University, Northwestern University, China

Email: xia@math.northwestern.edu

Abstract: At its core, AI and machine learning algorithms represent our mathematical communication with computers. Current algorithms are the product of iterative trial and error. In our work, we propose novel machine learning algorithms derived from and inspired by pure mathematics. First, our machine learning algorithm based on complex analysis are highly efficient in solving both mathematical and physical problems, surpassing existing Physical Informed Neural Networks (PINNs), for solving Partial Differential Equations (PDEs) and other scientific computations, achieving improvements in both speed and accuracy often by several orders of magnitude. It also shows strong performance in tasks like image recognition and other AI applications. Currently, we are testing our algorithms on Transformers and Large Language Models (LLMs). Initial results are promising. For example, on one task with MiniMind large language model, our algorithm, with only 0.1 billion (0.1B) parameters, achieves results comparable to the current model with 8 billion (8B) parameters—a huge efficiency improvement. However, it remains uncertain whether our algorithm can scale further.

Inspired by dynamical systems theory and Whitney embedding, we also created machine learning algorithms for time series predictions. To understand the essence of AI, we pose a simple question: Given a Sun-Earth-Jupiter three-body system, where we observe the position of Jupiter from Earth every night, and assume we know nothing about Newtonian mechanics, calculus, or universal gravitation, can a machine predict the future motion of Jupiter? The surprising answer is yes—provided there is enough data. We show that, more generally, for any dynamical system on a manifold, enough sequential data from a single, generic observable can fully recover the original system.

Biography: Zhihong Jeff Xia is the Arthur and Gladys Pancoe Professor of Mathematics at Northwestern University, as well as a Chair Professor at Great Bay University. He earned his Ph.D. in Mathematics from Northwest-

ern University in 1988. Professor Xia is renowned for solving the century-old Painleve Conjecture and, in collaboration with Jian Li, for discovering compelling evidence that a rogue planet once invaded our solar system a few hundred million years ago. His outstanding contributions have been recognized with several prestigious awards, including the Sloan Research Fellowship, the US National Young Investigator Award, the Blumenthal Award for the Advancement of Pure Mathematics, and the Monroe Martin Prize for Applied Mathematics.

Large Model-Powered Statistical Analysis

JIAN HUANG

The Hong Kong Polytechnic University, Hong Kong

Email: j.huang@polyu.edu.hk

Abstract: The advent of large-scale machine learning models, including deep neural networks and foundation models, is fundamentally reshaping the field of statistics. In this talk, we will examine how these powerful models can be leveraged to tackle contemporary statistical challenges. Through illustrative examples, including conditional generative learning, functional protein sequence generation, synthetic data augmentation, and code-free data analysis, we will highlight both the opportunities and the challenges that large models introduce to statistics.

Biography: Jian Huang is Chair Professor of Data Science and Analytics in the Departments of Data Science and AI, and Applied Mathematics at The Hong Kong Polytechnic University. He received his Ph.D. in Statistics from the University of Washington, Seattle. His current research interests include deep learning, generative models, representation learning, leveraging large models for statistical analysis, and AI for science. Professor Huang is a Fellow of the American Statistical Association and the Institute of Mathematical Statistics.

2 Tutorial Talks

Generative Modeling with Diffusion Models

JUHO LEE

Kim Jaechul Graduate School of AI, KAIST, South Korea

Email: juholee@kaist.ac.kr

Abstract: This tutorial introduces the fundamental principles behind diffusion-based generative models. Starting from the core mathematical ideas underlying denoising and score-based models, we will explore how these foundations lead to powerful generative modeling techniques. The tutorial will also cover several key advancements in the field, including:

- A simple mathematical framework for diffusion models unifying denoising diffusion models, score-based models, and flow matching.
- Latent diffusion models for scalable and controllable generation.
- Diffusion models for neural samplers.

Biography: Juho Lee is an associate professor at the Kim Jaechul Graduate School of AI at KAIST (Korea Advanced Institute of Science and Technology). His research focuses on Bayesian deep learning, generative models, and meta-learning. Prior to joining KAIST, he was a research scientist at AITRICS, an AI-based healthcare startup. He earned his Ph.D. in Computer Science and Engineering from POSTECH under the supervision of Professor Seungjin Choi, and completed a postdoctoral fellowship in the Computational Statistics & Machine Learning group at the University of Oxford with Professor Francois Caron.

Theory for Deep Generative Learning

JIAO YULING

Department of Artificial Intelligence, Wuhan University

Email: yulingjiaomath@whu.edu.cn

Abstract: Estimating underlying distributions from data is a fundamental task in machine learning. In the first part of this presentation, we will discuss the schemes and theoretical guarantees for various deep generative models,

including GANs, latent space diffusion models, simulation-free continuous normalized flow models, and a newly proposed one-step generator based on ODE flow. In the second part, I will focus on conditional distribution learning for controllable generation and uncertainty quantification.

Biography: Yuling Jiao, Professor and vice dean at the School of Artificial Intelligence, Wuhan University. His main research areas include machine learning and scientific computing. Recently, he has focused on the mathematical foundations of AI, publishing over thirty papers in flagship journals and conferences in fields such as computational mathematics, applied mathematics, statistics, electronic engineering, and artificial intelligence. His publications include: SIAM series, Appl. Comput. Harmon. Anal., Inverse Problems; Ann. Stat., J. Amer. Statist. Assoc.; IEEE Trans. Inf. Theory, IEEE Trans. Signal Process.; J. Mach. Learn. Res., ICML, NeurIPS as well as Nat. Commun..

A Physicist's Perspective on Generative Models

LEI WANG

Institute of Physics, Chinese Academy of Sciences, China

Email: wanglei@iphy.ac.cn

Abstract: I shall present a physicist's perspective to autoregressive and flow-based generative models. I will also mention their scientific applications based on these understandings.

Biography: Lei Wang got his Bachelor's degree from Nanjing University in 2006 and Ph.D. from the Institute of Physics, Chinese Academy of Sciences in 2011. He did postdoctoral research on computational quantum physics at ETH Zurich in the next few years. Lei Wang joined the Institute of Physics in 2016. His research interest is at the cross-section of deep learning and quantum many-body computation.

3 Invited Talks

Exploring the Crossroads of Machine Learning and Quantum Dynamics

YU CAO

Shanghai Jiao Tong University, Shanghai, China

Email: yucaoc@sjtu.edu.cn

Abstract: We could witness that advances in machine learning and quantum dynamics are converging to reveal new capabilities. This talk navigates the crossroads of these two fields. We will discuss a new paradigm of solving quantum machine learning, exploring how quantum algorithm might offer advantages for certain machine learning problems, e.g., some control problems. Simultaneously, we will also discuss how the machine learning could offer a tool for improving the simulation of quantum dynamics, along with a discussion on some open questions. By exploring the relationship – ML empowering quantum dynamical simulation and quantum dynamics reshaping ML – we believe that such a converging picture would play an increasingly more important role in the future.

Biography: I am currently a tenure-track Associate Professor at Institute of Natural Sciences and School of Mathematical Sciences at Shanghai Jiao Tong University (SJTU). I received the bachelor’s degree from City University of Hong Kong in 2015, and later graduated with a Ph.D. from Duke University in 2020. My research interest lies on the dynamical systems arising from e.g., quantum information and machine learning.

Reward-Directed Score-Based Diffusion Models via q-Learning

XUEFENG GAO

Department of Systems Engineering and Engineering Management, Chinese University of Hong Kong, Hong Kong

Email: xfgao@se.cuhk.edu.hk

Abstract: We propose a new reinforcement learning (RL) formulation for training continuous-time score-based diffusion models for generative AI to generate samples that maximize reward functions while keeping the generated distributions close to the unknown target data distributions. Different

from most existing studies, our formulation does not involve any pretrained model for the unknown score functions of the noise-perturbed data distributions. We present an entropy regularized continuous-time RL problem and show that the optimal stochastic policy has a Gaussian distribution with a known covariance matrix. Based on this result, we parameterize the mean of Gaussian policies and develop an actor critic type (little) q-learning algorithm to solve the RL problem. A key ingredient in our algorithm design is to obtain noisy observations from the unknown score function via a ratio estimator. Numerically, we show the effectiveness of our approach by comparing its performance with two state-of-the-art RL methods that fine tune pretrained models. Finally, we discuss extensions of our RL formulation to probability flow ODE implementation of diffusion models and to conditional diffusion models.

Biography: Xuefeng Gao is an Associate Professor at the Department of Systems Engineering and Engineering Management, Chinese University of Hong Kong. His research interests include Stochastic Modelling, Reinforcement Learning, Generative Diffusion Models, and Financial Engineering. He received his B.S. in Mathematics from Peking University, China, and his Ph.D. in Operations Research from Georgia Institute of Technology, USA.

Faster Convergence and Acceleration for Diffusion-Based Generative Models

GEN LI

Department of Statistics, The Chinese University of Hong Kong, Hong Kong

Email: genli@cuhk.edu.hk

Abstract: Diffusion models, which generate new data instances by learning to reverse a Markov diffusion process from noise, have become a cornerstone in contemporary generative modeling. While their practical power has now been widely recognized, theoretical underpinnings for mainstream samplers remain underdeveloped. Moreover, despite the recent surge of interest in accelerating diffusion-based samplers, convergence theory for these acceleration techniques remains limited. In this talk, I will introduce a new suite of non-asymptotic results aimed at better understanding popular samplers like DDPM and DDIM in discrete time, offering significantly improved conver-

gence guarantees over previous work. Our theory accommodates L2-accurate score estimates, and does not require log-concavity or smoothness on the target distribution. Building on these insights, we propose training-free algorithms that provably accelerate diffusion-based samplers, leveraging ideas from higher-order approximation similar to those used in high-order ODE solvers like DPM-Solver.

Biography: Gen Li is currently an assistant professor in the Department of Statistics at the Chinese University of Hong Kong. He received the Ph.D. in the Department of Electronic Engineering at Tsinghua University in 2021, and received the bachelor's degree from the Department of Electronic Engineering and Department of Mathematics at Tsinghua University in 2016. His research interests include diffusion based generative model, reinforcement learning, high-dimensional statistics, machine learning.

Consensus-based Optimization Methods with Adaptive Momentum Estimation

JINGRUN CHEN

School of Mathematical Sciences, University of Science and Technology of China, China

Email: jingrunchen@ustc.edu.cn

Abstract: In this presentation, we will discuss two developments in the framework of consensus-based optimization (CBO) method to solve: 1) high-dimensional nonconvex optimization problem; 2) high-dimensional stochastic control problem, based on the combination of CBO method and Adam, with adaptive momentum estimation (Adam-CBO).

Biography: Jingrun Chen is currently a professor at the School of Mathematical Sciences and the Suzhou Advanced Research Institute at the University of Science and Technology of China, specializing in scientific computing and artificial intelligence.

Flow Based Generative Models for Medical Image Syn-

thesis

XIAOQUN ZHANG

Shanghai Jiao Tong University, China

Email: xqzhang@sjtu.edu.cn

Abstract: This talk explores advancements in flow-based generative models for medical image synthesis, which are crucial for enhancing diagnostics, treatment planning, and data augmentation. Two novel approaches for bi-modality transfer are introduced. First, SyMOT-Flow minimizes discrepancies between distributions using optimal transport, enabling stable and interpretable image generation. Second, Bi-DPM improves efficiency and quality in bi-modality synthesis by avoiding complex ODE solvers and ensuring consistency across discrete time steps. Both methods are validated on MRI and CT datasets, demonstrating superior image quality and anatomical accuracy.

Biography: Xiaoqun Zhang received her Ph.D. degree in applied mathematics from University of South Brittany, France. She currently is a distinguished Professor with Institute of Natural Sciences and School of Mathematics Science, Shanghai Jiao Tong University, China. Her research interest includes data and imaging sciences, machine learning, inverse Problems, and optimization.

A Bidirectional DeepParticle Method for Efficiently Solving Low-dimensional Transport Map Problems

ZHIWEN ZHANG

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Abstract: In this talk, we introduce the Bidirectional DeepParticle (BDP) method, a novel approach for efficiently computing transport maps between probability distributions arising from particle-based simulations of bio-physical systems. The BDP method approximates solutions as empirical measures of adaptive particles that concentrate in high-gradient regions, enabling accurate modeling under varying physical parameters by learning both forward and reverse transport maps (from a uniform reference distribution to a target distribution) through minimizing the discrete 2-Wasserstein (W₂) distance

and optimizing transition maps via a mini-batch technique. We demonstrate the effectiveness of BDP for solving Keller–Segel chemotaxis systems in laminar flows and Kolmogorov flows with chaotic streamlines in 3D space, outperforming traditional single-step flow matching and generative models (e.g., rectified flow and shortcut diffusion models) with compact neural networks.

Biography: Z. Zhang’s research interests lie in scientific computation, with topics including uncertainty quantification (UQ), numerical methods for stochastic differential equations (SDEs) and stochastic partial differential equations (SPDEs), as well as numerical methods for partial differential equations (PDEs) arising from quantum chemistry, wave propagation, multiscale porous media, nonlinear filtering, and stochastic fluid dynamics. Recently, he has also been working on deep learning methods for solving SDEs and PDEs.

Recent Advances in Solving Imaging Inverse Problems using Diffusion Models

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Abstract: Imaging inverse problems involve reconstructing underlying images from noisy observations. Traditional approaches often rely on hand-crafted priors, which can fail to capture the complexity of real-world data. The advent of pre-trained generative models has introduced new paradigms, offering improved reconstructions by learning rich priors from data. Among these, diffusion models have emerged as a powerful framework, achieving remarkable reconstruction performance across numerous imaging inverse problems. In this talk, I will provide an overview of the latest advancements in leveraging diffusion models to address imaging inverse problems, highlighting their technical innovations and practical applications.

Biography: Zhaoqiang Liu serves as a professor at both the School of Computer Science and Engineering and the School of Mathematical Sciences, University of Electronic Science and Technology of China (UESTC). His current research focuses on diffusion models and their applications in solving inverse problems, along with theoretical aspects of large language models.

Previously, he was a postdoctoral researcher at the Department of Computer Science, National University of Singapore (NUS). He earned his Ph.D. in Mathematics from NUS in 2017 and obtained a Bachelor's degree in Mathematical Sciences from Tsinghua University in 2013.

Minimax Optimal Rates for Distribution Regression

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Abstract: Distribution regression seeks to estimate the conditional distribution of a multivariate response given a continuous covariate. This approach offers a more complete characterization of dependence than traditional regression methods. Classical nonparametric techniques often assume that the conditional distribution has a well-defined density, an assumption that fails in many real-world settings. These include cases where data contain discrete elements or lie on complex low-dimensional structures within high-dimensional spaces. In this work, we establish minimax convergence rates for distribution regression under nonparametric assumptions, focusing on scenarios where both covariates and responses lie on low-dimensional manifolds. We derive lower bounds that capture the inherent difficulty of the problem and propose a new hybrid estimator that combines adversarial learning with simultaneous least squares to attain matching upper bounds. Our results reveal how the smoothness of the conditional distribution and the geometry of the underlying manifolds together determine the estimation accuracy.

Biography: Rong Tang is an assistant professor in the Department of Mathematics at the Hong Kong University of Science and Technology (HKUST) since July, 2023. Prior to that, She received her Ph.D. in Statistics from the University of Illinois at Urbana-champaign (UIUC).

Advancing Spatial Intelligence from 3D4D Representa-

tion and Learning Process

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Abstract: 3D spatial intelligence—the ability to perceive, reason about, and manipulate geometric data—is fundamental to advancing AI applications in robotics, AR/VR, and autonomous systems. In this talk, I will showcase our endeavors to push the boundaries of this field, starting with the fundamental representation of 3D geometric data, the development of a cross-modal/structural learning mechanism, to the efficient yet effective loss function. These new perspectives are poised to unlock numerous possibilities.

Biography: Junhui Hou is an Associate Professor with the Department of Computer Science, City University of Hong Kong. His research interests include multi-dimensional visual computing, such as light field, hyperspectral, geometry, and event data. He received the Early Career Award from the Hong Kong Research Grants Council and the Excellent Young Scientists Fund from NSFC. He has served or is serving as an Associate Editor for IEEE TIP, TVCG, TMM, and TCSVT.

Towards AI Virtual Cell Through Dynamical Generative Modeling of Single-cell Omics Data

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Abstract: Reconstructing continuous cellular dynamics from sparse, high-dimensional single-cell omics data remains a fundamental challenge in systems biology. Recently, a paradigm shift has been witnessed by leveraging artificial intelligence—specifically, dynamical generative modeling—to develop an AI virtual cell, a predictive digital twin capable of simulating cellular behavior across time and space. In this talk, we introduce our recent attempts that integrate flow-based generative models with partial differential equations (PDEs) to infer latent dynamics from scRNA-seq data. For spatial transcriptomics data, we extend this method with stVCR, a generative model that aligns transcriptomic snapshots across biological replicates and

temporal stages. To further infer stochastic dynamics from static data, we explore a regularized unbalanced optimal transport (RUOT) formulation and its theoretical connections to the Schrödinger Bridge and diffusion models. I will also introduce a generative deep-learning solver designed for this problem. Together, these works suggest how generative AI could have the potential to unify dynamical modeling, spatial reconstruction, and stochastic inference—transforming fragmented omics data into a predictive virtual cell.

Biography: Peijie Zhou is a tenure-track assistant professor at the Center for Machine Learning Research and the Center for Quantitative Biology, Peking University. He earned his bachelor’s and Ph.D. degrees in computational mathematics from the School of Mathematical Sciences at Peking University in 2014 and 2019, respectively, under the supervision of Professor Tiejun Li. From 2020 to 2023, he served as a Visiting Assistant Professor in the Department of Mathematics at the University of California, Irvine, working with Professor Qing Nie. His research focuses on computational systems biology, particularly modeling and computation of complex biological systems driven by single-cell data and AI methodologies. His work has been published in interdisciplinary journals such as Nature Methods, Nature Climate Change, Nature Communications, Nature Machine Intelligence, Nature Genetics, Physical Review X, and Molecular Systems Biology. He also serves as a reviewer for journals including Nature Methods, PNAS, and Nature Communications.

Towards understanding the representation learning of diffusion models.

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Abstract: Diffusion models (DMs) excel in generative modeling, but their theoretical foundations and limitations remain underexplored. This talk addresses two key aspects: their feature learning dynamics and their ability to capture hidden inter-feature rules. First, I show that the denoising objective encourages DMs to learn balanced and comprehensive data representations, unlike classification models that prioritize easy-to-learn patterns. Theoretical analysis and experiments on synthetic and real-world datasets highlight

this distinction. Next, I explore a critical limitation: DMs often fail to learn fine-grained hidden rules between dependent features, such as the relationship between the height of the sun and shadow length in images. Empirical evaluations on models like Stable Diffusion reveal consistent failures, supported by synthetic tasks and theoretical insights showing that denoising score matching (DSM) is incompatible with enforcing rule conformity. I discuss potential solutions, such as classifier-guided sampling, and their limitations. This talk provides a deeper understanding of DMs' strengths and weaknesses, offering insights for building more robust and interpretable generative models.

Biography: Dr. Difan Zou is an assistant professor in computer science department and institute of data science at HKU. He has received his PhD degree in Department of Computer Science, University of California, Los Angeles (UCLA). His research interests are broadly in machine learning, deep learning theory, graph learning, mechanism interpretation, and interdisciplinary research between AI and other subjects. His research is published in top-tier machine learning conferences (ICML, NeurIPS, COLT, ICLR) and journal papers (IEEE Trans., JMLR, Nature Comm., PNAS, etc.). He serves as an area chair/senior PC member for NeurIPS, ICML and AAI, and PC members for ICLR, COLT, etc.

QCD matter exploration meets Generative AI

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Abstract: In this talk I will present some of the applications of generative AI models in exploring physics, including those towards QCD matter under extreme conditions. Several modern generative models, including GAN, autoregressive model, normalizing flow model and diffusion model will be covered for their physics application, especially in the context of lattice field theory configuration generation. I will introduce Fourier flow model for curing mode collapse in quantum anharmonic oscillator as demonstration. The connection between diffusion model and stochastic quantization in the context of lattice field theory will be explained. I will also mention the application of diffusion model in the form of point cloud to construct fast emulator for heavy ion collision simulation, which may promise the Bayesian inference

for physics from these complicated physical processes.

Biography: Dr. Kai Zhou received his B.Sc. degree in Physics from Xi’an Jiaotong University in 2009, and his PhD degree in Physics from Tsinghua University in 2014. After that, he worked as a Postdoctoral researcher in the Institute for Theoretical Physics (ITP) at Goethe University Frankfurt in Germany from 2014 to 2017. Since 2017 he started as a Research Fellow (W1 professor status) and Group Leader at the Frankfurt Institute for Advanced Studies (FIAS), leading the AI for Science group “Deepthinkers”, focusing on physics studies with modern computational paradigms Machine- and Deep-Learning, supervises Master/PhD students and Postdocs in AI for Science. He was then promoted to Fellow (W2 professor status) at FIAS from 2022. Since the end of 2023 he joined CUHK-Shenzhen as an Assistant Professor at SSE.

Dr. Zhou has broad interests in AI for Science, including high energy nuclear physics, statistical physics, energy, application oriented and other diverse fields. He remains committed to pushing the boundaries of physics and modern computational paradigms, especially machine learning, to provide new pathways and insights in exploring the physical world while also shaping the future of technological advances in computations with inspiration from physics knowledge.

Multimodal LLM for Protein Design

YUGUANG WANG

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Abstract: We introduce TourSynbio, a multimodal protein foundation model through which users can converse in natural language to interpret, design, recommend and generate reports on proteins. This 32-billion-parameter foundation model fuses biological knowledge with evolutionary theory and assembles multiple AI modules into a cohesive protein-design agent. Already deployed in partnerships with pharmaceutical and synthetic-biology companies, it has demonstrated marked success. TourSynbio also powers a full downstream ecosystem: its core TourSynbio-Agent automatically plans and orchestrates across models, while three tightly integrated modules provide end-to-end capability:

1. TourSynbio-Search (“the Perplexity AI of protein design”) gathers data and domain knowledge.
2. TourSynbio-GraDeIF (“the MidJourney of protein design”) generates novel sequences.
3. TourSynbio-AutoProteinEngine (“the Cursor of protein design”) trains, optimizes and validates models.

Together, they form a complete solution that significantly enhances both the efficiency and success rate of protein engineering.

Biography: Dr. Yuguang Wang is currently an Associate Professor at Shanghai Jiao Tong University, Co-Director of the Chongqing AI Research Institute at SJTU, and Founder of Toursun Synbio. He also holds adjunct appointments at Shanghai AI Laboratory and the University of New South Wales. Previously, he was a Research Scientist at the Max Planck Institute. He received his Ph.D. in Mathematics from the University of New South Wales in 2015. Dr. Wang has published over 80 papers in top journals and conferences in the field of scientific intelligence, with three selected as highlight papers at major AI conferences. In 2024, he released China’s first protein foundation model, TourSynbio, and received the 2025 Mega Engineer Award.

Physical AI Roadmap

ZENG JIA

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Abstract: What is Physical AI Roadmap? In this talk, we will briefly discuss the five levels roadmap of Physical AI.

Biography: Dr Zeng is an expert in “AI workload, optimization and compute” area. From 2013 to 2023, he was with Huawei Noah’s Ark Lab for strategic planning in AI foundation models, universal problem solver and embodied AI. He obtained Bachelor of Engineering from Wuhan University of Technology in 2003, and obtained PhD from City University of Hong Kong in 2007. He published several academic papers in AI top tier conferences and journals.

General reactive machine learning potentials for CHON elements

TONG ZHU

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Abstract: Accurate and efficient modeling of chemical reactions is vital for catalysis, materials design, and molecular simulations. Machine learning potentials (MLPs) provide a computationally efficient alternative to ab initio methods, but constructing broadly applicable reactive MLPs remains challenging due to chemical complexity. We present a scalable workflow for developing reactive MLPs tailored to C, H, O, and N systems. Using the Transition1x and RGD-1 datasets, we created the RXN-xTB dataset with over 17 million non-equilibrium structures. Through iterative active learning, about 19.9k representative structures were selected and refined using high-level quantum calculations at the ω B97X-D/def2-TZVP level, ensuring comprehensive chemical coverage. We evaluated multiple training strategies, including pretraining with finetuning and Δ -learning, demonstrating complementary strengths across tasks such as energy and force prediction, reaction barrier estimation, geometry optimization, and molecular dynamics. Incorporating DeePHF-based relabeling and multi-task learning further improved accuracy. Our best model achieved a mean absolute error of 0.97 kcal/mol in reaction energy prediction, matching CCSD(T)-F12/cc-pVDZ-F12 benchmarks. The resulting MLPs are robust and transferable, maintaining accuracy even in out-of-distribution chemical spaces. This work offers a practical, data-efficient framework for building high-accuracy reactive MLPs, enabling reliable simulations across diverse molecular systems.

Biography: Prof. Zhu is a full professor at East China Normal University and Shanghai Innovation Institute. His primary research focus is on the chemical reaction dynamics of complex systems. In recent years, he has developed a series of methods for constructing chemical reaction networks in gas-phase systems by combining machine learning and physical models. He has published more than 70 papers in journals such as Nature Machine Intelligence, Nature Communications, Advanced Science, and JACS Au, with over 1,000 citations.

Evolution of Discriminator and Generator Gradients in GAN Training: From Fitting to Collapse

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Abstract: Generative Adversarial Networks (GANs) are powerful generative models but often suffer from mode mixture and mode collapse. We propose a perspective that views GAN training as a two-phase progression from fitting to collapse, where mode mixture and mode collapse are treated as inter-connected. Inspired by the particle model interpretation of GANs, we leverage the discriminator gradient to analyze particle movement and the generator gradient, specifically “steepness,” to quantify the severity of mode mixture by measuring the generator’s sensitivity to changes in the latent space. Using these theoretical insights into evolution of gradients, we design a specialized metric that integrates both gradients to detect the transition from fitting to collapse. This metric forms the basis of an early stopping algorithm, which stops training at a point that retains sample quality and diversity. Experiments on synthetic and real-world datasets, including MNIST, Fashion MNIST, and CIFAR-10, validate our theoretical findings and demonstrate the effectiveness of the proposed algorithm. This is joint work with Ming Li.

Biography: Weiguo GAO is a full professor within the School of Data Science & School of Mathematical Sciences at Fudan University. His research interests cover a wide range of topics within machine learning, optimization and applied mathematics.

Wasserstein Bounds for Generative Diffusion Models with Gaussian Tail Targets

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Abstract: We present an estimate of the Wasserstein distance between the data distribution and the generation of score-based generative models. The sampling complexity (NFEs) with respect to dimension is $\mathcal{O}(d)$, with a log-

arithmetic constant. In the analysis, we assume a Gaussian-type tail behavior of the data distribution and an ϵ -accurate approximation of the score. Such Gaussian tail assumption is general. It can be derived from the bounded support distributions with early stopping techniques. The crux of the analysis lies in the global Lipschitz bound of the score, which is shown from the Gaussian tail assumption by a dimension independent estimate of the heat kernel. Consequently, our complexity bound scales linearly (up to a logarithmic constant) with the square root of the trace of the covariance operator, which relates to the invariant distribution of forward process. Our analysis also extends to the probabilistic flow ODE, as the sampling process.

Biography: Zhongjian is currently an assistant professor in the Division of Mathematical Sciences at Nanyang Technological University. Prior to that, he was a William H. Kruskal Instructor in the Committee on Computational and Applied Math, Department of Statistics, at the University of Chicago. He got his Ph.D. in mathematics from the University of Hong Kong under the supervision of Dr. Zhiwen Zhang. His research interests lie broadly in the computational methods and numerical analysis in the fields of applied math, physics and engineering.

Primal dual splitting methods for minimizing movement schemes with general nonlinear mobility transport distances

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Abstract: 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.

Biography: Chaozhen Wei is currently a "Hundred Talents Program" researcher from University of Electronic Science and Technology of China. He graduated from Sichuan University with a bachelor's degree and obtained his Ph.D. from the University at Buffalo, State University of New York. He has served as a postdoctoral scholar at the Hong Kong Jockey Club Institute for Advanced Study of the Hong Kong University of Science and Technology and Worcester Polytechnic Institute in the United States. His research focuses on the intersection of mathematics and materials science, specifically on multi-scale computable modeling and efficient algorithms for thin film materials, crystal defects, and interface problems related to biological tissues. Currently, he is the principal investigator of one National Natural Science Foundation of China general project and a participant in one key project.

HOT: An Efficient Halpern Accelerating Algorithm for Optimal Transport Problems

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Abstract: This talk introduces HOT, an efficient Halpern accelerating algorithm for solving the optimal transport (OT) problems with finite supports in \mathbb{R}^n , where the involved linear systems in the HOT algorithm can be efficiently solved in linear time complexity. Consequently, we can obtain an ε -approximate solution (in terms of the Karush-Kuhn-Tucker (KKT) residual) to the OT problem with M supports in $O(M^2/\varepsilon)$ flops, which improves the best-known computational complexity for the OT problem. For a class of important OT problems where the supports are in \mathbb{R}^2 with ground distances calculated by L_2^2 -norm, we prove that HOT can obtain an ε -approximate solution (in terms of the KKT residual) to the OT problem with M supports in $O(M^{1.5}/\varepsilon)$ flops by solving an equivalent reduced model of the discrete OT problem. We further propose an efficient procedure to recover an optimal

transport plan for the original OT problem based on a solution to the reduced model, thereby overcoming the limitations of the reduced OT model in applications that require the transport plan. We implement the HOT algorithm in PyTorch and numerical results show the superior performance of the HOT algorithm compared to existing state-of-the-art algorithms for solving the OT problems. This talk is based on the joint works with Guojun Zhang, Zhexuan Gu, and Defeng Sun from The Hong Kong Polytechnic University.

Biography: Yancheng Yuan is an Assistant Professor at the Department of Applied Mathematics, The Hong Kong Polytechnic University. His research focuses on continuous optimization, the mathematical foundation of data science, and data-driven applications. His research has been published in prestigious academic journals and conferences, including *SIAM Journal on Optimization*, *Mathematical Programming Computation*, *Journal of the American Statistical Association*, *Journal of Machine Learning Research*, *IEEE Transactions on Pattern Analysis and Machine Intelligence*, *NeurIPS*, *ICML*, *ICLR*, *ICCV*, *ACM WWW*, *ACM SIGIR*. His papers have been selected in Best Paper Award Finalist of *ACM WWW 2021* and *ACM SIGIR 2024*.

Balancing Diffusion and Lévy-Based Generative Modeling: A Hybrid Lévy-Diffusion Generative Model

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Abstract: This report explores the mathematical foundations of generative models based on stochastic processes, focusing on two primary frameworks: diffusion-based generative modeling and Lévy process-based generative modeling. While diffusion generative models have demonstrated remarkable success, they are prone to mode-collapse issues, particularly when handling imbalanced data. To address these limitations, Lévy generative modeling has emerged as a more diverse alternative. However, despite its enhanced diversity, training Lévy scores is computationally expensive, and the nonlocal operator inherent to Lévy processes introduces significant complexity, making it challenging

to derive invariant measures and obtain their samples. To strike a balance between the strengths and challenges of these two approaches, we propose the **Hybrid Lévy-Diffusion Model (HLDM)**, which combines the advantages of diffusion and Lévy generative models. In HLDM, the diffusion process is employed as the forward procedure to generate training data, simplifying computation due to the explicit availability of transition densities. For the reverse generative procedure, instead of directly using the reverse process, HLDM constructs a jump process whose probability flow matches the original reverse process exactly. This approach requires training the Lévy score, but its analytical expression, derived from known densities, significantly reduces complexity.

Biography: Yuanfei Huang received his Ph.D. degree from Huazhong University of Science and Technology in 2021 under the supervision of Professor Jinqiao Duan. His doctoral research focused on the analysis of transitions between metastable states in Gaussian and non-Gaussian stochastic dynamical systems. In February 2022, he joined Professor Adrian Rollin's team at the School of Data Science and Statistics, National University of Singapore, as a Research Fellow. During this period, his research concentrated on analyzing epidemic processes on dynamic random graphs. In August 2023, Dr. Huang became a Postdoctoral Researcher in Professor Xiang Zhou's group at City University of Hong Kong. His research topics include the Onsager-Machlup functional for non-Gaussian systems, entropy production in non-Gaussian active thermodynamic systems and its machine-learning-based computational methods, non-Gaussian transition path theory, and the study of generative models. Dr. Huang has published multiple papers in prestigious international journals, such as *SIAM Journal on Applied Mathematics* and *Nonlinearity*.

On Well-posedness of Mean Field Game Master Equations: A Unified Approach

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Abstract: It is well known that the global (in time) well-posedness of mean field game master equations relies on certain monotonicity conditions, and there have been several types of conditions proposed in the literature. In this

talk we intend to provide a unified understanding on the role of monotonicity conditions in the theory. Inspired by Lyapunov functions for dynamical systems, we propose a general type of monotonicity condition, which covers all the existing ones as special cases and is essentially necessary for the existence of Lipschitz continuous classical solutions. Our approach works for very general mean field games, including extended mean field games and mean field games with volatility control. In particular, for the latter a new notion of second order monotonicity condition is required. The talk is based on some ongoing joint works with Jianfeng Zhang and Jianjun Zhou.

Biography: Prof. Chenchen Mou received his bachelor's degree in math, actuarial science and risk management, from Jilin University, China, in 2009. He received master's degree in mathematics from Jilin University, China, in 2011. He received his PhD in mathematics from Georgia Institute of Technology, USA, in 2016. Before joining City University of Hong Kong in 2020, he worked as an assistant adjunct professor at UCLA.

Rethink Deep Learning with Invariance in Data Representation

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Abstract: 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.

Biography: Dr. Shuren Qi is currently a Postdoctoral Fellow with Department of Mathematics, The Chinese University of Hong Kong. His research focuses on robust and explainable representations in 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/>.

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