

# THE INTERNATIONAL CONFERENCE ON NEW TRENDS IN COMPUTATIONAL AND DATA SCIENCES

26-27 August 2023

in Honour of Professor Tonv Fan-cheona Chan's 70th

26 August at the Hong Kong University of Science and Technology (HKUST)



27 August at the Chinese University of Hong Kong (CUHK)

### **SPONSORS**

Department of Mathematics, HKUST Department of Mathematics, CUHK Hong Kong Society of Industrial and Applied Mathematics (HKSIAM)



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## BACKGROUND

With the rapid developments in technology, Computational and Data Science has played an ever increasingly important and unprecedented role in many scientific disciplines, with profound applications within nearly every applied discipline such as engineering, physics, biology, finance and more recently also imaging sciences, data sciences, and so on, often with transformative impacts. There has been a dramatic rise in the need for Computational and Data Science in Hong Kong.



The main objective of this conference is to bring together leading researchers, research students, as well as practitioners with interest in the core components of the community, including the theoretical, computational, and practical aspects in scientific computing, optimization, image processing, and data science. One of the aims of the conference is to promote data science in Hong Kong by providing a forum for participants to exchange ideas and discuss their latest research developments. This conference will cover recent progress, stimulate new ideas, and facilitate interdisciplinary collaborations. It will emphasize the crucial and unique role of mathematical insights in advanced algorithm design and novel real-world applications.

## **INVITED SPEAKERS**

Xavier Bresson, National University of Singapore Jianfeng Cai, The Hong Kong University of Science and Technology Zhiming Chen, Chinese Academy of Sciences Eric Chung, The Chinese University of Hong Kong Xianfeng Gu, Stony Brook University Shi Jin, Shanghai Jiao Tong University Sung Ha Kang, Georgia Institute of Technology Wen-wei Lin, Nanjing Center for Applied Mathematics Michael Ng, The University of Hong Kong Zuowei Shen, National University of Singapore Xue-cheng Tai, Norwegian Research Center Chi Keung Tang, The Hong Kong University of Science and Technology Gunther Uhlmann, The Hong Kong University of Science and Technology Yuan Yao, The Hong Kong University of Science and Technology Xiaoqun Zhang, Shanghai Jiao Tong University

## SCHEDULE AT A GLANCE



### Day 1 (August 26, 2023) at **HKUST**

Venue: Kaisa Group Lecture Theater (IAS LT), Lo Ka Chung Building, Lee Shau Kee Campus

9:15am-9:20am	Welcoming Remark
9:20am-10:00am	Gunther Uhlmann, The Hong Kong University of Science and Technology
10:00am-10:40am	Zhiming Chen, Chinese Academy of Sciences
10:40am-11:10am	Coffee Break
11:10am-11:50am	Michael Ng, The University of Hong Kong
12:00pm-2:00pm	Lunch* (China Garden Restaurant, G/F)
2:00pm-2:40pm	Xue-cheng Tai, Norwegian Research Center
2:40pm-3:20pm	Wen-wei Lin, Nanjing Center for Applied Mathematics
3:20pm-3:50pm	Coffee Break
3:50pm-4:30pm	Chi Keung Tang, The Hong Kong University of Science and Technology
4:30pm-5:10pm	Xavier Bresson, National University of Singapore
5:15pm-5:30pm	Group Photo
6:00pm	Banquet <sup>*</sup> (UniQue, Conference Lodge, HKUST)

### Day 2 (August 27, 2023) at **CUHK**

Venue: LT4, Yasumoto International Academic Park (YIA)

9:15am-9:55am	Shi Jin, Shanghai Jiao Tong University
9:55am-10:35am	Zuowei Shen, National University of Singapore
10:35am-11:05am	Coffee Break
11:05am-11:45am	Sung Ha Kang, Georgia Institute of Technology
12:00pm-2:00pm	Lunch* (Chung Chi College Staff Club)
2:00pm-2:40pm	Xianfeng Gu, Stony Brook University
2:40pm-3:20pm	Yuan Yao, The Hong Kong University of Science and Technology
3:20pm-4:00pm	Xiaoqun Zhang, Shanghai Jiao Tong University
4:00pm-4:30pm	Coffee Break
4:30pm-5:10pm	Jianfeng Cai, The Hong Kong University of Science and Technology
5:10pm-5:50pm	Eric Chung, The Chinese University of Hong Kong
6:00pm	Dinner#

\* For invited speakers and invited guests only

# For invited guests only

## TITLE AND ABSTRACT

### Gunther Uhlmann: Nonlinearity Helps for Inverse Problems

We show how the nonlinearity for several partial differential equations helps to solve several inverse problems associated with nonlinear equations which is not known for the corresponding linearized equations. We illustrate this for several examples including nonlinear elasticity and nonlinear acoustics.

### Zhiming Chen: Arbitrarily High-Order Space and Time Discretization for The Wave Equation on Arbitrarily Shaped Domains with Automatic Mesh Generation

We propose novel high-order space discretization methods for the acoustic wave equation with discontinuous coefficients. The space discretization is based on the unfitted finite element method which allows us to treat problems with complex interface geometry on Cartesian meshes. The strong stability and optimal error estimates of the semi-discrete problem are established based on a new unfitted finite element space without using the interface penalty. Efficient arbitrarily high-order algorithms are developed to solve the ODE systems resulting from the space discretization by the unfitted finite element methods. Numerical examples confirm our theoretical results. This talk is based on joint works with Yong Liu.

### Michael Ng: Quaternion Matrices and Imaging Science

In this talk, I discuss some recent results about quaternion matrices and their applications to imaging science. Theoretical results, mathematical models and numerical examples are provided.

## Xuecheng Tai: PottsMGNet: A Mathematical Explanation of Encoder-Decoder Based Neural Networks

For problems in image processing and many other fields, a large class of effective neural networks have encoderdecoder-based architectures. Although these networks have made impressive performances, mathematical explanations of their architectures are still underdeveloped. In this paper, we study the encoder-decoder-based network architecture from the algorithmic perspective and provide a mathematical explanation. We use the two-phase Potts model for image segmentation as an example for our explanations. We associate the segmentation problem with a control problem in the continuous setting. Then, multi-grid method and operator splitting scheme, the PottsMGNet, are used to discretize the continuous control model. We show that the resulting discrete PottsMGNet is equivalent to an encoder-decoder-based network. With minor modifications, it is shown that a number of the popular encoder-decoder-based neural networks are just instances of the proposed PottsMGNet. By incorporating the Soft-Threshold-Dynamics into the PottsMGNet as a regularizer, the PottsMGNet has shown to be robust with the network parameters such as network width and depth and achieved remarkable performance on datasets with very large noise. In nearly all our experiments, the new network always performs better or as well on accuracy and dice than existing networks for image segmentation. This talk is based on a joint work with Raymond Chan and Hao Liu.

### Wen-wei Lin: Volumetric Stretch Energy Minimization and its Associated Optimal Mass Transport with Applications

Volumetric stretch energy has been widely applied to the computation of volume-/mass-preserving parameterizations of simply connected tetrahedral mesh models M. However, this approach still lacks theoretical support. In this talk, we provide a theoretical foundation for volumetric stretch energy minimization (VSEM) to show that a map is a precise volume-/mass-preserving parameterization from M to a region of a specified shape if and only if its volumetric stretch energy reaches 3|M|/2, where |M| is the total mass of M. We use VSEM to compute an  $\varepsilon$ -volume-/mass-preserving map f\* from M to a unit ball, where  $\varepsilon$  is the gap between the energy of f\* and 3|M|/2. In addition, we prove the efficiency of the VSEM algorithm with guaranteed asymptotic R-linear convergence. Furthermore, based on the VSEM algorithm, we propose a projected gradient method for the computation of the  $\varepsilon$ -volume-/mass-preserving optimal mass transport map with a guaranteed convergence rate of O(1/m) and combined with Nesterov-based acceleration, the guaranteed convergence rate becomes  $O(1/m^2)$ . Numerical experiments are presented to justify the theoretical convergence behavior for various examples drawn from known benchmark models. Moreover, these numerical experiments show the effectiveness of the proposed algorithm, particularly in the processing of 3D medical MRI brain images.

### Chi-keung Tang: Toward Visual Object Recognition in the Open World

Recent advances in computer vision have focused on few-shot learning when only a few exemplars are given for recognizing objects in novel classes unseen during training. In this talk, we will present contemporary works of few-shot learning in image/video object detection (CVPR'20, ECCV'22), semantic Segmentation (ECCV'22), partially-supervised instance segmentation (ECCV'20), co-salient object detection (CVPR'21, PAMI'23) with extension to domain generalization (ICLR'23).

### Xavier Bresson: A Generalization of Transformers to Graphs

Graph Neural Networks (GNNs) have shown great potential in the field of graph representation learning. Standard GNNs define a local message-passing mechanism which propagates information over the whole graph domain by stacking multiple layers. This paradigm suffers from two major limitations, over-squashing and poor long-range dependencies, that can be solved using global attention but significantly increases the computational cost to quadratic complexity. In this work, we propose an alternative approach to overcome these structural limitations by leveraging the ViT/MLP-Mixer architectures introduced in computer vision. We introduce a new class of GNNs, called Graph MLP-Mixer, that holds three key properties. First, they capture long-range dependency as demonstrated on the long-range LRGB datasets and mitigate the over-squashing issue on the TreeNeighbour dataset. Second, they offer memory and speed efficiency, surpassing related techniques. Third, they show high expressivity in terms of graph isomorphism as they can distinguish at least 3-WL isomorphic graphs. As a result, this novel architecture provides significantly better results over standard message-passing GNNs for molecular datasets.

### Shi Jin: Quantum Computation of Partial Differential Equations

Quantum computers have the potential to gain algebraic and even up to exponential speed up compared with its classical counterparts, and can lead to technology revolution in the 21st century. Since quantum computers are designed based on quantum mechanics principle, they are most suitable to solve the Schrodinger equation, and linear PDEs (and ODEs) evolved by unitary operators. The most efficient quantum PDE solver is quantum simulation based on solving the Schrodinger equation. It became challenging for general PDEs, more so for nonlinear ones. We will first give a short "mathematician's survival kit" on quantum computing, then discuss three topics: (1) We introduce the "warped phase transform" to map general linear PDEs and ODEs to Schrodinger equation or with unitary evolution operators in higher dimension so they are suitable for quantum simulation; (2) For (nonlinear) Hamilton-Jacobi equation and scalar nonlinear hyperbolic equations we use the level set method to map them-exactly-to phase space linear PDEs so they can be implemented with quantum algorithms and we gain quantum advantages for various physical and numerical parameters. (3) For PDEs with uncertain coefficients, we introduce a transformation so the uncertainty only appears in the initial data, allowing us to compute ensemble averages with multiple initial data with just one run, instead of multiple runs as in Monte-Carlo or stochastic collocation type sampling algorithms. Finally, we will give some open problems.

### Zuowei Shen: Mathematics in Data Science

We currently live in the age of big data, where discovering, interpreting, learning, and utilizing the information, knowledge, and resources hidden in data can greatly benefit humanity and improve our daily lives. However, the vast amount of data we collect is incredibly complex, and our expectations of what we can achieve with it are high. As a result, this presents numerous challenges and opportunities for various fields, particularly in the realm of mathematical science. In this presentation, we will highlight specific examples, particularly in image and video processing, to demonstrate how mathematics has played a crucial role in the era of big data. Additionally, we will show how mathematics can push the boundaries of data science and explore the challenges that mathematicians face in this era of big data.

#### Sung Ha Kang: Variational Image Processing: Total Variation, Segmentation and Clustering

This talk will review variational image processing problems starting from color total variation and unsupervised image segmentation. Starting from Tony Chan's contribution to image processing, some extensions will be introduced, including regularized k-means and parallel adaptive clustering and its application to streaming data.

#### Xianfeng Gu: A Geometric Understanding of Generative Model in Deep Learning

Deep learning (DL) has achieved great successes, but understanding of DL remains primitive. In this talk, we try to answer some fundamental questions about DL through a geometric perspective: what does a DL system really learn? How does the system learn? Does it really learn or just memorize the training data sets? How to improve the learning process? Natural datasets have intrinsic patterns, which can be summarized as the manifold distribution principle: the distribution of a class of data is close to a low-dimensional manifold. DL systems mainly accomplish two tasks: manifold learning and probability distribution transformation. The latter can be carried out based on optimal transportation (OT) theory. This work introduces a geometric view of optimal transportation, which bridges statistics and differential geometry and is applied for generative adversarial networks (GANs) and diffusion models. From the OT perspective, in a GAN model, the generator computes the OT map, while the discriminator computes the Wasserstein distance between the real data distribution and the counterfeit; both can be reduced to a convex geometric optimization process. The diffusion model computes a transportation map from the data distribution to the Gaussian distribution by a heat diffusion, and focuses on the inverse flow. Furthermore, the regularity theory of the Monge-Ampere equation discovers the fundamental reason for mode collapse. In order to eliminate the mode collapses, a novel generative model based on the geometric OT theory is proposed, which improves the theoretical rigor and interpretability, as well as the computational stability and efficiency. The experimental results validate our hypothesis, and demonstrate the advantages of our proposed model.

#### Yuan Yao: Robust Statistical Learning and Generative Adversarial Networks

Robust learning under Huber's contamination model has become an important topic in statistics and theoretical computer science. Statistically optimal procedures such as Tukey's median and other estimators based on depth functions are impractical because of their computational intractability. In this talk, we present an intriguing connection between f-GANs and various depth functions through the lens of f-Learning. Similar to the derivation of f-GANs, we show that these depth functions that lead to statistically optimal robust estimators can all be viewed as variational lower bounds of the total variation distance in the framework of f-Learning. This connection opens the door of computing robust estimators using tools developed for training GANs. In particular, we show in both theory and experiments that some appropriate structures of discriminator networks with hidden layers in GANs lead to statistically optimal robust location estimators for both Gaussian distribution and general elliptical distributions where first moment may not exist. Some applications are discussed on financial data analysis and robust denoising of Cryo-EM images.

### Xiaoqun Zhang: On the Convergence of Continuous and Discrete Unbalanced Optimal Transport Models For 1-Wasserstein Distance

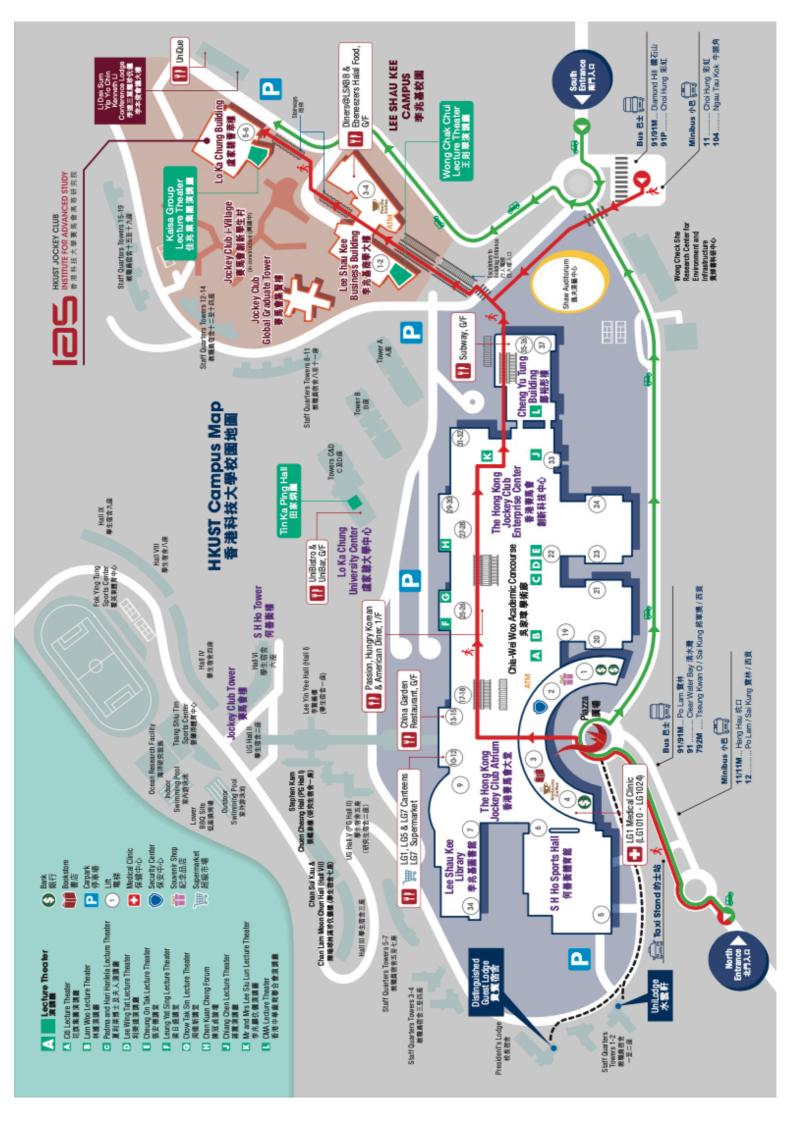
We consider a Beckmann formulation of an unbalanced optimal transport (UOT) problem. The  $\gamma$ -convergence of this formulation of UOT to the corresponding optimal transport (OT) problem is established as the balancing parameter  $\alpha$  goes to infinity. The discretization of the problem is further shown to be asymptotic preserving regarding the same limit, which ensures that a numerical method can be applied uniformly and the solutions converge to the one of the OT problem automatically. Particularly, there exists a critical value, which is independent of the mesh size, such that the discrete problem reduces to the discrete OT problem for  $\alpha$  being larger than this critical value. The discrete problem is solved by a convergent primal-dual hybrid algorithm and the iterates for UOT are also shown to converge to that for OT. Finally, numerical experiments on shape deformation and partial color transfer are implemented to validate the theoretical convergence and the proposed numerical algorithm.

### Jianfeng Cai: A Unified Framework for Non-Convex Low-Rank Matrix Recovery Problems

The challenge of recovering low-rank matrices from linear samples is a common issue in various fields, including machine learning, imaging, signal processing, and computer vision. Non-convex algorithms have proven to be highly effective and efficient for low-rank matrix recovery, providing theoretical guarantees despite the potential for local minima. This talk presents a unifying framework for non-convex low-rank matrix recovery algorithms using Riemannian gradient descent. We demonstrate that numerous well-known non-convex low-rank matrix recovery algorithms can be considered special instances of Riemannian gradient descent, employing distinct Riemannian metrics and retraction operators. Consequently, we can pinpoint the optimal metrics and develop the most efficient non-convex algorithms. To illustrate this, we introduce a new preconditioned Riemannian gradient descent algorithm, which accelerates matrix completion tasks by more than ten times compared to traditional methods.

#### Eric Chung: Computational Multiscale Methods and Applications

Many practical problems, especially those arising from geosciences, have multiscale features due to medium heterogeneities, nonlinearity and coupling of multiple models. The goal of multiscale methods or numerical upscaling techniques is to compute the solutions of these complicated problems efficiently by constructing coarse scale equations for some dominant components of the solutions. In this talk, we will present the latest development of a class of multiscale methods, which make use of solutions of local problems to obtain coarse scale equations and have rigorous convergence theories. For nonlinear problems, the macroscopic parameters in the coarse scale equations can be computed efficiently by the use of deep learning techniques. We will discuss the general concepts and present some applications.



### 香港中文大學校園地圖 CUHK Campus Map

指示 Guide:

前往康本國際學術園:

從港鐵大學站 A 出口離開,沿車站路往上走,康本國際學術園將在你的左方。

#### Going to Yasumoto International Academic Park,:

Leave at Exit A of University Station, go through the Station Road, Yasumoto International Academic Park will be on you left hand side.

