

# **Workshop on Graph Theory, Optimization and Scientific Computing**

2023.12.29-2024.1.1

The Hong Kong Polytechnic University

# Preface

Welcome to Workshop on Graph Theory, Optimization and Scientific Computing, as organized by the Department of Applied Mathematics of The Hong Kong Polytechnic University.

The primary aim of the workshop is to bring together researchers from diverse backgrounds to explore the intersection of graph theory, optimization, and scientific computing. This workshop aims to foster collaboration, exchange ideas, and promote advancements in these fields, with a particular focus on their applications in various domains such as computer science, operations research, engineering, and social sciences. We expect this workshop will provide an ideal platform for local students and researchers to access cutting-edge research.

We are grateful to the members of Organizing Committee and Local Organizing Committee for their hard work. We are also grateful to the staff members of the Department of Applied Mathematics for their time and effort making this conference possible.

The workshop gratefully acknowledges the patronage of The Hong Kong Polytechnic University, and the financial support of CAS AMSS-PolyU Joint Laboratory of Applied Mathematics (JLab).

We sincerely hope that this workshop will enhance international collaboration between applied mathematicians and provide an opportunity for young researchers to learn the current state of the art in scientific computing and PDEs.

Finally, we hope all participants have a fruitful workshop in The Hong Kong Polytechnic University and wish all overseas participants an enjoyable stay in Hong Kong.

Organizing Committee

Yanping Lin (PolyU), Zhonghua Qiao (PolyU), Guiying Yan (AMSS)

# Acknowledgements

We are very grateful for the support and contributions to Graph Theory, Optimization and Scientific Computing as given by

The Hong Kong Polytechnic University (PolyU)

Department of Applied Mathematics, PolyU

CAS AMSS-PolyU Joint Laboratory of Applied Mathematics (JLab)

We would also like to thank the staff members in the Department of Applied Mathematics who have worked together in handling the various arrangements related to the conference. Their assistance has been indispensable.

## Organizing Committees

### Organizing Committee

- Yanping Lin (The Hong Kong Polytechnic University)
- Zhonghua Qiao (The Hong Kong Polytechnic University)
- Guiying Yan (Chinese Academy of Sciences)

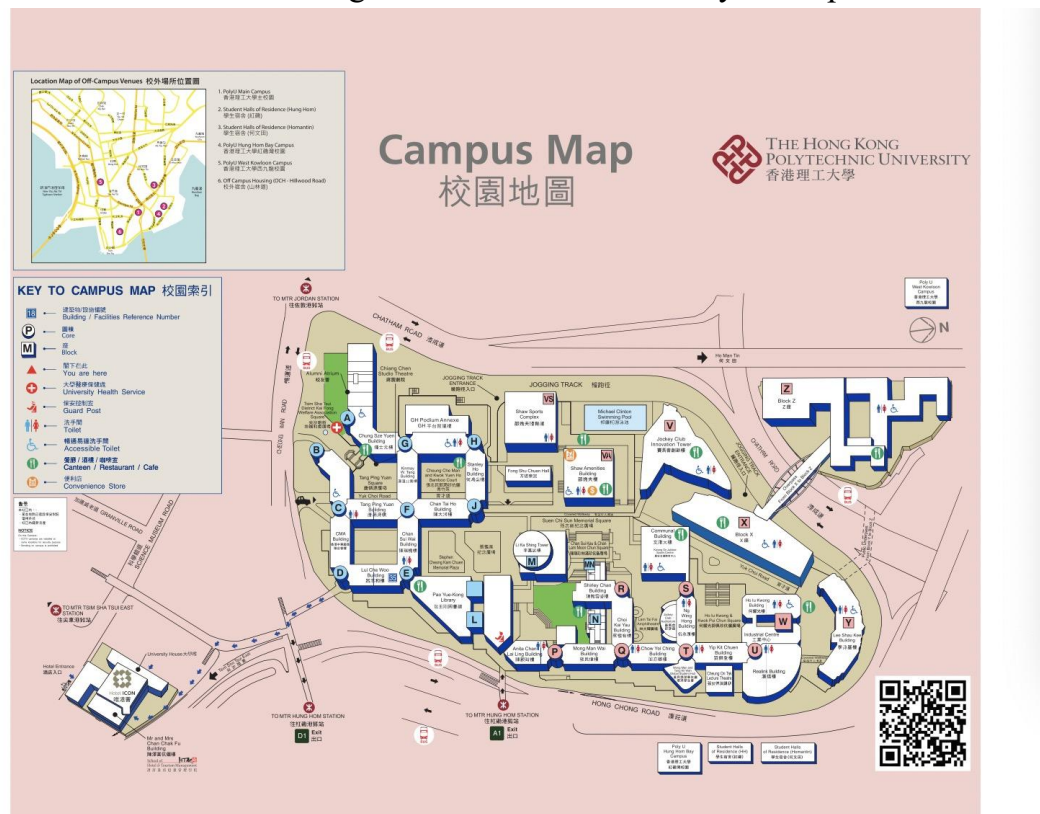
### Local Organizing Committee

- Jianbo Cui (The Hong Kong Polytechnic University)
- Zhonghua Qiao (The Hong Kong Polytechnic University)

# Conference Highlights

## Conference Venue

The workshop will be held on the PolyU campus. Please refer to the campus map. Please note that smoking is not allowed on the PolyU campus.



## Opening Ceremony & Group Photo

The opening ceremony and group photo will be held in Y302 at 9: 00 in the Saturday morning of 30 December 2023.

## Registration & Information Desk

Registration desk will be set up outside Y302 from 17:00-18:00 on 29 December 2023, 8:45-17:45 on 30 December 2023 and 8:45-11:45 on 31 December 2023.

## **On-campus Internet Access**

NetID: gstgtosc

Password: December2023

SSID: PolyUWLAN

Ref:

<https://www.polyu.edu.hk/en/its/it-services/wi-fi-services/how-to-connect-to-wifi/>

## **Registered participants are entitled to:**

- Attendance to all conference sessions
- Invitation to the welcome reception
- Invitation to the opening ceremony
- Invitation to the lunch and banquet
- Coffee breaks

## **Lunch**

Ju Yin House Restaurant, 4/F, Communal Building.

## **Banquet**

The Conference Banquet will be held on 30 December 2023 at 18:00 at SJ Cuisine (港晶軒), 2/F Harbour Crystal Centre, Tsim Sha Tsui East.

# Conference Venue

## 29<sup>th</sup> December 2023

Registration Desk will open from 17:00-18:00

Outside **Y302**, PolyU

Welcome Reception: 18:00-20:00

Sportful Garden Restaurant(陶源酒家), 1st Basement and G/F, No. 98 Granville Road, East Ocean Commercial Centre, TST, KLN

## 30<sup>th</sup> December 2023

Opening Ceremony & Group Photo: **Y302**

Registration & Information Desk: **outside Y302 (8:45-17:45)**

Invited Talks: **Y302 (9:15-12:15 & 14:00-17:45)**

Lunch: **12:15-14:00**

Ju Yin House Restaurant, 4/F, Communal Building

Banquet: **18:00-20:00**

SJ Cuisine (港晶軒), 2/F Harbour Crystal Centre, Tsim Sha Tsui East

## 31<sup>st</sup> December 2023

Registration & Information Desk: **outside Y302 (8:45-12:15)**

Invited Talks: **Y302 (9:00-12:15)**

Lunch: **12:20-14:00**

Ju Yin House Restaurant, 4/F, Communal Building

Dinner: **18:00-20:00**

Ju Yin House Restaurant, 4/F, Communal Building

# Conference schedule

<b>29 December 2023, Friday</b>	
17:00-18:00	<b>Registration</b>
18:00-20:00	<b>Reception dinner</b>

<b>30 December 2023, Saturday Y302</b>	
08:45-09:00	<b>Morning tea refreshment</b>
09:00-09:15	<b>Open Ceremony</b>
09:15-10:00	Tao Tang <b>Chair: Yanping Lin</b>
10:00-10:30	Yaojun Chen
10:30-10:45	<b>Tea break</b>
10:45-11:15	Qiumei Huang <b>Chair: Guiying Yan</b>
11:15-11:45	Bin Liu
11:45-12:15	Xin Liu
12:15-14:00	<b>Lunch</b>
14:00-14:30	Mei Lu <b>Chair: Yaojun Chen</b>
14:30-15:00	Zhengke Miao
15:00-15:30	Yuejian Peng
15:30-16:00	Yiqiao Wang
16:00-16:15	<b>Tea break</b>
16:15-16:45	Guiying Yan <b>Chair: Mei Lu</b>
16:45-17:15	Zhijian Yang
17:15-17:45	Tong Li
18:00-20:00	<b>Banquet</b>

<b>31 December 2023, Sunday Y302</b>	
08:45-09:00	<b>Morning tea refreshment</b>
09:00-09:30	Jiang Yang <b>Chair: Jianbo Cui</b>
09:30-10:00	Lei Zhang
10:00-10:30	Tao Zhou
10:30-10:45	<b>Tea break</b>
10:45-11:15	Jianbo Cui <b>Chair: Zhonghua Qiao</b>
11:15-11:45	Dianming Hou
11:45-12:15	Limin Ma
12:20-14:00	<b>Lunch</b>
14:00-17:00	<b>Free discussions</b>
18:00-20:00	<b>Dinner</b>



## Invited Talks

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**30 December 2023, Saturday**

**Chair:** Yanping Lin  
[Y302]

09:15-10:00 **Tao Tang** (BNU-HKBU United International College, China)  
*Nonlinear energy stability for phase-field models: numerics and analysis*

10:00-10:30 **Yaojun Chen** (Nanjing University, China)  
*The Ramsey numbers of two sets of cycles*

**Chair:** Guiying Yan  
[Y302]

10:45-11:15 **Qiumei Huang** (Beijing University of Technology, China)  
*Implicitly linear Jacobi spectral-collocation methods for weakly singular Volterra-Hammerstein integral equations*

11:15-11:45 **Bin Liu** (Ocean University of China, China)  
*Streaming algorithms for maximizing  $k$ -submodular functions under the multi-knapsack constraint*

11:45-12:15 **Xin Liu** (Chinese Academy of Sciences, China)  
*A continuous optimization approach to semi-supervised clustering problems*

**Chair:** Yaojun Chen  
[Y302]

14:00-14:30 **Mei Lu** (Tsinghua University, China)  
*Erdos-Ko-Rado theorem for multisets*

14:30-15:00 **Zhengke Miao** (Jiangsu Normal University, China)  
*Nowhere-zero 3-flows in toroidal graphs*

15:00-15:30 **Yuejian Peng** (Hunan University, China)  
*Minimum degree stability of graphs forbidding a family of odd Cycles*

15:30-16:00 **Yiqiao Wang** (Beijing University of Technology, China)  
*Linear 2-arboricity of planar graphs*

**Chair:** Mei Lu  
[Y302]

16:15-16:45 **Guiying Yan** (Chinese Academy of Sciences, China)  
*The Graph theoretic methods in coding theory*

16:45-17:15 **Zhijian Yang** (Wuhan University, China)  
*ML-aided multiscale modeling and simulation*

17:15-17:45 **Tong Li** (Chinese Academy of Sciences, China)  
*Two extremal problems in uniform hypergraphs*

**31 December 2023, Sunday**

**Chair:** Jianbo Cui  
[Y302]

09:00-9:30 **Jiang Yang** (Southern University of Science and Technology, China)  
*Higher-order energy stable exponential time differencing Runge–Kutta methods for gradient flows*

09:30-10:00 **Lei Zhang** (Peking University, China)  
*Construction of solution landscape for complex systems*

10:00-10:30 **Tao Zhou** (Chinese Academy of Sciences, China)  
*Deep adaptive sampling for numerical PDEs*

**Chair:** Zhonghua Qiao  
[Y302]

10:45-11:15 **Jianbo Cui** (The Hong Kong Polytechnic University, Hong Kong)  
*Structure-preserving numerical method of Wasserstein-Hamiltonian flow*

11:15-11:45 **Dianming Hou** (Jiangsu Normal University, China)  
*A linear second-order maximum bound principle-preserving BDF scheme for the Allen-Cahn equation with a general mobility*

11:45-12:15 **Limin Ma** (Wuhan University, China)  
*An energy stable and maximum bound principle preserving scheme for the dynamic Ginzburg–Landau equations under the temporal gauge*

## The Ramsey numbers of two sets of cycles

Yaojun Chen  
Nanjing University

**Abstract.** For two given sets  $C_1$  and  $C_2$  of cycles, the Ramsey number  $R(C_1, C_2)$  is the smallest integer  $N$  such that for any graph  $G$  on  $N$  vertices, either  $G$  contains a cycle from  $C_1$  or its complement contains a cycle from  $C_2$ . In this paper, we determine all Ramsey numbers  $R(C_1, C_2)$ , which confirms a conjecture due to Hansson recently, and extends the well known Ramsey numbers for two cycles.

## Structure-preserving numerical method of Wasserstein-Hamiltonian flow

Jianbo Cui  
The Hong Kong Polytechnic University

**Abstract.** We study discretizations of Hamiltonian systems on the probability density manifold equipped with the  $L_2$ -Wasserstein metric. Based on discrete optimal transport theory, several Hamiltonian systems on a graph (lattice) with different weights are derived, which can be viewed as spatial discretizations of the original Hamiltonian systems. We prove consistency of these discretizations. Furthermore, by regularizing the system using the Fisher information, we deduce an explicit lower bound for the density function, which guarantees that symplectic schemes can be used to discretize in time. Moreover, we show desirable long time behavior of these symplectic schemes, and demonstrate their performance on several numerical examples. Finally, we compare the present approach with the standard viscosity methodology.

## A linear second-order maximum bound principle-preserving BDF scheme for the Allen-Cahn equation with a general mobility

Dianming Hou  
Jiangsu Normal University

**Abstract.** In this talk, we will present and analyze a linear second-order numerical method for solving the Allen-Cahn equation with a general mobility. The proposed fully-discrete scheme is carefully constructed based on the combination of first and second-order backward differentiation formulas with nonuniform time steps for temporal approximation and the central finite difference for spatial discretization. The discrete maximum bound principle is proved of the scheme by using the kernel recombination technique under certain mild constraints on the time steps and the ratios of adjacent time step sizes. Furthermore, we rigorously derive the discrete  $H^1$  error estimate and energy stability for the classic constant mobility case and the  $L^\infty$  error estimate for the general mobility case. Various numerical experiments are also presented to validate the theoretical results and demonstrate the performance of the proposed method with a time adaptive strategy.

## Implicitly linear Jacobi spectral-collocation methods for weakly singular Volterra-Hammerstein integral equations

Qiumei Huang  
Beijing University of Technology

**Abstract.** In this talk, we use Jacobi spectral-collocation methods to solve two-dimensional weakly singular Volterra-Hammerstein integral equations. To overcome the reduction in the numerical accuracy of the spectral methods caused by the singularities of the solutions, we use the smoothing transformation to change the equation into a weakly singular equation with smooth solution. For the Hammerstein nonlinear term, we use the implicitly linear method to simplify the calculation and improve the accuracy. Convergence analysis in the  $L^\infty$ -norm is carried out and the exponential convergence rate is obtained. Finally, we demonstrate the efficiency of the proposed method by numerical examples.

## Two extremal problems in uniform hypergraphs

Tong Li  
Chinese Academy of Sciences

**Abstract.** In this talk, I will report some recent progress on two extremal problems in uniform hypergraphs. In the first part, we consider the rainbow Turán problem raised by Keevash, Mubayi, Sudakov and Verstraëte in 2007 and study the rainbow Turán number for hypergraph matchings and paths. In the second part, we consider the anti-Ramsey problem raised by Erdős, Simonovits and Sós in 1975 and determine the anti-Ramsey number for some classical hypergraphs such as paths and cycles. These results are based on joint work with Hao Huang, Yucong Tang, Guanghui Wang, Guiying Yan and Wenling Zhou.

## Streaming algorithms for maximizing k-submodular functions under the multi-knapsack constraint

Bin Liu  
Ocean University of China

**Abstract.** Submodular optimization, as the important branch of combinatorial optimization, is an interdisciplinary area of operational research, economics, computer science, etc. The general problem of optimizing a submodular function subject to different constraints captures many problems of interest both in theory and in practice, including maximum cut, facility location, maximum coverage, social welfare maximization, influence maximization in social networks, and sensor placement, etc. On the other hand, in the current big data environment, the input data of many applications is much larger than the storage capacity of individual computer. Therefore, it becomes of crucial importance to process the data in a streaming fashion. In this talk, I will show several streaming algorithms for the problem of maximizing k-submodular functions under the multi-knapsack constraint.

## A continuous optimization approach to semi-supervised clustering problems

Xin Liu

Chinese Academy of Sciences

**Abstract.** We propose a semi-supervised spectral clustering method with incomplete labels. Unlike existing methods, our method does not rely on an accurate number of clusters and can preserve the must link information. The main step of our method is to solve a continuous optimization problem with a block structure. Specifically, one block solves a linear programming problem, while the other involves a trace minimization problem. Through a block coordinate descent algorithm with finite convergence, we demonstrate that our method is more efficient than state-of-the-art semi-supervised spectral clustering methods.

## Erdos-Ko-Rado theorem for multisets

Mei Lu

Tsinghua University

**Abstract.** Let  $k, m, n$  be positive integers. A  $k$ -multiset of  $[n]_m$  is a collection of  $k$  integers from the set  $1, 2, \dots, n$  in which the integers can appear more than once but at most  $m$  times. A family of such  $k$ -multisets is called an intersecting family if every pair of  $k$ -multisets from the family have non-empty intersection. In this talk, we will present our result of intersecting family on  $k$ -multiset.

## An energy stable and maximum bound principle preserving scheme for the dynamic Ginzburg–Landau equations under the temporal gauge

Limin Ma

Wuhan University

**Abstract.** We propose a decoupled numerical scheme of the time-dependent Ginzburg–Landau equations under the temporal gauge. For the magnetic potential and the order parameter, the discrete scheme adopts the second type Nedelec element and the linear element for spatial discretization, respectively; and a linearized backward Euler method and the first order exponential time differencing method for time discretization, respectively. The maximum bound principle (MBP) of the order parameter and the energy dissipation law in the discrete sense are proved. The discrete energy stability and MBP-preservation can guarantee the stability and validity of the numerical simulations, and further facilitate the adoption of an adaptive time-stepping strategy, which often plays an important role in long-time simulations of vortex dynamics, especially when the applied magnetic field is strong. An optimal error estimate of the proposed scheme is also given.

## Nowhere-zero 3-flows in toroidal graphs

Zhengke Miao

Jiangsu Normal University

**Abstract.** Tutte’s 3-flow conjecture states that every 4-edge-connected graph admits a nowhere-zero 3-flow. The planar case of Tutte’s 3-flow conjecture is the classical Grötzsch’s Theorem (1959). Steinberg and Younger (1989) further verified Tutte’s 3-flow conjecture for projective planar graphs. We confirm Tutte’s 3-flow conjecture for all toroidal graphs. This talk is based on the joint work with Jiaao Li, Yulai Ma, Yongtang Shi, Weifan Wang and Cun-Quan Zhang.

## Minimum degree stability of graphs forbidding a family of odd cycles

Yuejian Peng  
Hunan University

**Abstract.** We determine what the tight bound on the minimum degree would be to guarantee an  $n$ -vertex graph forbidding a family of odd cycles to be bipartite. Let  $\mathcal{C}$  be a family of odd cycles. We discover that the length of the shortest odd cycle not in  $\mathcal{C}$  and the length of the longest odd cycle in  $\mathcal{C}$  determine what the tight bound is. Let  $l \leq k$  and  $n \geq 1000k^8$  be positive integers. Let  $\mathcal{C}$  be a family of odd cycles,  $C_{2l+1}$  be the shortest odd cycle not in  $\mathcal{C}$ , and  $C_{2k+1}$  be the longest odd cycle in  $\mathcal{C}$ . Let  $BC_{2l+1}(n)$  denote the graph obtained by taking  $2l+1$  vertex-disjoint copies of  $K_{\frac{n}{2(2l+1)}, \frac{n}{2(2l+1)}}$  and selecting a vertex in each of them such that these vertices form a cycle of length  $2l+1$ . Note that  $BC_{2l+1}(n)$  is  $\mathcal{C}$ -free and non-bipartite with minimum degree  $\frac{n}{2(2l+1)}$ . Let  $C_{2k+3}(\frac{n}{2k+3})$  denote the balanced blow up of  $C_{2k+3}$  with  $n$  vertices. Note that  $C_{2k+3}(\frac{n}{2k+3})$  is  $\mathcal{C}$ -free and non-bipartite with minimum degree  $\frac{2}{2k+3}n$ . We show that if  $G$  is an  $n$ -vertex  $\mathcal{C}$ -free graph with  $\delta(G) > \max\{\frac{n}{2(2l+1)}, \frac{2}{2k+3}n\}$ , then  $G$  is bipartite. The bound is tight evident by  $BC_{2l+1}(n)$  and  $C_{2k+3}(\frac{n}{2k+3})$ . Moreover, the only  $n$ -vertex  $\mathcal{C}$ -free non-bipartite graph with minimum degree  $\max\{\frac{n}{2(2l+1)}, \frac{2}{2k+3}n\} = \frac{n}{2(2l+1)}$  is  $BC_{2l+1}(n)$ , and the the only  $n$ -vertex  $\mathcal{C}$ -free non-bipartite graph with minimum degree  $\max\{\frac{n}{2(2l+1)}, \frac{2}{2k+3}n\} = \frac{2}{2k+3}n$  is  $C_{2k+3}(\frac{n}{2k+3})$ . Our result unifies stability results of Andrásfai, Erdős and Sós, and Häggkvist for large  $n$ . Our result is also related to the question of Erdős and Simonovits: For an integer  $r \geq 2$  and a family of non-bipartite graphs  $\mathcal{H}$ , what is the tight bound of  $\alpha$  such that any  $\mathcal{H}$ -free  $n$ -vertex graph with minimum degree at least  $\alpha n$  has chromatic number at most  $r$ ? Our result answers this question for  $r = 2$  and any family of odd cycles. This is a joint work with Xiaoli Yuan.

## Nonlinear energy stability for phase-field models: numerics and analysis

Tao Tang  
BNU-HKBU United International College

**Abstract.** The phase-field model, a powerful modeling tool for dealing with interface problems, has been widely used in various fields such as computational physics, computational biology, materials engineering, and even image processing. The dissipation of free energy is an important and fundamental property of the phase-field model. Our research will focus on the following three aspects based on the energy dissipation of the phase-field model: (1) High-order and efficient numerical methods that satisfy energy dissipation; (2) Energy dissipation of the time-fractional phase-field model; (3) Theoretical research on operator splitting methods that ensure energy dissipation.

## Linear 2-arboricity of planar graphs

Yiqiao Wang  
Beijing University of Technology

**Abstract.** The linear 2-arboricity of a graph  $G$  is the least integer  $k$  such that  $G$  can be partitioned into  $k$  edge-disjoint forests, whose components are paths of length at most 2. In this talk, we give a short survey on the research progress about the linear 2-arboricity of graphs. Better upper bounds of linear 2-arboricity of planar graphs, toroidal graphs, 1-planar graphs and other special graphs are also established.

## The Graph theoretic methods in coding theory

Guiying Yan  
Chinese Academy of Sciences

**Abstract.** The innovation of channel coding technology has promoted the upgrading of mobile communication, and mathematics has played an important role in the study of channel coding theory. In this talk, I will introduce the roles of Graph theoretic methods in coding theory, and our recent advances in coding theory research.

## Higher-order energy stable exponential time differencing Runge–Kutta methods for gradient flows

Jiang Yang  
Southern University of Science and Technology

**Abstract.** We present a general framework to construct higher-order unconditional energy stable exponential time differencing Runge–Kutta (ETDRK) methods for a class of gradient flows. More precisely, we identify a set of conditions that ETDRK schemes need to satisfy in order to have the energy stable property, show that the commonly used third-order and fourth-order ETDRK schemes do not satisfy these conditions, and construct, with proper stabilization, new third-order ETDRK schemes which satisfy the conditions and thus unconditionally decrease the energy. We present ample numerical experiments using the new schemes to validate their accuracy and stability, large time step behavior, long time evolution and the adaptive time stepping strategy for various gradient flows. This is the first work to study the unconditionally energy stability of arbitrarily high-order ETDRK methods, and it is hopeful that our general framework will lead to constructions of higher than third-order unconditional energy stable ETDRK schemes.

## ML-aided multiscale modeling and simulation

Zhijian Yang  
Wuhan University

**Abstract.** In the past several decades, multiscale modeling and simulation (MMS) has attracted many interests and demonstrated its power in many applications. However, there are still issues remaining in MMS which are the bottlenecks for its full application. With the help of machine learning techniques, I will demonstrate a couple of examples in the efforts of resolving these issues. Namely, I will show our recent work of deriving macroscopic constitutive relations from microscopic models based on learning techniques as well as learning boundary conditions.

## Construction of solution landscape for complex systems

Lei Zhang  
Peking University

**Abstract.** Energy landscape has been widely applied to many physical and biological systems. A long standing problem in computational mathematics and physics is how to search for the entire family tree of possible stationary states on the energy landscape without unwanted random guesses? Here we introduce a novel concept “Solution Landscape”, which is a pathway map consisting of all stationary points and their connections. We develop a generic and efficient saddle dynamics method to construct the solution landscape, which not only identifies all possible minima, but also advances our understanding of how a complex system moves on the energy landscape. We then apply the solution landscape approach to study two problems: One is construction of the defect landscapes of confined nematic liquid crystals, and the other one is to find the transition pathways connecting crystalline and quasicrystalline phases.

## Deep adaptive sampling for numerical PDEs

Tao Zhou  
Chinese Academy of Sciences

**Abstract.** Adaptive computation is of great importance in numerical simulations. The ideas for adaptive computations can be dated back to adaptive finite element methods in 1970s. In this talk, we shall propose a deep adaptive sampling method for solving PDEs where deep neural networks are utilized to approximate the solutions. In particular, we propose the failure informed PINNs (FI-PINNs), which can adaptively refine the training set with the goal of reducing the failure probability. Compared to the neural network approximation obtained with uniformly distributed collocation points, the developed algorithms can significantly improve the accuracy, especially for low regularity and high-dimensional problems.