华南数学应用与交叉研究中心
South China Research Center for Applied Mathematics and Interdisciplinary Studies

CAMIS-SCNU
Workshop

复杂系统中的变分方法研究论坛

Workshop on Variational Approaches in Complex Systems

Brochure

会议手册

South China Research Center for Applied Mathematics
and Interdisciplinary Studies (CAMIS), South China Normal University
华南师范大学华南数学应用与交叉研究中心

Guangzhou, China
April 12-14, 2019

Address: Zhong Shan Avenue West 55, Tianhe District, Guangzhou 510631, China
地址：广东省广州市天河区中山大道西55号 邮编：510631
Website: http://camis.scnu.edu.cn/

1. Useful Information

(1) Timetable

Workshop on Variational Approaches in Complex Systems April 12-14, 2019			
Time	**April 12 (Friday)**	**April 13 (Saturday)**	**April 14 (Sunday)**
8:50-9:00	Opening remarks		
9:00-10:00	Masao DOI	Chun LIU	Changyou WANG
10:00-10:30	Coffee break	Coffee break & Photos	Coffee break
10:30-11:00	**Xingkun MAN**	**Xingye YUE**	**Pingbing MING**
11:00-11:30	**Yana DI**	**Xiang ZHOU**	**Shuyang DAI**
11:30-12:00	**Xianmin XU**	**Zhen ZHANG**	**Chaozhen WEI**
12:00-14:00	Lunch	Lunch	12:00-12:10 Closing Remarks 12:10 Lunch
14:00-14:30	**Xinpeng XU**	**Aihui ZHOU**	**Departure**
14:30-15:00	**Jun LI**	**Lei ZHANG**	
15:00-15:30	**Wei JIANG**	**Yongyong CAI**	
15:30-16:00	Coffee break	Coffee break	
16:00-16:30	**Yan WANG**	Changjuan ZHANG Haiqin WANG	
16:30-17:00	**Quan ZHAO**	Qiong-ao HUANG Weijie HUANG	
17:30—20:00	Dinner	Banquet	

(2) Address

① **Accommodation:** Hanpudun Hotel（汉普敦酒店）

② **Hotel Address:** Hanpudun Hotel, No.61-65 Zhong Shan Avenue West, Tianhe District, Guangzhou 510631, China（广东省广州市天河区中山大道西 61-65 号汉普敦酒店 邮编：510631）

③ **Talk Avenue:** South China Research Center for Applied Mathematics and Interdisciplinary Studies (CAMIS), South China Normal University（华南师范大学华南数学应用与交叉研究中心）

(3) Map: Hanpudun Hotel-- CAMIS


South China Research Center for Applied Mathematics
and Interdisciplinary Studies (CAMIS)
华南师范大学华南数学应用与交叉研究中心
Hanpudun Hotel
汉普敦酒店
大道西

2.Programme (日程)

Date	Time	Activity	Venue
April 11th, Thurs.	16:00-18:00	Registration (注册)	**The hall of CAMIS** 交叉中心一楼大厅
	18:00	Welcome dinner	Taoyuan 陶园二楼自选区
April 12th, Fri.	08:30-08:50	Registration (注册)	**Room 111 of CAMIS**
	08:50-09:00	Opening remarks by **Prof. Weizhu BAO**	
	Session 1. Chairman: **Prof. Weizhu BAO**		
	09:00-10:00	*Application of Onsager Machlup integral in solving dynamic equations in non-equilibrium systems* **Prof. Masao DOI (Plenary talk)**	
	10:00-10:30	Coffee break	
	Session 2. Chairman: **Prof.** Masao DOI		
	10:30-11:00	*The Drying of Liquid Droplets* **Prof. Xingkun MAN (满兴坤)**	
	11:00-11:30	*Application of Onsager Principle in solving coating dynamic problem* **Prof. Yana DI (邸亚娜)**	
	11:30-12:00	*Onsager variational Principle as an approximation tools for complicated two-phase flow* **Prof. Xianmin XU（许现民）**	
	12:00-14:00	Lunch（午饭）	Taoyuan 陶园二楼自选区
	Session 3. Chairman: **Prof. Xianmin XU**		
	14:00-14:30	*Evaporation-induced phase dynamics of diblock copolymer solution films* **Prof. Xinpeng XU (徐新鹏)**	
	14:30-15:00	*The Generalized Onsager Principle and its Applications* **Prof. Jun LI（李君）**	
	15:00-15:30	Application of the Onsager's variational principle to surface diffusion-controlled problems **Prof. Wei JIANG (蒋维）**	

	15:30-16:00	Coffee break	
	Session 4. Chairman: **Prof. Wei JIANG**		
	16:00-16:30	*Solid-state dewetting: from flat to curved substrates* **Prof. Yan WANG（王燕）**	
	16:30-17:00	*Sharp-interface approach for simulating solid-state dewetting* **Dr. Quan ZHAO (赵泉)**	
	17:30	Dinner (晚饭)	Taoyuan 陶园二楼 餐厅
April 13th, Sat.	Session 1. Chairman: **Prof.** Jinkai LI		
	09:00-10:00	***Diffusion in Biological Environments: the Energetic Variational Approaches*** **Prof. Chun L/IU (柳春, Plenary Talk)**	
	10:00-10:30	Coffee break (Photos, 集体照)	
	Session 2. Chairman: **Prof. Tiezheng QIAN**		
	10:30-11:00	*Numerical methods for Porous Medium Equation by an Energetic Variational Approach* **Prof. Xingye YUE（岳兴业）**	
	11:00-11:30	*Control Perspective for Rare events* **Prof. Xiang ZHOU（周 翔）**	
	11:30-12:00	*Variational modeling of moving contact line problems with elastic membrane* **Prof. Zhen ZHANG（张振）**	
	12:00-14:00	Lunch (午饭)	Taoyuan 陶园二楼 自选区
	Session 3. Chairman: **Prof.** Zhilin LI		
	14:00-14:30	*Adaptive Finite Element Approximations for Density Functional Models* **Prof. Aihui ZHOU（周爱辉）**	
	14:30-15:00	*Solution landscapes of Nematic Liquid Crystal* **Prof. Lei ZHANG（张磊）**	
	15:00-15:30	*Ground states of Bose-Einstein condensates with higher order interaction* **Prof. Yongyong CAI（蔡勇勇）**	
	15:30-16:00	Coffee break	

	Session 4. Chairman: **Prof. X**inpeng XU		
	16:00-16:15	*Numerical simulation for a bubble rising in surrounding liquid and interacting with a horizontal solid wall* **Dr. Changjuan ZHANG (张昌娟）**	
	16:15-16:30	*Curvotaxis of droplets and cells: Directed migration guided by substrate curvature* **Ms. Haiqin WANG (王海钦)**	
	16:30-16:45	*An unconditionally energy stable scheme for simulating wrinkling phenomena of elastic thin films on a compliant substrate* **Dr. Qiongao HUANG（黄琼敖）**	
	16:45-17:00	*θ-L approach for solid-state dewetting problems* **Dr. Weijie HUANG（黄卫杰）**	
	17:30	Banquet (晚宴)	Taoyuan 陶园二楼餐厅
April. 14th, Sun	Session 1. Chairman: **Prof.** Shijin DING		
	09:00-10:00	***On Phases Transition between Isotropic and Nematic States*** **Prof. Changyou WANG（王长友, Plenary Talk）**	
	10:00-10:30	Coffee break	
	Session 2. Chairman: **Prof. X**iaoping WANG		
	10:30-11:00	*Cauchy-Born rule: from perfect crystal to bilayer graphene* **Prof. Pingbing MING (明平兵)**	
	11:00-11:30	*Dislocation network structures in 2D bilayer system* **Prof. Shuyang DAI（戴书洋）**	
	11:30-12:00	*A Continuum Model for the Disconnection Mechanism of Grain Boundary Dynamic* **Dr. Chaozhen WEI（魏朝祯）**	
	12:00-12:10	Closing Remarks	
	12:10	Lunch	Taoyuan 陶园二楼自选区

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2. Abstract & Title

Ground states of Bose-Einstein condensates with higher order interaction

Yongyong Cai (蔡勇勇) (Beijing Computational Science Research Center)

We analyze the ground states and dynamics of a Bose-Einstein condensate in the presence of higher-order interactions (HOI), modeled by a modified Gross-Pitaevskii equation (MGPE). In fact, due to the appearance of HOI, the ground state structures become very rich and complicated. We establish the existence and non-existence results under different parameter regimes, and obtain their limiting behaviors and/or structures with different combinations of HOI and contact interactions. Both the whole space case and the bounded domain case are considered, where different structures of ground states are identified.

Dislocation network structures in 2D bilayer system

Shuyang Dai (戴书洋) (Wuhan University)

We develop a multiscale continuum model to describe the interlayer defects in bilayer materials. The model incorporates both the anisotropy elasticity of each mono-layer in bilayer materials and the first-principle calculation informed interaction between two layers, i.e., the nonlinear atomistic potential energy between two layers. The equilibrium structures are obtained from the numerical simulations of the force balance differential equations. We apply this approach to determine the structure and energetics of twisted bilayer material. In tBLG, two distinct, modified Moiré structures are observed. We also investigated the dislocation structure in heterogeneous bilayer material such as G/BN. Our model agrees well with the atomistic results. An analytical description is developed based on the obtained structural features.

Application of Onsager Principle in solving coating dynamic problems

Yana Di (邸亚娜) (Institute of Computational Mathematics, CAS)

In 1931, Onsager proposed a variational principle which has become the base of many kinetic equations for non-equilibrium systems. We have been showing that this principle is useful in obtaining approximate solutions for the kinetic equation. And we also use it to determine the steady state in non-equilibrium system by a variational calculus.

Application of Onsager Machlup integral in solving dynamic equations in non-equilibrium systems

Masao Doi (Beihang University)

In 1931, Onsager proposed a variational principle which has become the base of many kinetic equations for non-equilibrium systems. We have been showing that this principle is useful in obtaining approximate solutions for the kinetic equation, but our previous method has a weakness that it can be justified, strictly speaking, only for small incremental time. Here we

propose an improved method which does not have this drawback. The new method utilizes the integral proposed by Onsager and Machlup in 1953, and can tell which of the approximate solutions is the best solution without knowing the exact solution. The new method has an advantage that it allows us to determined the steady state in non-equilibrium system by a variational calculus. We demonstrate this using three examples, (a) simple diffusion problem, (b) capillary problem in a tube with corners, and (c) free boundary problem in liquid coating, for which the kinetic equations are written in second or fourth order partial differential equations..

θ-L approach for solid-state dewetting problems

Weijie Huang (黄卫杰) (Beijing Computational Science Research Center)

We propose a θ−L approach for simulating solid-state dewetting of thin films. Solid-state dewetting belongs to a class of interface problems and the motion of the film/vapor interface is governed by surface diffusion and contact line migration. For solving the corresponding sharp-interface model, traditional methods usually suffer from severe stability constraints and/or mesh redistribution due to the high nonlinearity of the surface diffusion equation and the coupling with moving contact lines. The θ−L formulation introduces a proper tangential velocity along the evolving interface and utilizes a new frame of reference, i.e., the interface tangential angle θ and the interface length L, so that it both reduces the stiffness from surface diffusion and improves the performance in mesh equidistribution. Moreover, it could achieve high-order accuracy when implemented by a semi-implicit parametric finite element method.

An unconditionally energy stable scheme for simulating wrinkling phenomena of elastic thin films on a compliant substrate

Qiongao Huang (黄琼敖) (Wuhan University)

By introducing a scalar auxiliary variable (SAV), we propose a class of semi-implicit time-stepping, unconditionally energy stable numerical schemes for simulating wrinkling phenomena of an elastic thin films on a compliant substrate. These SAV schemes only need to solve, twice, a decoupled linear, fourth-order integro-differential equations with constant coefficients at each time step, and these linear equations can be efficiently implemented by using Fourier spectral method to discretize spatial derivatives. Numerical results have demonstrated that these SAV schemes (including first-order SAV/BDF1, second-order SAV/BDF2 and SAV/CN2) are highly efficient and accurate. Furthermore, many interesting wrinkling phenomena, such as pattern formations (e.g., stripes, checkerboards, labyrinths, herringbones) and pattern transitions under different loading processes, are investigated by using the proposed schemes.

Application of the Onsager's variational principle to surface diffusion-controlled problems

Wei Jiang (蒋维) (Wuhan University)

We apply the Onsager's variational principle to develop a general approach for describing surface diffusion-controlled problems. By some examples, e.g., a solid toroidal island on a substrate, and the migration of “small’’ particles on curved substrates, we show that this approach

represents a general tool for modeling interface diffusion-controlled morphology evolution.

the Generalized Onsager Principle and its Applications

Jun Li (李君) (Tianjin Normal University)

The Onsager principle is widely used in nonequilibrium thermodynamics or hydrodynamics. In this report, we’ ll articulate the generalized Onsager principle and its applications. The generalized Onsager principle can be used for active or passive system. It ensures fundamental variational structure of the models as well as dissipative properties of the passive component in the models, irrespective of the choice of scale (kinetic to continuum) and of the physical potentials. It also provides guidance for setting boundary conditions. Base on the generalized Onsager principle, it is convenient to design the entropy production rate preserving numerical scheme.

Diffusion in Biological Environments: the Energetic Variational Approaches

Chun Liu (柳春) (Illinois Institute of Technology)

Almost all biological activities involve transport and distribution of ionic particles in biological environments. In this talk, I will focus on two aspects: the dynamic boundary conditions which models the force balance on the boundaries and also the temperature effects.

The Drying of Liquid Droplets

Xingkun Man (满兴坤) (Beihang University)

The drying of liquid droplets is a common daily life phenomenon that has long held a special interest in scientific research. We propose an Onsager variational principle theory that describes the droplet shape evolution and predicts the deposit distribution of nonvolatile components on the substrate. It is shown that for the drying of a single droplet, the deposition pattern changes continuously from a coffee ring to volcanolike and to mountainlike depending on the mobility of the contact line and the evaporation rate. When drying of two neighboring droplets, asymmetrical ring-like deposition patterns are formed, including fanlike and eclipse-like deposition patterns. The same theoretical model is also used to explain the multi-ring patterns of the deposit that are formed when colloidal suspensions are dried on a substrate. Using a standard model for the stick-slip motion of the contact line, the theory predicts (a) the multi-ring patterns are not observed at high evaporation rate, (b) the spacing between rings decreases with the decrease of the ring radius, and (c) the multi-ring pattern is taken over by a disk pattern near the center. These results are in qualitative agreement with existing experiments, and the predictions of the theory about how the evaporation rate, droplet radius and receding contact angle affects the pattern can be tested experimentally.

Cauchy-Born rule: from perfect crystal to bilayer graphene

Pingbing Ming (明平兵) (Institute of Computational Mathematics, CAS)

In this talk we shall discuss the application of the Cauchy-Born rule to two typical systems. The first is the perfect crystal with simple or complex lattice structures. The second is the bilayer graphene, which is a system with dislocation-type defect. The validity of the Cauchy-Born rule will be underpinned by various stability conditions.

Curvotaxis of droplets and cells: Directed migration guided by substrate curvature

Haiqin Wang (王海钦) (Guangdong Technion-Israel Institute of Technology)

Directed migration induced by substrate curvature has recently attracted much attention because of their importance in both material processing and biological systems. Such curvature-guided migration is usually called curvotaxis. It is interesting to note that although animal cells are much more complex than simple liquid droplets, their curvotaxis shows some similarities, particularly in average migration direction (both toward the region of smaller curvature or concave region of negative curvature). We are particularly interested in micro-droplets and adherent animal cells on substrates of micron-scale curvature. This is the natural curvature condition that most micro-droplets and animal cells are interacting with. Many experiments have been done for the curvotaxis of both liquid droplets and animal cells on microstructure substrates such as micro-pillars, micro-cones, 2D micro-sinusoidal substrates and sphere-with-skirt substrates etc. However, an appropriate theory to understand curvotaxis of droplets and cells at low Reynolds number is still missing. In this talk, I will present our efforts in theory to understand the statics and dynamics of the curvotaxis. We predict by using Onsager's variational principle that directed migration of droplets is given by the balance between conservative capillary forces and dissipative forces from liquid viscosity and contact line slip. In contrast, curvotaxis of animal cells is much more complex. We propose a liquid-like cell model and an elastic cell model to explain the interplay between cell activity and substrate curvature. We have also proposed several new cell experiments to justify our predictions. For example, one can examine the effects of the contractility of basal stress fibers by adding blebbistatin or reducing substrate stiffness. One can check the correlation between cell motility and stress fiber orientations by reducing the integrin molecules on the substrates. One can vary the thickness of the cell to justify the validity of elastic model and liquid-like model of adherent cells; the thicker the cell is, the better the elastic cell model is. In addition, it will be also very interesting to see the effects of substrate curvature on the spreading area of adherent cells.

On Phases Transition between Isotropic and Nematic States

Changyou Wang (王长友) (Purdue University)

In this talk, I will discuss the interfacial problem of liquid crystals between the isotropic state and nematic state. As the Frank elasticity constants are sufficiently small, a sharp interface can form. We will present some results concerning the asymptotical limit in the frame of Gamma convergence. This is a joint work with Professor Fanghua Lin.

Solid-state dewetting: from flat to curved substrates

Yan Wang (王燕) (Central China Normal University)

Employing a thermodynamic variational method, we propose sharp interface models combined with relaxed contact angle boundary conditions for simulating solid-state dewetting of thin films on rigid flat and curved substrates. In the models, film/vapor interfacial anisotropy is easily included, and the movement of the contact line can be explicitly described by the relaxed boundary conditions. We apply the models to study the equilibrium configuration of small islands and the pinch-off of large island, the migration of tiny particles and the templated solid-state dewetting on inverted pyramidal pits. The simulation results capture many of the complexities associated with solid-state dewetting experiments.

A Continuum Model for the Disconnection Mechanism of Grain Boundary Dynamics

Chaozhen Wei (魏朝祯) (Hong Kong University of Science and Technology)

We propose a novel approach to simulate the evolution of polycrystalline microstructures based upon a disconnection model for grain boundary (GB) kinetics. Disconnections are line defects that lie solely with GB and are characterized by both a Burgers vector and a step height, as set by the GB bicrystallography. The model incorporates surface tension, applied stress, and jumps in chemical potential across GBs. The model also includes disconnection nucleation and mobility. We first derive a continuum equation of motion for individual GBs and then for GB triple junctions (TJ) within a polycrystalline microstructure that rigorously accounts for conservation of disconnection Burgers vectors and step heights and couples the GBs meeting at the TJ. We then perform continuum simulation of GB dynamics without TJs, and with TJs in a polycrystalline microstructure. The resultant simulations provide clear demonstrations of the importance of including a crystallography-respecting microscopic model of microstructure evolution and the intrinsic coupling between stress, capillarity, and microstructure connectivity in microstructure evolution.

Onsager variational Principle as an approximation tools for complicated two-phase flow

Xianmin Xu (许现民) (Chinese Academy of Sciences)

Many two-phase flow problems are quite complicated due to the existence of moving contact lines and shape transition of two-phase interfaces. Both numerical simulations and analytical study for these problems are very challenging, especially to quantitatively compare with physical experiments. In this talk, we will show that the Onsager principle could be used as a powerful approximation tool in these problems. This is illustrated by examples like sliding droplets on an inclined surface, capillary rising for a thin soap film, etc.

Evaporation-induced phase dynamics of diblock copolymer solution films

Xinpeng Xu (徐新鹏) (Guangdong Technion-Israel Institute of Technology)

Many soft matter systems exist as solutions, e.g., polymer solutions and colloidal suspensions. Solutions are made by dissolving a material in a liquid. They show fascinating phase structure and dynamic properties. In this talk, I will show modeling efforts from simple binary solutions, to polymer solutions, and to diblock copolymer solutions. The idea of two-fluid model formulated by Onsager's variational principle will be the key to the modeling of these different soft matter solutions. Particular attention will be placed on evaporation-induced phase dynamics of diblock copolymer solution films.

Numerical methods for Porous Medium Equation by an Energetic Variational Approach

Xingye Yue (岳兴业) (Soochow University)

We study numerical methods for porous media equation. There are two important characteristics: the finite propagation of the free boundary and the potential waiting time, which make the problem not easy to handle. Based on different dissipative energy laws, we develop two numerical schemes by an energetic variational approach, which keeps the balance of the least action principle and the maximum dissipation principle. Firstly, based on $f \log f$ form of the total energy, we obtain the trajectory equation, and then construct a fully discrete scheme. We prove that the numerical scheme of the trajectory equation is uniquely solvable on a convex set and keeps the discrete energy dissipation law. Next, based on $1/f$ form of total energy, we construct a linear numerical scheme for the corresponding trajectory equation, which also keeps the discrete dissipation law. Each scheme yields a good approximation for the solution and the free boundary. No oscillation is observed for the numerical solution around the free boundary. Furthermore, the waiting time problem could be treated naturally, which is hard for all the existence methods. As a linear scheme, the second scheme is more efficient.
This is joint work with Chenghua Duan, Chun Liu and Cheng Wang

Numerical simulation for a bubble rising in surrounding liquid and interacting with a horizontal solid wall

Changjuan Zhang (张昌娟) (Beijing Computational Science Research Center)

A bubble is driven by buoyancy force to rise in a viscous liquid toward a horizontal flat rigid wall, impinging on and possibly bouncing from the wall. First, we carry out numerical simulations of an axisymmetric bubble interacting with a solid flat wall using arbitrary Lagrangian-Eulerian finite element method (ALE-FEM). We validate the ALE-FEM simulation with existing experimental and numerical data, investigate the bubble dynamics to explore four different dynamic behaviors, and compare the thin film dynamics with the predictions by the lubrication approximation. Second, bubble dynamics in two space dimensions are investigated by the ALE-FEM and the adaptive mesh refinement lattice Boltzmann method (AMR-LBM). We validate the two methods, investigate the dynamics of suspended bubbles, and study the dynamics of rising bubbles. The capabilities and numerical accuracy are discussed for the two methods.

Solution landscapes of Nematic Liquid Crystal

Lei Zhang (张磊) (Peking University)

Topological defect plays an important role in the physics of liquid crystals. Although a large amount of previous studies is devoted to understand and compute the stable defect structures in liquid crystals as a consequence of geometric frustration, less attention has been paid to investigate the transition states between stable defect structures and the solution landscapes of nematic liquid crystals. In this talk, we first show that a combination of the Landau-de Gennes model and the multi-scale string method can systematically investigate the transition pathways between different defect patterns of nematic liquid crystals confined in a 3D cylinder with homeotropic boundary condition in 3D cylinder. Next, we proposed a High index Optimization-based Shrinking Dimer (HiOSD) method to compute the complete defect landscape of Nematic Liquid Crystals in 2D square. The joint work with Pingwen Zhang (PKU), Yucheng Hu (Tsinghua).

Variational modeling of moving contact line problems with elastic membrane

Zhen Zhang (张振) (Southern University of Science and Technology)

We introduce a sharp interface models for moving contact lines with elastic membrane. A continuous model with the boundary conditions is derived for the dynamics of two immiscible fluids with moving contact lines based on thermodynamic principles. Both static configuration and dynamic models are developed. Perturbation analysis is conducted for the 2D static configuration to reveal the multiscale structure. We also discuss related models on surfactants and polymers.

Sharp-interface approach for simulating solid-state dewetting

Quan Zhao (赵泉) (National University of Singapore)

We consider the solid-state dewetting of thin films in three dimensions by using a sharp-interface approach. Based on the thermodynamic variation, a speed method is used for performing the first variation to the total surface energy functional. This method shares more advantages than the traditional use of parameterized curves (or surfaces), e.g., it is more intrinsic and its variational structure (related with Cahn-Hoffman $\boldsymbol{\xi}$-vector) is clearer and more direct. By making use of the first variation, necessary conditions for the equilibrium shape of the solid-state dewetting problem is given, and a kinetic sharp-interface model which includes the surface energy anisotropy is also proposed. Numerical simulations demonstrate the accuracy and efficacy of the sharp-interface approach to capture many of the complexities observed in solid-state dewetting experiments.

Adaptive Finite Element Approximations for Density Functional Models

Aihui Zhou (周爱辉) (Chinese Academy of Sciences)

Density functional models are powerful, widely used approaches for computation of ground state electronic energies and densities in chemistry, materials science, biology, and nanosciences. In this presentation, we will talk about adaptive finite element approximations of orbital-free and Kohn-Sham density functional models, including the construction and analysis of the residual type a posteriori error estimators as well as the convergence and complexity of the adaptive finite element approximations.

We will demonstrate several typical numerical experiments that show the robustness and efficiency of the adaptive finite element computations in electronic structure calculations. This presentation is based on some joint works with H. Chen, X. Dai, X. Gong, L. He, and B. Yang.

Control Perspective for Rare events

Xiang Zhou (周翔) (City University of Hong Kong)

The rare events in randomly perturbed dynamical systems are very important in physics, chemistry and biology, since they describe the random and infrequent hoppings between metastable states. The traditional studies are based on the large scale nonlinear optimisation in path space, due to the large deviation principle and the underlying Lagrangian or Hamiltonian variational structure. In addition, the recent advancement of importance sampling and saddle point methods also have new characterization from the optimal control perspective. This talk will summarize these connections of rare events (minimum action method, gentlest ascent dynamics and dynamical importance) with the various forms of optimal control. We discuss the application to new problems such as rare events in active matters, as well as a new method for solving optimal control problem. The project is supported by Hong Kong GRF.

4.Participants List

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