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
Conference

科学计算与交叉研究论坛

Forum in Scientific Computing and Interdisciplinary Research

Conference 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
November14-18, 2018

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/

Contents

1. Information for Participants

1.1 Address

（1） **Conference Address:** South China Research Center for Applied Mathematics and Interdisciplinary Studies (CAMIS), South China Normal University, Zhong Shan Avenue West 55, Guangzhou 510631, China

会议地址：广东省广州市天河区中山大道西 55 号华南师范大学 邮编：510631

（2） **Hotel address:** Hanpudun Hotel, No.61-65 Zhong Shan Avenue West, Tianhe District, Guangzhou 510631,China

酒店地址： 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

1.2 Travel Information

Guangzhou Baiyun International Airport—Hanpudun Hotel (汉普敦酒店)

(1) **Taxi** (**Suggest**): Guangzhou Baiyun International Airport -- Airport Avenue -- Guangzhou Airport Expressway -- South China Expressway -- Zhongshan Avenue West – Hanpudun Hotel（汉普敦酒店）

Distance: 43km Time: about 42 minutes **Fare: about RMB¥150-160**

(see Map-1.1)

(2) **Airport Bus** (Line 2B): Gate A4 station at Baiyun Airport A area arrival hall / Gate B11 station at Baiyun Airport B area arrival hall -- Hanpudun Hotel（汉普敦酒店）

Distance: 43km Time: about 50 minutes **Fare: RMB¥24**

(see Map-1.1)

(3) **Metro**: Guangzhou Baiyun International Airport (633 meters walk) -- North extension of Metro Line 3 (Direction of Tiyu Xilu) -- Tiyu Xilu (14 stations) -- Transfer Line 3 (Direction of Tianhe Coach Terminal) -- Exit E of Huashi (3 stations) -- South China Normal University (300 meters)

Distance: 37km Time: about 1.5hours **Fare: RMB¥8**

(see Map-1.2)

(1) **出租车（建议）：**广州白云国际机场——机场大道——广州机场高速——华南快速干线——中山大道西——华南师范大学

距离：43 公里　　时间：42 分钟　　费用：约 150-160 元

(2) **机场快线（空港快线 2b 线 华师大厦酒店方向）：**广州白云国际机场 A 区到达大厅 A4 号门——B 区到达大厅 B11 号门——汉普敦酒店

距离：43 公里　　时间：50 分钟　　费用：24 元

(3) **地铁：**广州白云国际机场（步行 633 米）——地铁 3 号线北延段（体育西路方向）——体育西路（14 站）——同站换乘 3 号线（天河客运站方向）——华师（3 站）E 出口——华南数学应用与交叉研究中心（300 米）

距离：37 公里　　时间：1.5 小时　　票价：8 元

1.3 Map

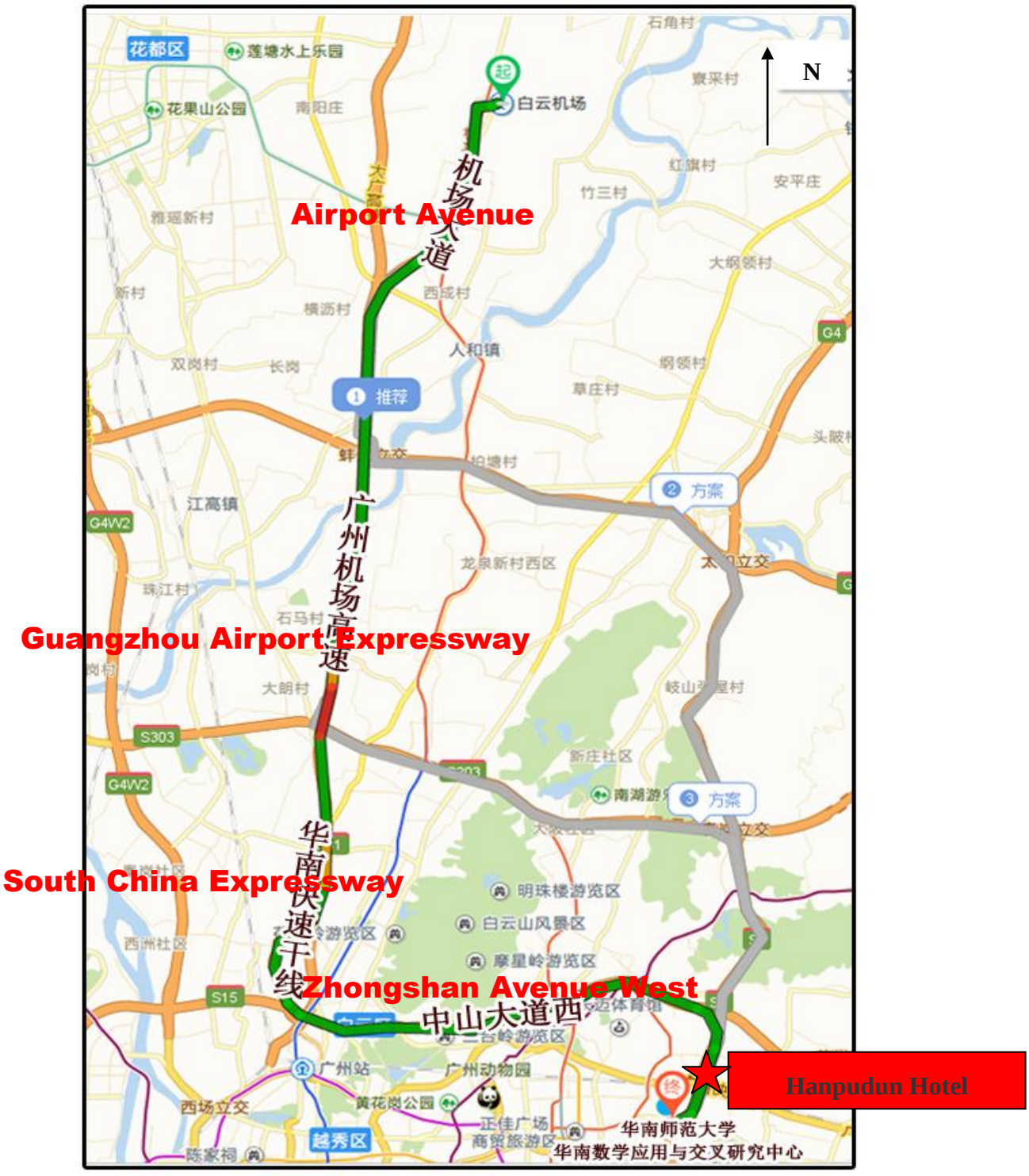
(1) Guangzhou Baiyun International Airport—Hanpudun Hotel(汉普敦酒店)

①If you take taxi or airport bus please see Map-1.1

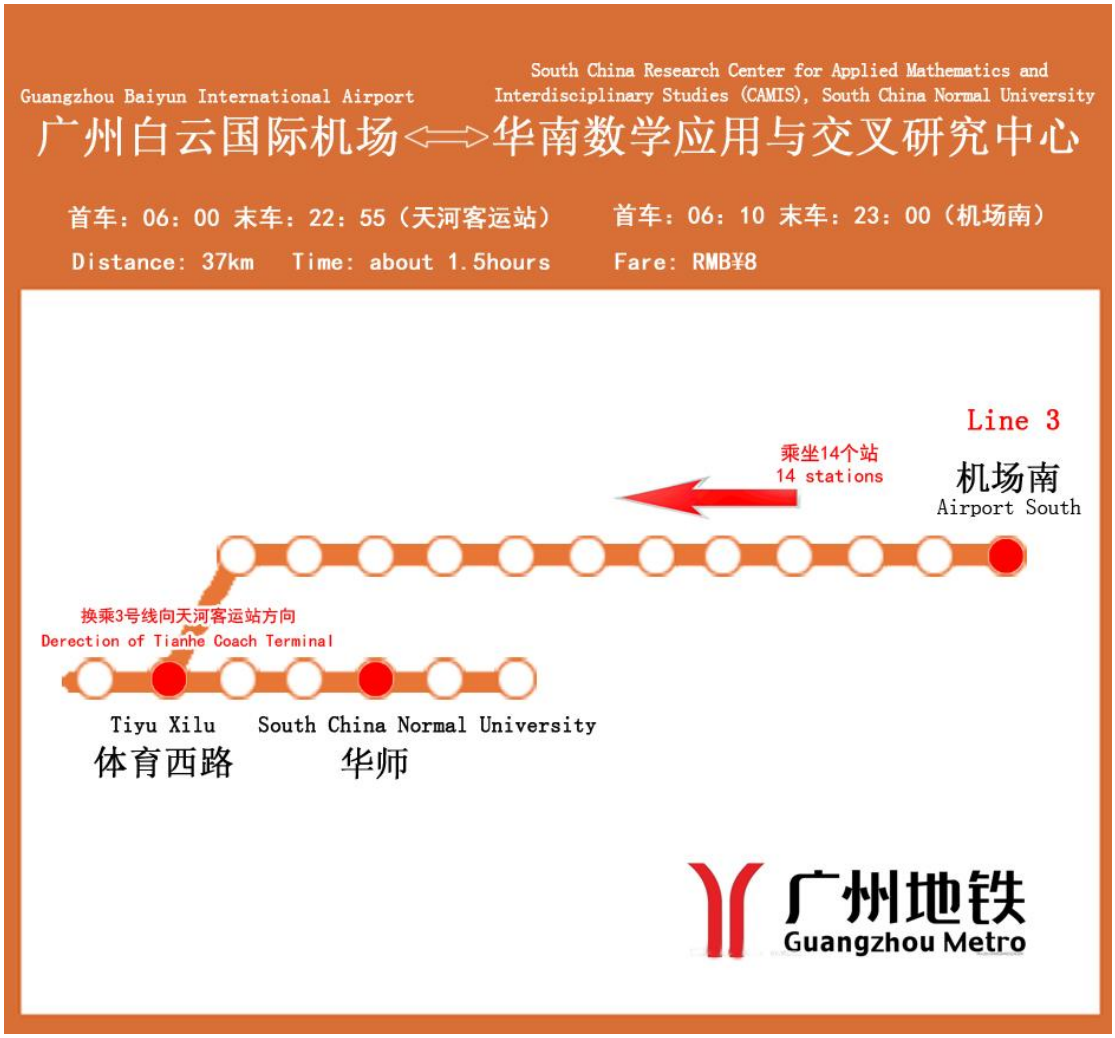
②If you take metro please see Map-1.2

(2) Hanpudun Hotel(汉普敦酒店) —South China Research Center for Applied Mathematics and Interdisciplinary Studies (CAMIS)

Please see campus map Map-1.3


N
Airport Avenue
机场大道
Guangzhou Airport Expressway
广州机场高速
South China Expressway
华南快速干线
Zhongshan Avenue West
中山大道西
Hanpudun Hotel
花都区
莲塘水上乐园
花果山公园
白云机场
南阳庄
雅瑶新村
横沥村
西城村
人和镇
双岗村
长岗
草庄村
大纲领村
竹三村
红旗村
安平庄
寮采村
石角村
推荐
方案
江高镇
龙泉新村西区
珠江村
石马村
大朗村
S303
G4W2
S15
G4
明珠楼游览区
白云山风景区
摩星岭游览区
广州站
广州动物园
黄花岗公园
正佳广场
商贸旅游区
华南师范大学
华南数学应用与交叉研究中心
西场立交
越秀区
陈家祠
西洲社区
新庄社区

Map-1.1


Guangzhou Baiyun International Airport
South China Research Center for Applied Mathematics and Interdisciplinary Studies (CAMIS), South China Normal University
广州白云国际机场⟺华南数学应用与交叉研究中心
首车：06：00 末车：22：55（天河客运站）
首车：06：10 末车：23：00（机场南）
Distance: 37km
Time: about 1.5hours
Fare: RMB¥8
Line 3
乘坐14个站
14 stations
机场南
Airport South
换乘3号线向天河客运站方向
Derection of Tianhe Coach Terminal
Tiyu Xilu
体育西路
South China Normal University
华师
广州地铁
Guangzhou Metro

Map-1.2


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

1.4 Notes

(1) Registration： Office 107, Camis

(2) Accommodation: Hanpudun Hotel 汉普敦酒店

(3) Meals:

Lunch (Huashi Hotel, buffet)

Dinner (Tao Yuan (桃园))

(4) Telephone helplines:

①Health Center: 020-85211120

②Security Office: 020-85211100

③Contact the CAMIS staffs if necessary:

Qingrong Yang（阳青蓉）: jczx1@m.scnu.edu.cn 15898517230

Wenjing Liang（梁文静）: jczx1@m.scnu.edu.cn 13622866875

Kaihua Huang（黄凯华）: 58419842@qq.com 13719046746

Jinkai Li（李进开）: jklimath@m.scnu.edu.cn 13128801297

Shijin Ding（丁时进）: dingsj@scnu.edu.cn 13650861899

2. Organizing Committee

Weizhu Bao (包维柱)（Chair）	National University of Singapore and South China Normal University
Shijin Ding (丁时进)	South China Normal University
Tiezheng Qian (钱铁铮)	The Hong Kong University of Science and Technology
Xiaoping Wang (王筱平)	Hong Kong University of Science and Technology and South China Normal University
Zhouping Xin (辛周平)	The Chinese University of Hong Kong and South China Normal University


知行荣新


华南数学应用与交叉研究中心


应用数学与交叉科学高端论坛暨华南师范大学华南数学应用
与交叉研究中心成立揭牌仪式 2018年5月11日——5月13日

3. Conference Schedule

November 14, 2018 (Wednesday)		
14:00-17:30	Registration---Office 107, Camis（中心 107 办公室）	
November 15, 2018 (Thursday)		
8:50-9:00	**Opening Ceremony**	
9:00-9:30	Zhonghua QIAO	Thermodynamic-consistent multiple-relaxation-time lattice Boltzmann equation model for two-phase fluids with Peng-Robinson equation of state
9:30-10:00	Hongyu LIU	Localization and geometrization in wave scattering and applications
10:00-10:30	Coffee/tea break	
10:30-11:00	Yana DI	Dynamic simulations of Q-tensor model of nematic liquid crystal flows
11:00-11:30	Yang XIANG	Energy and Dynamics of Grain Boundaries Based on Underlying Mircrostructure
11:30-12:00	Xinpeng XU	Dynamics of several soft matter solutions: multiscale modeling and simulations
12:00-14:00	Lunch---Huashi Hotel, buffet	
14:00-14:30	Xiang ZHOU	Simplified Gentlest Ascent Dynamics for Transition State in Non-Gradient Systems
14:30-15:00	Zhen ZHANG	Modeling and simulation of moving contact line problems with surfactant
15:00-15:30	Jun HU	A new simple adaptive finite element method for eigenvalue problems
15:30-16:00	Coffee/tea break	
16:00-16:30	Yanping CHEN	Two-grid methods for semilinear elliptic interface problems by immersed finite element methods
16:30-17:00	Qinglin TANG	An efficient numerical method to compute the ground state of rotating dipolar Bose-Einstein Condensates
17:00-17:30	Chunxiong ZHENG	Formulation of Nonlocal Boundary Value Problem and Its Asymptotic Analysis
18:00	Dinner---Tao Yuan (桃园)	
November 16, 2018 (Friday)		
8:30-9:00	Yufeng NIE	Nodes Placement Method by Bubble Simulation and Its' Application
9:00-9:30	Shuai LU	Filter based methods for statistical linear inverse problems
9:30-10:00	Jingzhi LI	Shape derivatives for scattering problems
10:00-10:20	Coffee/tea break	
10:20-10:30	Group Photo	
10:30-11:00	Xiaoqing JIN	Riemannian Method for Inverse Eigenvalue Problem

11:00-11:30	Yanren HOU	On the Weak Solutions to the Steady Navier-Stokes Equations with Mixed Boundary Conditions
11:30-12:00	Yongyong Cai	Nested Picard Iterative Integrators for Dirac equation in the nonrelativistic limit
12:00-14:00	Lunch---Huashi Hotel, buffet	
14:00-14:30	Dan HU	Weighted Least Square Analysis Method for Free Energy Calculation and Its Applications
14:30-15:00	Hui ZHANG	A positivity-preserving, energy stable and second order BDF scheme for the Cahn-Hilliard equation
15:00-15:30	Weiying ZHENG	Electromagnetic scattering problem in a two-layer medium
15:30-16:00	Coffee/tea break	
16:00-16:30	Hanquan WANG	A Chebyhev spectral element method and its application
16:30-17:00	Zhijian YANG	Effective boundary conditions for molecular dynamics simulations
17:00-17:30	Zhenli XU	Harmonic surface mapping algorithm for fast electrostatic sums
18:00	Dinner---Tao Yuan (桃苑)	
November 17, 2018 (Saturday)		
8:30-9:00	Ziqing XIE	A Globally Convergent Barzilai-Borwein-type Local Minimax Method for Finding Multiple Saddle Points
9:00-9:30	Weiwei SUN	Recent development on maximal L^p analysis of parabolic finite element solutions
9:30-10:00	Zhiwen ZHANG	Computing effective diffusivity of chaotic and stochastic flows using structure preserving schemes
10:00-10:30	Coffee/tea break	
10:30-11:00	Zaiwen WEN	Second-Order Type Optimization Methods For Data Analysis
11:00-11:30	Wei JIANG	Solid-state dewetting: modeling, numerics and analysis
11:30-12:00	Zhongyi HUANG	Asymptotic analysis and numerical method for singularly perturbed eigenvalue problems
12:00-14:00	Lunch---Huashi Hotel, buffet	
14:00-14:30	Guanghui HU	Towards the efficient and robust numerical methods for Kohn-Sham equation
14:30-15:00	Ran ZHANG	A weak Galerkin nite element scheme for the Cahn-Hilliard equation
15:00-15:30	Liwei XU	Numerical investigation for electromagnetic waves in fluids
15:30-16:00	Coffee/tea break	
16:00-17:30	Free Discussion and closing ceremony	
18:00	Dinner---Tao Yuan (桃苑)	
November 18, 2018 (Sunday)		
	Departure	

4. Titles&Abstracts

1. **Thermodynamic-consistent multiple-relaxation-time lattice Boltzmann equation model for two-phase fluids with Peng-Robinson equation of state**

Qiao Zhonghua

The Hong Kong Polytechnic University

In this work, a multiple-relaxation-time (MRT) lattice Boltzmann (LB) equation model with Beam-Warming (B-W) scheme is proposed to simulate multi-phase fluid system with Peng-Robinson (P-R) equation of state (EOS). The mathematical model of the multi-phase fluid flow is derived based on the NVT-based framework, where the Helmholtz free energy of P-R fluid is introduced. The non-ideal force in multi-phase flow is directly computed from the free energy so that a more compact formulation of hydrodynamic equations, which is termed as potential form, can be obtained. The MRT-LB model is developed based on the potential form of hydrodynamic equations, which can eliminates the parasitic currents effectively. In addition, to capture the tiny nonconvex perturbation from the linear trend of P-R model precisely, the B-W scheme is utilized in the present MRT-LB model, which leads to an adjustable Courant-Friedrichs-Lewy (CFL) number and the second order accuracy can be naturally achieved by this scheme without any other requirement and numerical boundary conditions. In the numerical experiments, a realistic hydrocarbon component, such as isobutane, in three dimensional space is simulated by the proposed MRT-LB model. Numerical results show that the magnitude of parasitic currents can be significantly reduced by the present MRT-LB model. In addition, our numerical predictions of surface tension agree well with the experimental data, which verify the effectiveness of the proposed MRT-LB model.

2. Localization and geometrization in wave scattering and applications

Hongyu Liu

Hong Kong Baptist University

In this talk, the speaker shall discuss their recent discovery on the localization and geometrization in wave scattering as well as the corresponding applications in invisibility, inverse scattering and plasmon resonances.

3. **Dynamic simulations of Q-tensor model of nematic liquid crystal flows**

Yana DI

Institute of Computational Mathematics and Scientific/Engineering Computing

We present a linear energy-stabled numerical scheme for the hydrodynamic Beris-Edwards model. Several numerical examples are shown to demonstrate the effectiveness of the model and the numerical scheme in simulating the dynamics of defects in flows of nematic liquid crystals.

4. Energy and Dynamics of Grain Boundaries Based on Underlying Mircrostructure

XIANG Yang

Hong Kong University of Science and Technology

Grain boundaries are the interfaces of grains with different orientations in polycrystalline materials. Energetic and dynamic properties of grain boundaries play essential roles in the mechanical and plastic behaviors of the materials. These properties of grain boundaries strongly depend on their microscopic structures. We present continuum models for the energy and dynamics of grain boundaries based on the continuum distribution of the line defects (dislocations or disconnections) on them. The long-range elastic interaction between the line defects is included in the continuum models to maintain stable microstructure on grain boundaries during the evolution. The continuum models are able to describe both normal motion and tangential translation of the grain boundaries due to both coupling and sliding effects that were observed in atomistic simulations and experiments.

5. Dynamics of several soft matter solutions: multiscale modeling and simulations

Xinpeng Xu

Guangdong Technion (广东以色列理工学院)

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 usually show fascinating phase structure and dynamic properties. In this talk, I will show modeling efforts from simple binary solutions, to polymer solutions, to diblock copolymer solutions, and to colloidal suspensions. 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. Some simulations results will also be shown during the talk.

6. Simplified Gentlest Ascent Dynamics for Transition State in Non-Gradient Systems

周翔

City University of Hong Kong

The transition states on potential energy surface belong to a class of special saddle points having only one unstable direction. They play key roles in the understanding the rare events like phase transitions and noise-induced transitions escaping a stable point. We first review our work on theoretic and numerical progresses: the gentlest ascent dynamics (GAD) and the iterative minimization algorithm. We then present the recent work of the simplified GAD (joint with Shuting Gu) for the non-gradient system which reduces the cost of GAD by half. The application of the Allen-Cahn equation subject to the shear flow is presented to investigate the influence of the shear on the morphology of the transition state. The work is supported by HK GRF.

7. Modeling and simulation of moving contact line problems with surfactant

ZHANG Zhen

Southern University of Science and Technology

We introduce a sharp interface models for moving contact lines with surfactant. A continuous model with the boundary conditions is derived for the dynamics of two immiscible fluids with moving contact lines based on thermodynamic principles. FEM-based numerical method is developed to solve the resulting free boundary problem. We also discuss related models on elastic materials.

8. A new simple adaptive finite element method for eigenvalue problems

Hu Jun

Peking University

A new simple adaptive finite element method is proposed to solve the eigenvalue problems of the second order elliptic self-adjoint operators. The proposed algorithm consists of two steps. In the first step, the standard adaptive finite element method is used to solve a source problem (with a properly chosen right-hand side function) associated to the eigenvalue problem, whose main purpose is to design an adaptive locally refined mesh which can captures the singularity caused by the operator and the boundary of the domain. In the second step, the eigenvalue problem is approximately solved by some finite element methods defined over the final adaptive mesh from the first step. Compared with the standard adaptive finite element method for the eigenvalue problem in the literature, a distinctive feature of our algorithm herein is that, instead of solving the eigenvalue problem over and over again, our method only solves one discrete (generalized) eigenvalue problem in the whole procedure. We perform several numerical examples in both 2D and 3D, and results shows that the computational cost of our method is much less than standard method without losing accuracy of the approximation of the eigenpairs. This demonstrate the efficiency and superiority of the new algorithm, and its potential to be applied to large-scale adaptive computations.

9. Two-grid methods for semilinear elliptic interface problems by immersed finite element methods

Yanping Chen

South China Normal University

In this talk, three efficient two-grid algorithms are proposed and analyzed for semi-linear interface problems with discontinuous diffusion coefficients in two dimension. Because of the advantages of simple structure of Cartesian grids and the finite element formulation, we use immersed finite element discretization. To linearize the finite element method equations, two-grid algorithms based on some Newton iteration approach and residual-correction technique are

applied. It is shown that the coarse space can be extremely coarse, and yet one can still achieve asymptotically optimal approximations as good as solving the original nonlinear problem on the fine mesh. As a result, solving such a large class of nonlinear equation will not be much more difficult than solving one linearized equation.

10. An efficient numerical method to compute the ground state of rotating dipolar Bose-Einstein Condensates

Qinglin Tang

Sichuan University

In this talk, we will present an efficient numerical method for computing the ground state of the rotating dipolar Bose-Einstein Condensates (BEC). The method consists two main merits: (i) efficient and accurate numerical methods will be proposed to evaluate the nonlocal dipole-dipole interaction. (ii). a nonlinear conjugate gradient method, accelerated by some well-adapted preconditioners, will be developed to compute the ground states. This work is realised in collaboration with Xavier ANTOINE (IECL, Lorraine, France), Antoine LEVITT (Inria, Paris, France) and Yong ZHANG (Tianjin University, Tianjin, China).

11. Formulation of Nonlocal Boundary Value Problem and Its Asymptotic Analysis

Chunxiong Zheng

Tsinghua University & Xinjiang University

12. Nodes Placement Method by Bubble Simulation and Its' Application

Yufeng Nie

Northwestern Polytechnical University

Nodes placement method by bubble simulation (NPBS) and its parallel version are introduced in this talk. Local mesh can be easily produced based on the nodes set developed by NPBS. Through introducing Riemann matrix, anisotropic meshes satisfying the size function can also be generated easily. As an application, adaptive finite element combined with NPBS is also introduced.

Keywords: Node placement; Local mesh; Anisotropic mesh; Load balancing; Adaptive finite element

13. Filter based methods for statistical linear inverse problems

Shuai Lu

Fudan University

Ill-posed inverse problems are ubiquitous in applications. Understanding of algorithms for their solution has been greatly enhanced by a deep understanding of the linear inverse problem. In the applied communities ensemble-based filtering methods have recently been used to solve inverse problems by introducing an artificial dynamical system. This opens up the possibility of using a range of other filtering methods, such as 3DVAR and Kalman based methods, to solve inverse problems, again by introducing an artificial dynamical system. The aim of this talk is to analyze such methods in the context of the ill-posed linear inverse problem.

Statistical linear inverse problems are studied in the sense that the observational noise is assumed to be derived via realization of a Gaussian random variable. We investigate the asymptotic behavior of filter based methods for these statistical linear inverse problems. Rigorous convergence rates are established for 3DVAR and for the Kalman filters, including minimax rates in some instances. Blowup of 3DVAR and its variant form is also presented, and optimality of the Kalman filter is discussed. These analyses reveal close connection between (iterative) regularization schemes in deterministic inverse problems and filter based methods in data assimilation. It is a joint work with Dr. M. A. Iglesias (U. of Nottingham, UK), Dr. K. Lin (Fudan U., China) and Prof. A. M. Stuart (Caltech, USA).

14. Shape derivatives for scattering problems

Jingzhi Li

Southern University of Science and Technology

This talk studies the “derivative” of solutions of second-order boundary value problems and of output functionals based on them with respect to the shape of the domain. A rigorous approach relies on encoding shape variation by means of deformation vector fields, which will supply the directions for taking shape derivatives. These derivatives and methods to compute them numerically are key tools for studying shape sensitivity, performing gradient based shape optimization, and small-variation shape uncertainty quantification. A unifying view of second-order elliptic boundary value problems recasts them in the language of differential forms (exterior calculus). Fittingly, the shape deformation through vector fields matches the concept of Lie derivative in exterior calculus. This paves the way for a unified treatment of shape differentiation in the framework of exterior calculus. Applications in scattering problems reveals the extraordinary power of the machinery.

15. Riemannian Method for Inverse Eigenvalue Problem

金小庆

University of Macau

In this talk, I will use the Riemannian optimization method to solve inverse eigenvalue problems. The convergence rate and numerical results will be given.

16. On the Weak Solutions to the Steady Navier-Stokes Equations with Mixed Boundary Conditions

Yanren Hou

Xi'an Jiaotong University

In this talk, for the Navier-Stokes equations in a bounded polygon or polyhedron $\Omega\subset R^d$, $d=2,3$, with a homogenous stress type mixed boundary condition, we first try to establish an a priori estimate for possible weak solutions by means of expanding the original system. Then the existence result without small data and/or large viscosity restriction is obtained. Finally, a global uniqueness result of the weak solution is an obvious result based on the a priori estimate obtained.

17. Nested Picard Iterative Integrators for Dirac equation in the nonrelativistic limit

蔡勇勇

北京计算科学研究中心

We present the construction and analysis of uniformly accurate nested Picard iterative integrators (NPI) for the Dirac equation in the nonrelativistic limit regime, which involves high frequency waves in time. To overcome the difficulty induced by the rapid temporal oscillation, we present the construction of several NPI methods which are uniformly first-, second- and third-order convergent in time w.r.t. the oscillation. The general idea is applying nested Picard iterations to the integral form of the Dirac equation and using exponential wave integrators to approximate the temporal integrals.

18. Weighted Least Square Analysis Method for Free Energy Calculation and Its Applications

Dan Hu

Shanghai Jiao Tong University

Free energy calculation is an efficient way for studying rare event dynamics. For a complex rare event dynamics, multiple reaction coordinates may be required to describe the transition path between equilibrium states. Theoretically, a one dimensional sampling along the transition path can provide sufficient information to calculate the potential of mean force (PMF) along the transition path. In the widely used free energy analysis method Wham, the sample data are divided

into a series of bins to calculate PMF. However, bin segmentation in Wham is coupled with the umbrella potentials applied in each window, because each umbrella potential is assumed to have a close value for all sample points in each bin. This coupling makes it difficult to perform one-dimensional bin segmentation along the transition path when multi-variable umbrella potentials are used in sampling. Here we develop a \underline{we}ighted \underline{l}east \underline{s}quare \underline{a}nalysis \underline{m}ethod (Welsam) to take the place of Wham for free energy analysis. In the new method Welsam, bin segmentation is decoupled from application of umbrella potentials. As a result, it becomes very convenient to perform one-dimensional bin segmentation and calculate one-dimensional potential of mean force along the transition path. Our simulation results suggest that Welsam has a comparable statistical error with Wham. Furthermore, Welsam can be used to reduce waste of sample data obtained during exploration of reaction coordinates. Examples including the applications in transmembrane permeation of ions will be discussed to illuminate the convenience of Welsam.

19. A positivity-preserving, energy stable and second order BDF scheme for the Cahn-Hilliard equation

张辉

北京师范大学

Here we present and analyze a new second-order energy stable Backward Differentiation Formula (BDF) finite difference scheme for the Macromolecular Microsphere Composite, Time-Dependent Ginzburg-Landau (MMC-TDGL) equation, a Cahn-Hilliard equation with Flory-Huggins-deGennes energy potential. One major challenge for the higher-order-in-time discretization is how to ensure an unconditional energy stability without compromising numerical efficiency or accuracy. We propose a second-order numerical scheme with unconditional energy stability using the BDF method with Douglas-Dupont regularization term. In addition, we drive an estimated bound for the numerical solution, which satisfies the maximum principle. For the error convergent analysis, to deal with the nonlinear logarithmic terms, we treat three nonlinear logarithmic terms as a whole and deal with all logarithmic terms directly by using the property that the nonlinear error inner product is always non-negative. Moreover, we present the detailed convergence analysis and multigrid method to solve the nonlinear numerical scheme, and various numerical results are presented, including the numerical convergence test, positivity-preserving property test, spinodal decomposition, energy dissipation and mass conservation properties.

20. Electromagnetic scattering problem in a two-layer medium

Weiying Zheng

Academy of Mathematics and Systems Science, Chinese Academy of Mathematics

This talk is focused on scattering problems in two-layer media, particularly, on PML

(perfectly matched layer) boundary conditions on the truncation boundary of the unbounded domain. The PML method is widely used in the engineering literature and proves to be very efficient for solving wave propagating problems. Since the pioneering work of Berenger, remarkable progresses have been made in the study of PML methods for acoustic, electromagnetic, and elastic scattering problems in homogeneous background media. However, the results for PML methods are still rare in inhomogeneous media, particularly, in stratified media. In this talk, I mainly focus on the stability and exponential convergence of PML methods for scattering problems in two-layer media.

21. A Chebyhev spectral element method and its application

王汉权
云南财经大学

We mainly discusses Chebyshev collocation-based spectral element method for the boundary value problem of the elliptic equations. There are few literature on how to implement collocation-based spectral element method for the elliptic problems. We describe how to apply the Chebyshev collocation-based spectral element method to numerically solve the boundary value problems of the elliptic equations. Firstly, the method constructed here uses the idea of the finite element method to decompose the domain of the equation, and divides the domain into several connected subdomains. Secondly, it uses the collocation-based method to discretize the elliptic equations in each subdomain. Thirdly, using the ideology of the finite element method assembles the unit stiffness matrix into a total stiffness matrix. Finally, the numerical solution of the unknown function can be found from the discretized system. This method can be used to deal with elliptic equations with the variable coefficients. It can also solve the boundary value problems for the elliptic equations defined in complex regions. Another benefit of the method lies on that it can achieve comparably simple programming. This is undoubtedly a value of this method. Extension of the numerical method to investigate the elliptic boundary value problem with singular solution and how to solve the time-dependent nonlinear Schrodinger equation with nonzero boundary condition are also discussed.

22. Effective boundary conditions for molecular dynamics simulations

Zhijian Yang
Wuhan University

This talk presents an absorbing boundary condition for molecular dynamics simulations of materials defects. The purpose of the boundary condition is to eliminates spurious reflections of phonons at the boundary and minimize the finite size effect. In contrast to other existing methods, our emphasis is placed on the ease of implementation. In particular, we propose a method for which the implementation can be done within existing molecular dynamics code, and it is

insensitive to lattice structure, the geometry and space dimension of the computational domain. To demonstrate the effectiveness, the results from two test problems are presented.

23. Harmonic surface mapping algorithm for fast electrostatic sums

Zhenli Xu

Shanghai Jiao Tong University

The fast and accurate evaluation of electrostatic interactions for particle systems at microscale has been one of the core topics for molecular simulations. We present a harmonic surface mapping algorithm (HSMA) for fast electrostatic sums of finite sources and infinite image sources. Compared to the popular PME method, this algorithm is be useful for more general boundary conditions rather than periodic boundary, and it is much easier for parallelization. The HSMA uses the property that the induced potential due to infinite images is harmonic and can be expanded into a Harmonic series. The analytical harmonic series is mapped into a boundary integral over a surface containing the simulation box, which is approximated by a particle system composed of the point sources and a finite number of point image charges, and thus can be efficiently calculated by FMM or the GPU calculations. The performance of the algorithm is shown by numerical examples.

24. A Globally Convergent Barzilai-Borwein-type Local Minimax Method for Finding Multiple Saddle Points

Ziqing Xie

Hunan Normal University

Saddle points, which are unstable critical points, have a widely range of applications in many fields of nonlinear science, such as nonlinear optics, condensed matter physics, chemical reactions, and materials science etc.. Owning to the nonlinearity of model problems, the multiplicity and instability of saddle points, it is extremely challenging to design a stable, efficient and globally convergent numerical algorithm for finding saddle points. In this talk, a globally convergent Barzilai-Borwein-type local minimax method (GBB-LMM) is proposed for finding multiple saddle points of nonconvex functionals in Hilbert space, where the idea of the Barzilai-Borwein gradient method combining with the nonmonotone line search strategy in optimization in Euclidean space is applied to solve a two-level local optimization problem. Actually, the Barzilai-Borwein-type step-size is explicitly constructed as a trial step-size at each iteration step of the local minimax method, and the nonmonotone step-size search rule is introduced to guarantee the global convergence. The feasibility and global convergence of the GBB-LMM are rigorously verified. The GBB-LMM is then implemented to solve several typical nonlinear boundary value problems with variational structures for multiple unstable solutions. The numerical results indicate that our approach may greatly speed up the convergence of traditional local minimax methods.

Keywords: global convergence, local minimax method, nonmonotone search rule, Barzilai-Borwein method, multiple saddle points

(Joint work with Yongjun Yuan, Wei Liu, and Ying Tang)

25. Recent development on maximal L^p analysis of parabolic finite element solutions

Weiwei Sun

City University of Hong Kong

The maximal L^p regularity/stability analysis is an important tool in the study of parabolic PDEs, particularly for nonlinear problems. The analysis on the discrete settings,such as finite element parabolic system, is incomplete andlimited to simple linear problems, although the L^p approach has shown its potential and advantage over the traditional L^2 analysis in dealing with strongly nonlinear equations. In this talk, we shall give a review on recent development of the maximal L^p regularity/stability estimates of parabolic finite element solutions. Also we present our recent works on establishing a solid framework of the maximal L^p regularity of fully-discrete finite element solutions of general linear parabolic PDEs and L^p-norm optimal error estimates for several nonlinear physical equations.

26. Computing effective diffusivity of chaotic and stochastic flows using structure preserving schemes

Zhiwen Zhang

The University of Hong Kong

We study the problem of computing the effective diffusivity for a particle moving in chaotic and stochastic flows. In addition, we numerically investigate the residual diffusion phenomenon in chaotic advection. Instead of solving the Fokker-Planck equation in the Eulerian formulation, we compute the motion of particles in the Lagrangian formulation, which is modeled by stochastic differential equations (SDEs).

We propose an effective numerical integrator based on a splitting method to solve the corresponding SDEs in which the deterministic subproblem is symplectic-preserving while the random subproblem can be viewed as a perturbation. We provide rigorous error analysis for the new numerical integrator using the backward error analysis (BEA) technique and show that our method outperforms standard Euler-based integrators. Numerical results are presented to demonstrate the accuracy and efficiency of the proposed method for several typical chaotic and stochastic flow problems of physical interests. The existence of residual diffusivity for these flow problems is also investigated.

27. Second-Order Type Optimization Methods For Data Analysis

Zaiwen Wen

Peking University

Optimization models are ubiquitous in data analysis. In this talk, we will review Gauss-Newton methods for phase retrieval, semi-smooth Newton methods for composite convex programs and its application to large-scale semi-definite program problems, sub-sampled semismooth Newton method for nonsmooth composite minimization problems from large-scale machine learning, as well as an adaptive regularized Newton method for Riemannian Optimization.

28. Solid-state dewetting: modeling, numerics and analysis

蒋维

武汉大学

In this talk, I will talk about our recent works about mathematical modeling, numerical simulations and theoretical analysis for solid-state dewetting problems.

29. Asymptotic analysis and numerical method for singularly perturbed eigenvalue problems

Zhongyi Huang

Tsinghua University

In this talk, we study the asymptotic analysis and numerical method for singularly perturbed eigenvalue problems (SPEP) which arise in fluid mechanics and quantum mechanics. We first make a close asymptotic analysis on the SPEP, and prove the main theorems about the asymptotic behavior of the eigenvalues and eigenfunctions. Then we propose a new tailored finite point method (TFPM) for numerical solutions of SPEP with higher accuracy. Our numerical examples verify our theory and show the feasibility and efficiency of our method.

30. Towards the efficient and robust numerical methods for Kohn-Sham equation

HU Guanghui

University of Macau

In this talk, we will introduce our recent work on the adaptive finite element framework for Kohn-Sham density functional theory. The background of Kohn-Sham DFT, as well as the challenges in developing robust and efficient numerical methods will be briefly described. In our work, an h-adaptive finite element framework has been proposing, and several numerical techniques such as the algebraic multigrid method, imaginary time propagation preconditioning, and multilevel correction, has been successfully applied on the algorithm towards the efficiency and robustness. A variety of numerical experiments will be demonstrated to show the effectiveness

of our method.

31. A weak Galerkin nite element scheme for the Cahn-Hilliard equation

Ran Zhang

Jilin University

This talk presents a weak Galerkin (WG) nite element method for the Cahn- Hilliard equation. The WG method makes use of piecewise polynomials as approximating functions, with weakly de ned partial derivatives (first and second order) computed locally by using the information in the interior and on the boundary of each element. A stabilizer is constructed and added to the numerical scheme for the purpose of providing certain weak continuities for the approximating function. A mathematical convergence theory is developed for the corresponding numerical solutions, and optimal order of error estimates are derived. Some numerical results are presented to illustrate the e?fficiency and accuracy of the method.

32. Numerical investigation for electromagnetic waves in fluids

Liwei Xu

University of Electronic Science and Technology of China

In this talk, we first introduce several models describing electromagnetic waves in fluids and electromagnetic waves in metals. We design and analyze discontinuous or continuous Galerkin schemes for numerical solutions of these models, and numerical results will be presented to illustrate the accuracy and efficiency of the model and the proposed scheme.

5. List of Participants

No.	Name	Institute	E-mail	Remark
1	Weizhu BAO	National University of Singapore and South China Normal University	matbaowz@nus.edu.sg	
2	Yongyong CAI	Beijing Computational Science Research Center	yongyong.cai@csrc.ac.cn	
3	Yanping CHEN	South China Normal University	yanpingchen@scnu.edu.cn	
4	Shijin DING	South China Normal University	dingsj@scnu.edu.cn	
5	Yana DI	Institute of Computational Mathematics, CAS	yndi@lsec.cc.ac.cn	
6	Wenyong GAN	Foshan University	gan.wyong@aliyun.com	
7	Xiaojing GAO	South China Normal University	780012428@qq.com	
8	Guanghui HU	University of Macau	garyhu@umac.mo	
9	Zhongyi HUANG	Tsinghua University	zhuang@math.tsinghua.edu.cn	
10	Yanren HOU	Xi'an Jiaotong University	yrhou@mail.xjtu.edu.cn	
11	Dan HU	Shanghai Jiaotong University	hudan80@sjtu.edu.cn	
12	Xiaoqing JIN	University of Macau	xqjin@umac.mo	
13	Chaolong JIANG	Yunnan University of Finance and Economics	Chaolong_jiang@126.com	
14	Jun HU	Peking University	hujun@math.pku.edu.cn	
15	Weijie HUANG	Beijing Computational Science Research Center	huangwj@csrc.ac.cn	
16	Wei JIANG	Wuhan University	jiangwei1007@whu.edu.cn	
17	Jingzhi LI	Southern University of Science and Technology	lijz@sustc.edu.cn	
18	Ying LIN	South China Normal University	linying@live.cn	
19	Hongyu LIU	Hong Kong Baptist University	hongyuliu@hkbu.edu.hk	
20	Shuai LU	Fudan University	slu@fudan.edu.cn	
21	Mingyu Mo	South China Normal University	84026925@qq.com	
22	Yufeng NIE	Northwest Polytechnic University	yfnie@nwpu.edu.cn	
23	Tiezheng QIAN	The Hong Kong University of Science and Technology	maqian@ust.hk	

24	Zhonghua QIAO	Hong Kong Baptist University	zhonghua.qiao@polyu.edu.hk	
25	Weiwei SUN	City University of Hong Kong	maweiw@cityu.edu.hk	
26	Qinglin TANG	Sichuan University	tang@scu.edu.cn	
27	Xiaoping WANG	The Hong Kong University of Science and Technology and South China Normal University	mawang@ust.hk	
28	Hanquan WANG	Yunnan University of Finance and Economics	wang_hanquan@hotmail.com	
29	Zaiwen WEN	Peking University	wenzw@pku.edu.cn	
30	Tingchun WANG	Nanjing University of Information Science & Technology	Wangtingchun2010@gmail.com	
31	Yan WANG	Central China Normal University	wang.yan@mail.ccnu.edu.cn	
32	Yang WANG	Xiangtan University	Wy2010ang@163.com	
33	Jianchen WEI	South China Normal University	445361959@qq.com	
34	Yang XIANG	Hong Kong University of Science and Technology	maxiang@ust.hk	
35	Ziqing XIE	Hunan Normal University	ziqingxie@hunnu.edu.cn	
36	Liwei XU	University of Electronics and Technology	xul@uestc.edu.cn	
37	Xinpeng XU	Guangdong Technion—Israel Institute of Technology	xu.xinpeng@gtiit.edu.cn	
38	Zhenli XU	Shanghai Jiaotong University	xuzl@sjtu.edu.cn	
39	Zhijian YANG	Wuhan University	zjyang.math@whu.edu.cn	
40	Qi YE	South China Normal University	yeqi@m.scnu.edu.cn	
41	Hui ZHANG	Beijing Normal University	hzhang@bnu.edu.cn	
42	Ran ZHANG	Jilin University	zhangran@jlu.edu.cn	
43	Zhen ZHANG	Southern University of Science and Technology	zhangz@sustc.edu.cn	
44	Zhiwen ZHANG	Hong Kong University	zhangzw@hku.hk	
45	Chunxiong ZHENG	Tsinghua University	czheng@math.tsinghua.edu.cn	
46	Weiying ZHENG	Institute of Computational Mathematics	zwy@lsec.cc.ac.cn	
47	Xiang ZHOU	City University of Hong Kong	xizhou@cityu.edu.hk	