

# Modeling and Numerical Methods for Interfacial Dynamics 界面动力学的建模和数值方法研讨会

# **Conference Brochure**

# 会议手册

Shenzhen, China Dec 15-17, 2018

Southern University of Science and Technology of China 中国南方科技大学

Address: Xue Yuan Avenue 1088, Nanshan District, Shenzhen, China 地址: 广东省深圳市南山区学苑大道 1088 号

# Catalogue

| 1. Information of Participants2 |    |  |  |  |
|---------------------------------|----|--|--|--|
| 1.1 Date                        | 2  |  |  |  |
| 1.2 Address                     | 2  |  |  |  |
| 1.3 Travel Information          | 3  |  |  |  |
| 1.4 Notes                       | 7  |  |  |  |
| 2. Conference Schedule          | 8  |  |  |  |
| 3. List of Participants         | 11 |  |  |  |
| 4. Title&Abstracts              | 13 |  |  |  |

# **1. Information of Participants**

# 1.1 Date

December 15-17, 2018

# 1.2 Address

1.2.1 Conference Address: Conference Room 415, Block 3, Hui Yuan, Southern University of Science and Technology Xue Yuan Avenue 1088, Nanshan District, Shenzhen

**会议地址:** 广东省深圳市南山区学苑大道 1088 号 南方科技大学 慧园 3 栋 415 报告厅

1.2.2 Hotel Address: Wen Hang Hotel, Li Shui Road 1128, Nanshan District, Shenzhen

酒店地址:广东省深圳市南山区丽水路1128号 文航酒店

# **1.3 Travel Information**

# 1.3.1 Shenzhen Baoan International Airport — Wen Hang Hotel

(1) Taxi (Suggest): Distance: 32km Time: About 45 minutes

# Fare: about RMB ¥80

出租车 (建议): 距离: 32km 时间: 约45分钟

# 费用:约80元

If the taxi driver doesn't familiar with the name of the hotel, please show him the Chinese address directly.

若司机不熟悉酒店名字,请直接告知中文地址。

(2) Metro & Bus: Shenzhen Baoan International Airport (350m walk) --Metro Line 11 (Direction of Futian, 3 stations) -- Qian Hai Wan
--Transfer to Metro Line 5 (Direction of Huang Bei Ling, 10 stations) -- Exit C of University Town -- Transfer to Bus m169 (170m walk to Lishan road south station, 7 stations) -- Chunyuan crossing station (210m walk) -- Wen Hang Hotel
Distance: 28.8km Time: About 70 minutes

#### Fare: RMB ¥9

**地铁&公交:**深圳宝安国际机场(步行350m)-- 地铁11号线(福田方向,3站)-- 前海湾站-- 站内转乘地铁5号线(黄贝岭方向, 10站)-- 大学城站C出口-- 转乘公交m169(步行170m至丽山路南站,7站)-- 春园路口站(步行210m)-- 文航酒店 距离: 28.8km 时间: 约70分钟

# 费用:9元

## **1.3.2 Hongkong International Airport** — Wen Hang Hotel

- (1) Transit Bus & Taxi: Hongkong International Airport -(Transit Bus)-Kingkey Banner Center -(Taxi)- Wen Hang Hotel Time: about 2 hours Fare: about HKD \$150 + RMB ¥40 P.S. Please refer to Pic-1 过境商务巴士&出租车: 香港国际机场 - (过境商务巴士) - 京基 百纳广场-(出租车)-文航酒店 时间:约2小时 费用:约150港币+40元 P.S. 请参考图 1
- (2) Ferry & Taxi: Hongkong International Airport -(Automated People Mover)- SkyPier Port -(Ferry)- Shekou Port -(Taxi)- Wen Hang Hotel Time: about 2 hours Fare: about HKD \$220 + RMB ¥60
  P.S. Please refer to Pic-2
  轮渡 & 出租车: 香港国际机场 (旅客捷运) 海天客运码头-(轮渡) 深圳蛇口口岸-(出租车) -文航酒店 时间: 约2小时 费用: 约220 港币+60 元
  P.S. 请参考图 2

| igkey be   | mont Conta   | 万 Skill  | 間日岸<br>nSay Poet                 | 港國際  | 祭機均   |
|--|--|--|----------------------------------|--|---|
|  | 開車時間   | )Departu   | ure time                         |  |   |
| 每天早  | 上06:3  | 80到晚_  | £21:45                           | (約15分  | 鐘一班   |
| 價FA  | RE   | -  | 來回豐價                             | OUDVOC   |   |
| pla Trip :                                       | MB¥150   | -  | Round Trip:                      | KWB ¥ 28   | 0 20  |
| 持京基  | 荣回車事設<br>享用送達住<br>1月33、14日31   | 代現来車日<br>所服務<br>Emilan   | 来回<br>Round                      | RMB¥   | 320   |
|  | State of the second state of the second  | Real of the Association of the A |                                  |  |   |
|  |  |  |                                  |  | -   |
| <b>F港国</b>                                       | 國際機均   | 易题   | 和学 方                             | 基百編  | 内廣均   |
| F港国<br>C Interna                                 | 國際機<br>ational Airpo<br>関車時間   | 場<br>IDepart   | III Kin<br>Kin                   | 基百編<br>gkey Banne  | 内廣均<br>er Center  |
| F港国<br>K. Interna<br>07:00                       | 國際機<br>ational Airpo<br>関車時間<br>07:30  | 示<br>(Deport.<br>08:00   | においた<br>Kin<br>Ire time<br>08:30 | 基百編<br>gkey Banne<br>09:00                                     | 内廣均<br>r Center<br>シン<br>09:30                                |
| F港国<br>C Interna<br>07:00<br>10:00               | 國際機<br>ational Airpo<br>開車時間<br>07:30<br>10:30                                   | 日本語の の の の の の の の の の の の の の の の の の の   | にで time<br>08:30<br>11:30        | 基百約<br>gkey Banne<br>09:00<br>12:00                            | 内廣均<br>r Center<br>09:30<br>12:30                             |
| F港国<br>07:00<br>10:00<br>13:00                   | 國際機<br>ational Airpo<br>開車時間<br>07:30<br>10:30<br>13:30                          | 日本語の の の の の の の の の の の の の の の の の の の   | に日本<br>11:30<br>14:30            | 基百約<br>gkey Banne<br>09:00<br>12:00<br>15:00                   | 内廣均<br>r Center<br>09:30<br>12:30<br>15:30                    |
| 5港国<br>07:00<br>10:00<br>13:00<br>16:00          | 即祭機<br>ational Airpo<br>開車時間<br>07:30<br>10:30<br>13:30<br>16:30                 | Deport<br>08:00<br>11:00<br>14:00<br>17:00   | 11:30<br>17:30                   | 基百約<br>gkey Banne<br>09:00<br>12:00<br>15:00<br>18:00          | 内廣均<br>r Center<br>09:30<br>12:30<br>15:30<br>18:30           |
| F港国<br>07:00<br>10:00<br>13:00<br>16:00<br>19:00 | <b>國際機</b><br>ational Airpo<br>開車時間<br>07:30<br>10:30<br>13:30<br>16:30<br>19:30 | Deport<br>08:00<br>11:00<br>14:00<br>17:00<br>20:00  | 11:30<br>17:30<br>20:30          | 基百約<br>gkey Banne<br>09:00<br>12:00<br>15:00<br>18:00<br>21:00 | 内廣均<br>or Center<br>09:30<br>12:30<br>15:30<br>18:30<br>21:30 |

Pic-1 图 1



Pic-2 图 2

# 1.3.3 SUSTech —— Wen Hang Hotel

We offer the transport services between SUSTech and Wen Hang Hotel every morning and evening.

Dec 15-17 Morning 8:30 a.m. Wen Hang Hotel to SUSTech Dec 15-17 Evening 18:10 p.m. SUSTech to Wen Hang Hotel

# 1.4 Notes

- 1.4.1 Registration: Conference Room 415, Block 3, Hui Yuan
- 1.4.2 Accommodation: Wen Hang Hotel 文航酒店
- 1.4.3 Meals: Breakfast (Wen Hang Hotel)

Lunch (SUSTech)

Dinner (Wen Hang Hotel) Dec 15

(SUSTech) Dec 14/16/17

# 1.4.4 Assistants

| Meya | 葛玥  | 13825249547 | gey@mail.sustc.edu.cn |
|------|-----|-------------|-----------------------|
|      | 柴树清 | 18682060116 |                       |
|      | 王陈希 | 13631695261 |                       |

# 2. Conference Schedule

| December 14, 2018 (Friday) |                 |  |  |  |
|----------------------------|-----------------|--|--|--|
| All Day                    | Arrive and Rest |  |  |  |
| 18:00 Dinner (SUSTech)     |                 |  |  |  |

| December 15, 2018 (Saturday) |   |  |  |  |  |
|------------------------------|---|--|--|--|--|
| 8:509:00                     | <b>Opening Ceremony</b>   |  |  |  |  |
| 9:009:40                     | SHEN Jie Structure preserving schemes for a class of nonline problems   |  |  |  |  |
| 9:4010:20                    | YANG XiaofengEfficient schemes with unconditionally energy<br>stabilities for anisotropic phase field models: S-II<br>and S-SAV |  |  |  |  |
| 10:2010:50                   | Coffee/Tea Break  |  |  |  |  |
| 10:5011:30                   | LI Zhilin Augmented Immersed Boundary/Interface m<br>and error analysis   |  |  |  |  |
| 11:3012:10                   | ZHANG Qinghai An Analytic Framework of Interface Tracking<br>Topology Computing for Multiphase Flow                             |  |  |  |  |
| 12:1014:00                   | Lunch and Break (SUSTech)   |  |  |  |  |
| 14:0014:40                   | WANG Xiaoping TBA   |  |  |  |  |
| 14:4015:20                   | ZHANG Hui   | A positivity-preserving, energy stable and second<br>order BDF scheme for the Cahn-Hilliard equation |  |  |  |
| 15:2015:50                   | Coffee/Tea Break  |  |  |  |  |
| 15:5016:30                   | FENG Xiaobing   | TBA  |  |  |  |
| 16:3017:10                   | LIU Chun  | Thermal Effects on Charge Transport in Biological<br>Environments                                    |  |  |  |
| 17:1017:50                   | WU Hao The Cahn-Hilliard Equation with Dynamic Boundary<br>Conditions   |  |  |  |  |
| 18:00                        | Dinner (Wen Hang Hotel)   |  |  |  |  |

| December 16, 2018 (Sunday) |  |  |  |  |
|----------------------------|--|--|--|--|
| 9:009:40                   | CHEN Wenbin A Second Order Energy Stable Linear Scheme for a<br>Thin Film Model Without Slope Selection                |  |  |  |
| 9:4010:20                  | YUE Pengtao Numerical simulations of contact-angle hysteresis  |  |  |  |
| 10:2010:50                 | Coffee/Tea Break (Group photo)   |  |  |  |
| 10:5011:30                 | WANG Qi TBA  |  |  |  |
| 11:3012:10                 | QIAO Zhonghua Exponential time differencing methods for phase equations  |  |  |  |
| 12:1014:00                 | Lunch and Break (SUSTech)  |  |  |  |
| 14:0014:40                 | TANG Huazhong         Physical-constraints-preserving schemes for<br>special relativistic magnetohydrodynamic equation |  |  |  |
| 14:4015:20                 | ZHANG Lei Phase field modeling of membrane fusion  |  |  |  |
| 15:2015:50                 | Coffee/Tea Break   |  |  |  |
| 15:5016:30                 | XU Xianmin   | XU Xianmin       Sharp-interface limit of a phase-field model for two-phase flow with moving contact lines |  |  |
| 16:3017:10                 | DI Yana Thin film dynamics in coating problems using Onsager principle   |  |  |  |
| 17:1017:50                 | YING Wenjun  | YING Wenjun Analysis on the potential theory based Cartesian grid method for interface problems            |  |  |
| 18:00                      | Dinner(SUSTech)  |  |  |  |

| December 17, 2018 (Monday) |                  |  |  |  |
|----------------------------|------------------|--|--|--|
| 0.00 0.40                  | HUANG Huaviong   | Modeling and Computation of Free Boundary        |  |  |
| 9:009:40                   | HUANO Huaxiolig  | Problems   |  |  |
|                            |                  | An Immersed Boundary method for mass             |  |  |
| 9:4010:20                  | GONG Xiaobo      | transfer through porous biomembranes under large |  |  |
|                            |                  | deformation                                      |  |  |
| 10:2010:50                 | Coffee/Tea Break |  |  |  |
| 10:5011:30                 | REN Weiqing TBA  |  |  |  |
| 11.20 12.10 VIANC V        |                  | Energy and Dynamics of Grain Boundaries Based on |  |  |
| 11:3012:10                 | XIANG Yang       | Underlying Mircrostructure                       |  |  |
| 12:1014:00                 |                  | Lunch and Break (SUSTC)                          |  |  |
| 14:0014:40                 | ZHOU Zhi         | ni TBA   |  |  |
| 14.40 15.20                | ZUANC Zhan       | Modeling and simulation of moving contact line   |  |  |
| 14:4015:20                 |                  | problems with surfactant                         |  |  |
| 18:00                      | Dinner (SUSTC)   |  |  |  |

| No. | Name           | Institute   | E-mail                     |
|-----|----------------|---|----------------------------|
| 1   | CHEN Wenbin    | Fudan University  | wbchen@fudan.edu.cn        |
| 2   | DI Yana        | Academy of Mathematics and<br>Systems Science of Chinese Academy<br>of Sciences | yndi@lsec.cc.ac.cn         |
| 3   | FENG Xiaobing  | The University of Tennessee   | xfeng@utk.edu              |
| 4   | GONG Xiaobo    | Shanghai Jiao Tong University   | x.gong@sjtu.edu.cn         |
| 5   | HE Dongdong    | The Chinese University of Hong Kong<br>(Shenzhen)                               | hedongdong@cuhk.edu.cn     |
| 6   | HUANG Huaxiong | York University   | hhuang@mathstat.yorku.ca   |
| 7   | LI Wenbin      | Harbin Institute of Technology  | liwenbin@hit.edu.cn        |
| 8   | LI Zhilin      | North Carolina State University   | zhilin@ncsu.edu            |
| 9   | LIU Chun       | Illinois Institute of Technology  | cliu124@iit.edu            |
| 10  | QIAO Zhonghua  | The Hong Kong Polytechnic University  | zhonghua.qiao@polyu.edu.hk |
| 11  | REN Weiqing    | National University of Singapore  | matrw@nus.edu.sg           |
| 12  | SHEN Jie       | Purdue University   | shen7@purdue.edu           |
| 13  | TANG Huazhong  | Xiangtan University   | hztang@xtu.edu.cn          |
| 14  | WANG Qi        | University of South Carolina  | qwang@math.sc.edu          |
| 15  | WANG Xiaoming  | Southern University of Science and<br>Technology                                | wangxm@sustc.edu.cn        |
| 16  | WANG Xiaoping  | Hong Kong University of Science and<br>Technology                               | mawang@ust.hk              |
| 17  | WU Hao         | Fudan University  | haowufd@fudan.edu.cn       |
| 18  | XIANG Yang     | Hong Kong University of Science and<br>Technology                               | maxiang@ust.hk             |
| 19  | XU Xianmin     | Academy of Mathematics and<br>Systems Science of Chinese Academy<br>of Sciences | xmxu@lsec.cc.ac.cn         |

# **3. List of Participants**

| 20 | YANG Jiang    | Southern University of Science and<br>Technology | yangj7@sustc.edu.cn     |
|----|---------------|--|-------------------------|
| 21 | YANG Xiaofeng | University of South Carolina                     | XFYANG@math.sc.edu      |
| 22 | YAO Jin       | National University of Singapore                 | yaojin@u.nus.edu        |
| 23 | YING Wenjun   | Shanghai Jiao Tong University                    | wying@sjtu.edu.cn       |
| 24 | YUE Pengtao   | Virginia Tech University                         | ptyue@math.vt.edu       |
| 25 | ZHANG Hui     | Beijing Normal University                        | hzhang@bnu.edu.cn       |
| 26 | ZHANG Lei     | Peking University                                | zhangl@math.pku.edu.cn  |
| 27 | ZHANG Qinghai | Zhejiang University                              | 0015089@zju.edu.cn      |
| 28 | ZHANG Zhen    | Southern University of Science and<br>Technology | zhangz@sustc.edu.cn     |
| 29 | ZHOU Zhi      | The Hong Kong Polytechnic University             | zhi.zhou@polyu.edu.hk   |
| 30 | ZHONG Hua     | Guangxi Normal University                        | mahzhong@connect.ust.hk |

# 4. Title&Abstracts

# A Second Order Energy Stable Linear Scheme for a Thin Film Model Without Slope Selection

# CHEN Wenbin

Fudan University

In this talk, we present a second order accurate, energy stable numerical scheme for the epitaxial thin film model without slope selection, with a mixed finite element approximation in space. Some issues on stable schemes and convergence analysis are discussed.

# Thin film dynamics in coating problems using Onsager principle

# DI Yana

Academy of Mathematics and Systems Science of Chinese Academy of Sciences

A new variational method is proposed to investigate the dynamics of the thin film in a coating flow where a liquid is delivered through a fixed slot gap onto a moving substrate. A simplified ODE system has also been derived for the evolution of the thin film whose thickness hf is asymptotically constant behind the coating front. We calculate the phase diagram as well as the film profiles and approximate the film thickness theoretically, and agreement with the well-known scaling law as  $Ca^2/3$  is found.

## **FENG Xiaobing**

The University of Tennessee

#### TBA

# An Immersed Boundary method for mass transfer through porous biomembranes under large deformation

# GONG Xiaobo

#### Shanghai Jiao Tong University

In this talk, a novel method for modeling convection and diffusion mass transfer through a deformable membrane with porosity is proposed based on the immersed boundary method. A hyperbolic function is introduced for formulating a concentration jump over the interface. An extra diffusive flux equation is derived and coupled with the concentration equation so that both the diffusion and convection of solvent and solute are treated in a self-consistent and general way. Validations proved that the present numerical method is robust enough to predict the concentration field with arbitrary membrane oscillations. The effect of the fluid-membrane interaction on the mass transfer through a porous membrane with large deformations was investigated using oxygen unloading from red blood cells (RBCs) in capillary vessels as an example. Numerical results suggest that for the cells with large deformation in micro channels, transmembrane fluid flow arises and changes the flow field encapsulated in the porous membrane. With the increase of the permeability coefficient, the vorticity near the front and rear regions of cell membrane increases, which increases the diffusion flux across cell membrane. The proposed method is applicable for studying mass transfer through porous membranes with large deformation such as red blood cells and liposomes (drug deliveries) in microcirculatory systems.

# **Modeling and Computation of Free Boundary Problems**

# HUANG Huaxiong

#### York University

In this talk, I will present some of the work done by my collaborators and myself in the area of free boundary problems, with application in industry and physiology. Some of these problems can be simplified using asymptotic analysis and others have to be solved using numerical methods.

# Augmented Immersed Boundary/Interface methods and error analysis

# LI Zhilin

#### North Carolina State University

The immersed boundary method (IB) is well-known, popular, and has had vast areas of applications due to its simplicity and robustness even though it is only first order accurate near the interface. In this talk, I will explain a newly developed immersed boundary-augmented method for elliptic boundary value problems on arbitrary domains (exterior or interior) with a Dirichlet boundary condition. The new method inherits the simplicity, robustness, and first order convergence of the IB method. We also show an asymptotically first order convergence of the first partial derivatives obtained from the method. Numerical examples are provided to confirm the analysis.

# Thermal Effects on Charge Transport in Biological Environments

#### LIU Chun

#### Illinois Institute of Technology

Almost all biological activities involve transport of charged ions. Ion channels play critical roles in biological systems including heart and nerves. The study of the dynamic properties of these system provide formidable challenges and exciting opportunities for interdisciplinary researches and collaborations. Among them, the thermal effects play crucial role in the dynamics. In this talk, I will discuss a unified energetic variational approach developed specifically for these multiscale-multiphysics FFSI (field-fluid-structure interaction) problems. I will present some relevant theories, approaches and methods developed in the area.

# **Exponential time differencing methods for phase field equations**

# QIAO Zhonghua

#### The Hong Kong Polytechnic University

Exponential time differencing (ETD) methods will be developed for solving phase field equations. ETD method is a very efficient ordinary differential equation solver, which solves the linear part of the equation exactly by using the exponential integral factors and keep exponential behavior of the system. Our numerical schemes preserve the property of energy decay in the discrete sense, which is the fundamental physical feature of the solutions to phase field models as the gradient flows.

## **REN** Weiqing

National University of Singapore

TBA

# Structure preserving schemes for a class of nonlinear problems

## SHEN Jie

#### Purdue University

I will present the scalar auxiliary variable (SAV) approach to deal with nonlinear terms in a large class of gradient flows and Hamiltonian systems. The technique is not restricted to specific forms of the nonlinear part of the free energy. It leads to linear and unconditionally energy stable schemes which only require solving decoupled linear equations with constant coefficients. Hence, these schemes are extremely efficient and very accurate when combined with higher-order BDF schemes.

# Physical-constraints-preserving schemes for special relativistic magnetohydrodynamic equations

#### TANG Huazhong

#### Xiangtan University

We first study the admissible state set G of special relativistic magneto hydrodynamics(RMHD). It paves a way for developing physical-constraintspreserving (PCP) schemes for the special RMHD equations with the solutions in G. To overcome the difficulties arising from the extremely strong nonlinearities and no explicit formulas of the primitive variables and the flux vectors with respect to the conservative vector, two equivalent forms of G with explicit constraints on the conservative vector are skillfully discovered. The first is derived by analyzing roots of several polynomials and transferring successively them, and further used to prove the convexity of G with the aid of semi-positive definiteness of the second fundamental form of a hypersurface. While the second is derived based on the convexity, and then used to show the orthogonal invariance of G. The LxFsplitting property does not hold generally for the nonzero magnetic field, but by a constructive inequality and pivotal techniques, we discover the generalized LxF splitting properties, combining the convex combination of some LxF splitting terms with a discrete divergence-free condition of the magnetic field. Based on the above analyses, several 1D and 2D PCP schemes are then studied. In the 1D case, a first-order accurate LxF-type scheme is

first proved to be PCP under the CFL condition, and then the high-order accurate PCP schemes are proposed via a PCP limiter. In the 2D case, the discrete divergence-free condition and PCP property are analyzed for a first-order accurate LxF-type scheme, and two sufficient conditions are derived for high-order accurate PCP schemes. Our analysis reveals in theory for the first time that the discrete divergence-free condition is closely connected with the PCP property. Several numerical examples demonstrate the theoretical findings and the performance of numerical schemes.

# WANG Qi

University of South Carolina

TBA

# WANG Xiaoping

Hong Kong University of Science and Technology

TBA

# The Cahn-Hilliard Equation with Dynamic Boundary Conditions

## WU Hao

Fudan University

In this talk, we first recall some results for the Cahn-Hilliard equation subject to classical boundary conditions. Then we introduce a new class of dynamic boundary conditions that accounts for nontrivial short-range interactions near the solid wall. The derivation is based on an energetic variational approach that combines the least action principle and Onsager's principle of maximum dissipation. We will discuss well-posedness of the initial boundary value problem and the asymptotic behavior of global solutions as time goes to infinity.

# 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.

# Sharp-interface limit of a phase-field model for two-phase flow with moving contact lines

### XU Xianmin

Academy of Mathematics and Systems Science of Chinese Academy of Sciences

Moving contact line is a classical problem that falls beyond the framework of conventional hydrodynamics. Standard no-slip boundary condition leads to infinite energy dissipation. To overcome the difficulties, many models are proposed. One of them is proposed by T. Qian, X.-P. Wang & S. Sheng, which is a phase-field model that can describe slipping of the contact line on solid boundary due to uncompensated Young stress and is consistent the molecular dynamics simulations. In this talk, we will show some recent study on the sharp-interface limit of the model. By asymptotic analysis, we show that the model will converge to different sharp-interface limits under different choices for the mobility parameter and a relaxation parameter in the boundary condition. Numerical results are consistent with the analysis results and also illustrate the different convergence rates of the sharp-interface limits for different scalings of the two parameters. This is a joint work with Yana Di and Haijun Yu.

# Efficient schemes with unconditionally energy stabilities for anisotropic phase field models: S-IEQ and S-SAV

# YANG Xiaofeng

#### University of South Carolina

We consider numerical approximations for anisotropic phase field models, by taking the anisotropic Cahn-Hilliard/Allen-Cahn equations with their applications to the faceted pyramids on nanoscale crystal surfaces and the dendritic crystal growth problems, as special examples. The main challenge of constructing numerical schemes with unconditional energy stabilities for these type of models is how to design proper temporal discretizations for the nonlinear terms with the strong anisotropy. We combine the recently developed IEQ/SAV approach with the stabilization technique, where some linear stabilization terms are added, which are shown to be crucial to remove the oscillations caused by the anisotropic coefficients, numerically. The novelty of the proposed schemes is that all nonlinear terms can be treated semi-explicitly, and one only needs to solve some coupled/decoupled, but linear equations at each time step. We further prove the unconditional energy stabilities rigorously, and present various 2D and 3D numerical simulations to demonstrate the stability and accuracy.

# Analysis on the potential theory based Cartesian grid method for interface problems

# YING Wenjun

Shanghai Jiao Tong University

In the past years, we have been working on a potential theory based Cartesian gri d method for interface problems. The method solves interface problems on irregular d omains with Cartesian grids. It takes advantages of fast elliptic solvers on Cartesian gr ids and well-conditioning properties of reformulated boundary integral equations. In t his talk, I will present some theoretical results on the potential theory based Cartesian grid method for interface problems of the Poisson equation and Stokes equations. Ana lysis on both stability and accuracy of the method are considered.

# Numerical simulations of contact-angle hysteresis

## YUE Pengtao

#### Virginia Tech University

When a fluid interface slides on a solid substrate, the advancing and receding contact angles may differ, which is known as the contact angle hysteresis. In the phase-field framework, the relation between the microscopic dynamic contact angle and the prescribed equilibrium contact angle is embedded in the chemical potential on the solid wall. Following this observation, we propose a novel boundary condition for contact angle hysteresis by manipulating phase-field wall energy relaxation. Our method identifies pinning, advancing, and receding conditions automatically, without the explicit knowledge of contact-line velocity or contact angle. The same idea can be easily extended to numerical methods other than the phase-field method, as long as the generalized Navier boundary condition is used for contact line motion. We will provide some recent results on contact angle hysteresis from both a phase-field method and a level-set method. Code validations and 3D simulations of sliding drops will be presented.

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

# ZHANG Hui

#### Beijing Normal University

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. 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.

# Phase field modeling of membrane fusion

# ZHANG Lei

Beijing International Center for Mathematical Research, Peking University

Membrane fusion is involved in many cellular processes such as endocytosis and exocytosis, synaptic release, etc. Many efforts have been made in studying membrane fusion process, however, the application of atomistic model is greatly restricted by the short time interval and limited length scale and the bilayer structure has not been studied in continnum model. We developed phase field model containing both short-range and long-range free energy derived from particle model to study the process of membrane fusion. The transition path from two separate membranes to a fusion pore is constructed using a combination of Cahn-Hilliard equation and string method. With solvent between two apposed membrane, a leaky transition path is derived through an asymmetrical configuration stalk-hole complex. Without solvent, the classical symmetry transition pathway and the pathway through IMI(inverted micellar intermediate) configuration are found. The joint work with Anchang Shi (McMaster).

# An Analytic Framework of Interface Tracking and Topology Computing for Multiphase Flows

# ZHANG Qinghai

#### Zhejiang University

Interface tracking (IT) is a fundamental problem in simulating multiphase ows, yet current IT methods have a number of serious limitations. First, there is no rigorous analytic framework for explicit IT methods such as VOF methods and front-tracking methods. Second, all popular IT methods suer from lack of control on topological changes. Third, their IT accuracy are at best second-order. Fourth, their accuracy of curvature estimation is often less than satisfactory. All the aforementioned issues stem from the fact that current IT methods avoid geometrical and topological problems by converting them into problems of numerical PDEs. In drastic comparison, our approach is to tackle geometric and topological problems with tools in geometry and topology. For this purpose, we propose MARS, a novel analytic framework based on a topological space (the Yin space) that models physically meaningful material regions. This Yin space is further strengthened by the donating region theory for analyzing current IT methods, and it is also equipped with Boolean algebra and corresponding algorithms for developing new IT methods. MARS is the rst of its kind in that it relates dierent branches of mathematics to serve the simulation of multiphase ows. For standard benchmark problems on both IT and curvature estimation, our MARS methods are more accurate and ecient than current methods by many orders of magnitudes. We also show that, for certain water-wave problems with topological changes, our model converges to experimental results while those based on current IT methods cannot.

# 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.

# ZHOU Zhi

#### The Hong Kong Polytechnic University

TBA

