北京国际数学研究中心
BEIJING INTERNATIONAL CENTER FOR MATHEMATICAL RESEARCH

Workshop on Phase Field Method and Modeling

Dates:
July 24: Registration; July 25: Workshop

Venue:

Room 77201, Jingchunyuan 78, BICMR

Organizers:

Lei Zhang (Peking University)

Workshop Program

Morning Session		
9:00-12:00	**Discussion**	
12:00-14:00	**Lunch**	
Afternoon Session **Chair: Lei Zhang**		
Time	**People**	**Titles /Activities**
13:50-14:00	**Opening remarks**	
14:00-14:40	**Lili Ju** (U. of South Carolina)	Stabilized Compact Exponential Time Differencing Methods for Gradient Flow Problems and Scalable Implementation
14:45-15:25	**Xiaofeng Yang** (U. of South Carolina)	IEQ approach--A novel numerical approach to solve the Gradient flow problem with high nonlinearity
15:30-15:50	**Break**	
Chair: Lili Ju		
15:50-16:30	**Sungrim Lee** (Hiroshima University)	A New Application of Phase-field Method for Multicellular Pattern Formation
16:35-17:15	**Yanxiang Zhao** (George Washington U.)	A new phase field variational implicit solvent model of molecular solvation with Coulomb-filed approximation
18:00	**Dinner**	

Abstract

- **Stabilized Compact Exponential Time Differencing Methods for Gradient Flow Problems and Scalable Implementation**

Lili Ju (University of South Carolina)

Abstract: In this talk, we will present stabilized compact exponential time differencing methods (ETD) for numerical solutions of a family of gradient flow problems, which have wide applications in materials science, fluid dynamics and biological researches. These problems often form a special class of parabolic equations of different orders with high nonlinearity and stiffness, thus are often very hard to solve efficiently and robustly over large space and time scales. The proposed methods achieve efficiency, accuracy and provable energy stability under large time stepping by combining linear operator splittings, compact discretizations of spatial operators, exponential time integrators, multistep or Runge-Kutta approximations and fast Fourier transform. We will also discuss the corresponding localized ETD methods based on domain decomposition, which are highly scalable and therefore very suitable for parallel computing. Various numerical experiments are carried out to demonstrate superior performance of the proposed methods, including extreme scale phase field simulations of coarsening dynamics on the Sunway TaihuLight supercomputer.

- **IEQ approach--A novel numerical approach to solve the Gradient flow problem with high nonlinearity**

Xiaofeng Yang (University of South Carolina)

Abstract: The free energies of gradient flow systems usually consist of various nonlinear potentials formulated in diverse complex formats which present a major challenge in the construction of efficient and accurate time discretization schemes. We overcome this challenge by developing a flexible and robust IEQ approach which enables us to develop time discretization schemes for a large class of gradient flow systems. More precisely, the developed schemes (i) are accurate (up to second order in time); (ii) are stable (unconditional energy dissipation law holds); and (iii) are efficient and easy to implement (only need to solve some positive definite linear system at each time step.

- **A New Application of Phase-field Method for Multicellular Pattern Formation**

Sungrim Seirin-Lee, Department of Mathematics, Hiroshima University, JAPAN

Pattern formation in development biology is one of the fundamental processes by which cells change their functions. It is based on the communication of cells via intra- and intercellular dynamics of bio-chemicals. Thus, the cell is directly involved in biochemical interactions. However, many theoretical approaches describing biochemical pattern formation have usually neglected the cell's role or have simplified the subcellular process without considering cellular aspects despite the cell being the environment where bio-chemicals interact. Here we develop a mathematical model using the combination of multi-phasefield method and reaction-diffusion system by which biochemical dynamics can be directly observed with explicitly expressed cell structure and geometry in higher dimensions, and reconsider pattern formation by lateral inhibition of the Notch–Delta signaling pathway. We explore how the physical characteristic of cell, such as cell geometry or size, influences the bio-chemical pattern formation in a multi-cellular system.

- **A new phase field variational implicit solvent model of molecular solvation with Coulomb-filed approximation**

Yanxiang Zhao, George Washington University

Abstract: A phase field variational implicit-solvent approach is developed for the solvation of charged molecules. All the surface energy, the solute-solvent van der Waals interaction, and the electrostatic interaction are coupled together self-consistently through a phase field. The proposed method is different from our previous work in the sense that our new model here capture the consistency between phase field model and sharp interface model not only in the free-energy formulation but also in the corresponding Euler-Lagrange equation. By introducing a new phase field term in the long-range interaction (van der Waals interaction and electrostatic interaction), we make the variational force terms in the Euler-Lagrange equation all confined in the phase field transition layer region and no contributions in the region away from transition layer. An efficient and stable method is adopted to solve the gradient flow system to determine the equilibrium conformations and free energies of an underlying charged molecular system. Applications to single ions, a two-plate system, reveal that the new theory and methods can capture capillary evaporation in hydrophobic confinement and corresponding multiple equilibrium states as found in molecular dynamics simulations. Comparisons of the phase field and the original sharp interface variational approaches are discussed.