Forum on Modeling of Nonequilibrium Phenomena

会议日程 Program
Dec 20, 2015

Time	Title	Speaker	Host
10:00-10:50	Onsager principle and its applications to flow-diffusion phenomena in soft matter	Masao Doi	Qi Wang
10:50-11:40	Modeling, simulation and analysis of non-equilibrium complex fluids	Aiguo Xu	
11:40-1:30	**Lunch, CSRC Canteen**		
1:30-2:20	Proton polarity of interfacial water inhibits heterogeneous ice nucleaIon	Xin Zhou	Weizhu Bao
2:20-3:10	Optimization, Adaptation, and Initiation of Biological Transport Networks	Dan Hu	
3:10-3:40	**Coffee Break**		
3:40-4:30	Flow-mediated interactions between two self-propelled flapping filaments in tandem configuration	Xing Zhang	Tiezheng Qian
4:30-5:20	Nonequilibrium stochastic dynamics at single cell level	Hao Ge	
5:30-7:00	**Banquet for invited speakers at CSRC Canteen Dinner Room**		

会议日程 Program
Dec 21, 2015

Time	**Title**	**Speaker**	**Host**
9:40-10:30	Computational methods for the dynamics of nonlinear Schrodinger/Gross- Pitaevskii equations and applications	Weizhu Bao	Weiqing Ren
10:30-11:20	Nonequilibrium phenomena of free and confined spherical polymer micelle	Hui Zhang	
11:30-1:30	**Lunch at CSRC Canteen**		
1:30-2:20	Modeling and simulation of moving contact lines in multi-phase fluids	Weiqing Ren	Hui Zhang
2:20-3:10	Dynamic van der Waals theory and its applications	Tiezheng Qian	
3:10-3:40	**Coffee Break**		
3:40-4:30	Modeling and simulation of active liquid crystals with applications in cell mitosis	Jia Zhao	
5:30-7:00	**Dinner at a Restaurant at Shangdi**		

Onsager principle and its applications to flow-diffusion phenomena in soft matter

Masao Doi
Beihang University

Onsager principle is a general principle which governs the dynamics of soft matter[1,2]. Many basic equations which describe non-linear and non-equilibrium phenomena in soft matter have been derived from this principle. Here I will show that the principle is quite useful in analyzing the coupled problems of flow and diffusion in soft matter, such as wetting, drying and gelation processes.

REFERENCES

1. Masao Doi, Soft Matter Physics, Oxford University Press, p1-257 (2013)

2. Masao Doi, Onsager's variational principle in soft matter dynamics, in Non-Equilibrium Soft Matter Physics ed S. Komura and T. Ohta, World Scientific p 1-35 (2012)

Modeling, Simulation and Analysis of Non-equilibrium Complex Fluids

Aiguo Xu[1,2], Guangcai Zhang[1]

Laboratory of Computational Physics,
1, Institute of Applied Physics and Computational Mathematics,
No.6, Huayuan Road, Haidian District, Beijing 100088, P. R. China

2, Center for Applied Physics and Technology and
MOE Key Center for High Energy Density Physics Simulations,
College of Engineering, Peking University, Beijing 100871, China

Complex flows are ubiquitous in nature and play an important role in both the engineering fields and our daily lives. The existing various interfaces, complex forcing and relaxation processes results in very complicated hydrodynamic and thermodynamic responses. It is known that a Navier-Stokes(NS) model is not sufficient to capture the complicated non-equilibrium behaviors, and the spatial and temporal scales which the microscopic molecular dynamics simulation can access are too small to be comparable with experiments. The Monte Carlo simulation has a similar constraint on the system size and evolution time. Under such cases, a kinetic model based on the Boltzmann equation is more preferable.

In this talk, we will briefly review the progress of discrete Boltzmann modeling, simulation and analysis of non-equilibrium complex fluids in our group in recent years. The topics are relevant to multiphase flows, shock waves, combustions and hydrodynamic instabilities. Mathematically, the only difference of discrete Boltzmann from the traditional hydrodynamic modeling is that the NS equations are replaced by a discrete Boltzmann equation. But physically, besides the macroscopic behaviors described by the NS model, the discrete Boltzmann model(DBM) presents more kinetic information on the Thermodynamic Non-Equilibrium (TNE). Via the DBM, it is convenient to perform simulations on systems with flexible Knudsen number. The observations on TNE have been used to estimate the deviation amplitude from thermal equilibrium state, to recover the main feature of real distribution function, to distinguish different stages of phase transition, to discriminate and capture various interfaces, etc.

Proton polarity of interfacial water inhibits heterogeneous ice nucleation

Xin Zhou
School of Physical Sciences,
University of Chinese Academy of Sciences, China

Pure bulk water can keep liquid state without freezing until -40°C, almost all of water freezing appeared in nature happen on various surfaces of materials. It is still not very clear which aspects of materials impede or promote water freezing. The answer of the questions are very important not only in theory but in applications, such as designing anti-freezing materials. A common sense on that is the ice-matched lattice of materials facilitates ice nucleation, and is regarded as the reason that silver iodide (AgI) is employed in cloud seeding. However, many materials or surfaces have almost similar ice lattice as AgI, such as, barium fluoride (BaF2), but very different ability on ice nucleation. More recent experiments and simulations show many aspects of substrates affect water freezing. In the work, based on atomistic molecular dynamics (MD) simulations, we show the effect of substrates on ice nucleation could be universally understood from the reconstruction of interfacial water layers induced by the substrates. While oxygen atoms in the layers form the ice-like lattice induced by the lattice-matched substrates, the slight polarization of hydrogen atoms inside the layers could significantly inhibit the formation of ice nucleation. The effect of proton polarity in interfacial water can be understood under the classical nucleation theory.

Optimization, Adaptation, and Initiation of Biological Transport Networks

Dan Hu

Shanghai Jiao Tong University

Blood vessel systems and leaf venations are typical biological transport networks. The energy consumption for such a system to perform its biological functions is determined by the network structure. In the first part of this talk, I will discuss the optimized structure of vessel networks, and show how the blood vessel system adapts itself to an optimized structure. Mathematical models are used to predict pruning vessels in the experiments of zebra fish. In the second part, I will discuss our recent modeling work on the initiation process of transport networks. Simulation results are used to illustrate how a tree-like structure is obtained from a continuum adaptation equation system, and how loops can exist in our model. Possible further application of this model will also be discussed.

Flow-mediated interactions between two self-propelled flapping filaments in tandem configuration

Xing Zhang
The State Key Laboratory of Nonlinear Mechanics,
Institute of Mechanics,
Chinese Academy of Sciences

The mechanism by which aggregates of active swimmers are formed is an intriguing problem. In this talk I will show that, for two tandem self-propelled filaments driven by harmonic plunging motions of identical frequency and amplitude, stable configurations can be spontaneously formed by locking the trajectories onto the vortex centers. Further analysis indicates that the grouping energetics is also dictated by the wake vortex structure. The rationale behind the energetic advantage of the follower is found to be the interplay among actuation, self-propulsion, and the vortical fluid environment.

Nonequilibrium stochastic dynamics at single cell level

Hao Ge
Beijing International Center for Mathematical Research
Peking University

Stochastic processes become more and more popular to model the mesoscopic nonequilibrium biophysical dynamics, which well fit the recent development of advanced experimental techniques at single-cell level.

Here I will take about two short stories. One is the molecular mechanism of transcriptional burst, which is uncovered by both single-molecule in vitro experiments and stochastic models. The other is a new rate formula for phenotype transition at the intermediate region of gene-state switching for single cells, the rigorous proof of which needs to integrate the well-known Donsker-Varadhan theory and Feidlin-Wentzell theory of large deviation principle. The new rate formula can explain a "noise enhancer" therapy for HIV reported in a Science paper last year, which motivated a future project of us.

Computational methods for the dynamics of the nonlinear Schrodinger/Gross-Pitaevskii equations and applications

Weizhu Bao
Department of Mathematics
National University of Singapore & CSRC

In this talk, I begin with the nonlinear Schrodinger/Gross-Pitaevskii equations (NLSE/GPE) for modeling Bose-Einstein condensation (BEC), nonlinear optics, etc., and review some dynamical properties of NLSE/GPE including conserved quantities, dispersion relation, center-of-mass dynamics, soliton solutions and semiclassical limits. Different numerical methods will be presented including finite different time domain (FDTD) methods and time-splitting spectral method, and their error estimates and comparison will be discussed. Extensions to NLSE/GPE with an angular momentum rotation term and/or non-local dipole-dipole interaction as well as random potential will be presented. Finally, applications to quantum transport, subdifusive spreading of a BEC in a random potential, and quantized vortex interaction will be investigated

Nonequilibrium phenomena of free and confined spherical polymer micelle

Hui Zhang
School of Mathematical Sciences,
Beijing Normal University

Here we will present nonequilibrium phenomena of free spherical polymer micelle and confined spherical polymer micelle in a tube tunnel.

Firstly, we use the Time-Dependent Ginzburg–Landau (TDGL) mesoscopic model to simulate the phase transition process of macromolecule microsphere composite (MMC) hydrogel. We propose a free energy for such a reticular structure according to the structures of MMC hydrogel and entropy theory. This work generalizes the meanfield theory confined by Flory–Huggins for free energy in a polymer blend system. A spectral method is adopted to numerically solve the MMC-TDGL equation. The numerical results are consistent with chemical experiments, showing the network structure. According to the numerical results at different temperatures, we understand that the system shows intermittent phenomenon with increasing reaction temperature, which is a very good explanation of chemical experiments.

Secondly, phase behavior of the blends composed of diblock copolymer (AB) and homopolymer (A) micelles confined in a tube tunnel was studied using the self-consistent field theory. AB diblock copolymer and A homopolymer blend can form micelles of different shapes (lamellar, cylindrical, and spherical) because they have different critical micelle concentration (CMC). According to the CMC, we can find a stable spherical micelle morphology with a set of molecular parameters. When the spherical polymer micelle was confined in a channel, the shape of the micelles may differ from that of the bulk micelles. We study the shape variation of a spherical micelle under confinement with different A-homopolymer length. The results reveal depletion effect and capillary condensation. And these results are consisted with the physical experiment.

Modeling and simulation of moving contact lines in multi-phase fluids

Weiqing Ren
Department of Mathematics,
National University of Singapore and CSRC

The moving contact line problem is a classical problem in fluid mechanics. The difficulty stems from the fact that the classical Navier-Stokes equation with the no-slip boundary condition predicts a non-physical singularity at the contact line with infinite rate of energy dissipation.

In this talk, we will discuss how the continuum theory, molecular dynamics and the more recently developed multiscale techniques can be combined to give us a better understanding of the fundamental physics of the moving contact line and formulate simple and effective models. We also illustrate how this model can be used to analyze the behavior of the apparent contact angle, hysteresis and other important physical problems for the moving contact line.

Dynamic van der Waals theory and its applications

Tiezheng Qian
Department of Mathematics,
Hong Kong University of Science and Technology

The dynamic van der Waals theory [Phys. Rev. E 75, 036304 (2007)] is employed to model the growth of a single vapor bubble in a superheated liquid on a flat homogeneous substrate. The bubble spreading dynamics in the pool boiling regime has been numerically investigated for one-component van der Waals fluids, with a focus on the effect of the substrate wettability on bubble growth and contact line motion.

Mathematical Modeling and simulation of active liquid crystals with applications in cell mitosis

Jia Zhao
Department of Mathematics,
University of South Carolina, Columbia, USA

Active liquid crystals solutions and gels are complex fluids whose anisotropic molecules undergo self-propelled motion by either burning ATP or reacting with the host matrix. The self-propelled motion introduces new active stresses to the momentum balance together with self-propelled velocity, which can lead to spontaneous flows and symmetry breaking flow patterns.

In this talk, I will present how to model active liquid crystal solutions using continuum theory. Then, I will show numerical results of free surface flows of active liquid crystals. Finally, I will discuss the employment of this active liquid crystal model in the development of a whole cell model to simulate cell mitosis and motility. 3D numerical simulations of cytokinesis and cell motion will be presented.