Location: Four Points by Sheraton Shanghai Daning
Address: 1928 Gonghexin Rd., Zhabei District, Shanghai 200072, China
Nearest Subway Station: Yanchang Rd. of Line 1 ("Red Line")
Reference: http://www.travelchinaguide.com/cityguides/shanghai/transportation

Registration details:
Sep. 20, 2015, 15:00pm, Registration is open in the Lobby of Shanghai University Lehu Lou.
Sep. 20, 2015, 16:00pm, Registration is open in the Lobby of Four Points by Sheraton Shanghai Daning.
Sep. 21, 2015, 8:00am-9:00am, Registration is open at the entrance of the conference room.

PROGRAM OF 2015 DPD WORKSHOP

DAY ONE

DATE	TIME	TALKS
Sep. 21, 2015 Monday	9:00am - 9:15am	Welcome by **Zhe-Wei Zhou** & **George Karniadakis**
	9:15am - 10:15am (45min + 15min)	Chair: **Zhe-Wei Zhou** (Shanghai University, China) **Invited:** **Jia-Ping Lin** (East China University of Science and Technology, China) Simulations of Cooperative Self-Assembly of Polypeptide-Based Copolymers
	10:15am - 10:35am **Coffee Break**	
	Session ONE	Chair: **Shuo Chen** (Tongji University, China)
	10:35am - 11:00am (20min + 5min)	**Nicolas Moreno** (King Abdullah University of Science and Technology, Saudi Arabia) Large-scale simulations of block copolymer self-assembly in selective solvents
	11:00am - 11:25am (20min + 5min)	**Ding-Yi Pan** (Zhejiang University, China) Rheology studies on droplet and polymer suspensions with Dissipative Particle Dynamics method
	11:25am - 11:50am (20min + 5min)	**Yu-Ying Wang** (Chinese Academy of Science, China) Dissipative Particle Dynamics Simulation of Flow within Nanochannels
	11:50am - 12:15pm (20min + 5min)	**Guo-Hui Hu** (Shanghai University, China) Mesoscopic Study of DNA Translocation Through Nanopore
	12:15pm - 14:00pm **Lunch Break**	

PROGRAM OF 2015 DPD WORKSHOP

DAY ONE

DATE	TIME	TALKS
Sep. 21, 2015 Monday	14:00pm - 15:00pm (45min + 15min)	Chair: **George Karniadakis** (Brown University, USA) **Invited: Dmitry A. Fedosov** (Research Center Juelich, Germany) From single cells to intricate multi-cell interactions in blood flow
	15:00pm - 16:00pm (45min + 15min)	Chair: **George Karniadakis** (Brown University, USA) **Invited: Marco Ellero** (Swansea University, United Kingdom) Smoothed Dissipative Particle Dynamics: theory and applications to complex fluids
	16:00pm - 16:30pm **Coffee Break**	
	Session TWO	Chair: **Jia-Ping Lin** (East China University of Science and Technology, China)
	16:30pm - 16:55pm (20min + 5min)	**Yu-Hang Tang** (Brown University, USA) *In Silico* Investigation on the Self-Assembly Dynamics of Thermo-Responsive Smart Material
	16:55pm - 17:20pm (20min + 5min)	**Ting Ye** (Jilin University, China) Numerical modeling of a file of red blood cells in tube flow using dissipative particle dynamics
	17:20pm - 17:45pm (20min + 5min)	**Jian-Hua Huang** (Zhejiang Sci-Tech University, China) Dissipative particle dynamics simulations on the self-assembly of confined rod-coil block copolymers

PROGRAM OF 2015 DPD WORKSHOP

DAY TWO

DATE	TIME	TALKS
Sep. 22, 2015 Tuesday	9:00am - 10:00am (45min + 15min)	Chair: **Zhong-Yuan Lu** (Jilin University, China) **Invited: Hong-Xia Guo** (Chinese Academy of Sciences, China) The application of dissipative particle dynamics simulation techniques to complex fluids
	10:00am - 11:00am (45min + 15min)	Chair: **Zhong-Yuan Lu** (Jilin University, China) **Invited: Alexander Alexeev** (Georgia Institute of Technology, USA) Mesoscale simulations of stimuli-sensitive polymer networks
	11:00am - 11:15am **Coffee Break**	
	Session THREE	Chair: **Xian-Ren Zhang** (Beijing University of Chemical Technology, China)
	11:15am - 11:40am (20min + 5min)	**Ikuya Kinefuchi** (The University of Tokyo, Japan) New formulation of dissipative particle dynamics: Non-Markovian models
	11:40am - 12:05pm (20min + 5min)	**Ming-Ge Deng** (Brown University, USA) Modeling of mesoscopic electrokinetic phenomena using charged dissipative particle dynamics
	12:05pm - 12:30pm (20min + 5min)	**Yu-Xiang Wang** (Tongji University, China) Mesoscopic study on droplet by using Many-body dissipative particle dynamics
	12:30pm - 14:00pm **Lunch Break**	
	14:00pm - 15:00pm (45min + 15min)	Chair: **Hong-Xia Guo** (Chinese Academy of Sciences, China) **Invited: Xian-Ren Zhang** (Beijing University of Chemical Technology, China) The interaction between nanoparticles and membranes: from cytotoxicity to drug delivery

PROGRAM OF 2015 DPD WORKSHOP

DAY TWO

DATE	TIME	TALKS
Sep. 22, 2015 Tuesday		Chair: **Hong-Xia Guo** (Chinese Academy of Sciences, China)
	15:00pm - 16:00pm (45min + 15min)	**Invited: Changho Kim** (Brown University, USA) Quantifying uncertainties in equilibrium particle dynamics simulations
	16:00pm - 16:30pm **Coffee Break**	
	Session FOUR	Chair: **Dmitry A. Fedosov** (Research Center Juelich, Germany)
	16:30pm - 16:55pm (20min + 5min)	**Dmitrii Azarnykh** (Technische Universität München, Germany) Measurement technique of macroscopic parameters in DPD solvent
	16:55pm - 17:20pm (20min + 5min)	**Qing-Lin Hu** (Chinese Academy of Science, China) Impacts of Graphene Oxide Nanosheets on Structure and Biophysical Properties of Pulmonary Surfactant Film
	17:20pm - 17:45pm (20min + 5min)	**Wu-Ming Li** (Northwestern Polytechnical University, China) 3D dissipative particle dynamics simulations of microstructure of ferromagnetic fluids

PROGRAM OF 2015 DPD WORKSHOP

DAY THREE

DATE	TIME	TALKS
Sep. 23, 2015 Wednesday	9:00am - 10:00am (45min + 15min)	Chair: **Marco Ellero** (Swansea University, United Kingdom) **Invited: Alexandre Tartakovsky** (Pacific Northwest National Laboratory, USA) Stochastic Smoothed Particle Hydrodynamics and its applications for multiphase flow and reactive transport in porous media
	10:00am - 11:00am (45min + 15min)	Chair: **Marco Ellero** (Swansea University, United Kingdom) **Invited: Zhong-Yuan Lu** (Jilin University, China) Multiscale Simulation Study of Polymer Systems Based on Dissipative Particle Dynamics
	11:00am - 11:30am **Coffee Break**	
	11:30am - 12:30pm	Chair: **Zhe-Wei Zhou & George Karniadakis** **Panel Discussion: Future of DPD**
	12:30pm - 14:00pm **Lunch Break**	
	14:00pm - 18:00pm	**Tutorial Session** **Yu-Hang Tang**: Practicing Dissipative Particle Dynamics **Changho Kim**: Calculating material properties from LAMMPS

DETAILS OF THE TALKS

[1] **Jia-Ping Lin**, East China University of Science and Technology, China.

Title: Simulations of Cooperative Self-Assembly of Polypeptide-Based Copolymers

Abstract: Polypeptides bearing rich conformations are excellent building blocks for constructing self-assembled structures. For example, mixtures of polypeptide-based copolymers and polypeptide homopolymers are able to self-assemble into various hierarchical structures such as chiral super-helices by taking advantage of the rigid -helix conformation of the polypeptides. However, due to the limitations of current experimental characterization techniques, many issues remain unsolved, for example, the molecular packing details of the hierarchical structures and the chiral transfer from molecular level to microstructures. To address these issues, we employed computer simulations beyond the experiments to study the self-assembly of polypeptide-based copolymers. The simulations not only reproduced the experimental findings, but also revealed the structures and formation conditions of the self-assembled structures. Computer simulation is powerful in revealing the structural details and guiding experimental designs.

[2] **Nicolas Moreno**, King Abdullah University of Science and Technology, Saudi Arabia.

Title: Large-scale simulations of block copolymer self-assembly in selective solvents.

Abstract: We study the hierarchical self-assembly of block copolymers AB and AB/AC blends in solution with large-scale DPD simulations. For AB block copolymers, we adopt a model reduction methodology for DPD chains, where the properties governing the phase equilibria such as the characteristic size of the chain, compressibility, density, and temperature are preserved. The reduction in the number of degrees of freedom required compared with traditional DPD representations, allow us to capture long-range self-assembled structures. For AB/AC blends we use the traditional DPD schemes to investigate the mechanisms involved in the co-assembly of the two different block copolymers.

[3] **Ding-Yi Pan**, Dept. Engineering Mechanics, Zhejiang University, China.

Title: Rheology studies on droplet and polymer suspensions with Dissipative Particle Dynamics method.

Abstract: The Dissipative Particle Dynamics method is used to study both droplet and polymer suspension and their constitutive properties. The deformation of a single droplet and the collision process of two droplets are first studied to validate the method. A larger repulsion force is imposed between particles from different droplet to prevent two droplets from coalescing. The viscoelastic fluid, Oldroyd-B fluid, is produced by adding the dumbbell polymer beads into the Newtonian solvent. A modified Lee-Edwards boundary condition model is created to correct the spring force for dumbbell beads crossing the boundary. The rheological behaviors of dilute to semi-dilute emulsion, i.e. droplet suspension in both Newtonian fluid and Oldroyd-B fluid, as well as their correlation to the microstructures are investigated.

[4] **Yu-Ying Wang**, Institute of Process Engineering, Chinese Academy of Science, China.

Title: Dissipative Particle Dynamics Simulation of Flow within Nanochannels.

Abstract: The basic law of flow within nanochannels is investigated by the dissipative particle dynamics (DPD) simulation and theoretical analysis. The influences of wall/fluid interactions and the dimensions of the channels are discussed respectively by examining the density profiles, velocity profiles and the fluxes. The results show density and viscosity inhomogeneities near the wall/fluid

interfaces, which are determined by the wall/fluid interactions while the dimensions or the flow rates have no effect. Special flow patterns can be observed in a hydrophobic and highly confined channel. Furthermore, the fluid transport is significantly enhanced. The enhancement, defined as the ratio of the simulated flux to the flux calculated by the Hagen-Poiseuille relation, keeps increasing with the decrease of the dimension, and the increase of the wall/fluid interactions. A systematic investigation of the fluxes in nanochannels is conducted in this work. Several calculation methods, including the friction model and the modification of the Hagen-Poiseuille relation, are discussed for their validity in different dimensions. The calculated results are in good accordance with the simulation by DPD.

[5] **Guo-Hui Hu**, Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, China.

Title: Mesoscopic Study of DNA Translocation Through Nanopore.

Abstract: DNA sequencing technology has achieved a leapfrog development in recent years. As a new generation of DNA sequencing technology, nanopore sequencing has shown a broad application prospect and attracted vast research interests since it was proposed. To investigate the resistance forces of DNA in the nanopore, density functional theory (DFT) combined with the continuum NavierCStokes (NS) equations is utilized to investigate electro-osmotic flow and the viscous drag force acting on the DNA inside a nanopore. Surface charge on the walls of the nanopore is also taken into account in our model. The consistence between our calculation and the previous experimental measurement indicates that the present theoretical model is an effective tool to predict the hydrodynamic resistance on DNA. Results show that charge inversion, which cannot be obtained by the PoissonCBoltzmann (PB) model, will reduce electro-osmotic velocity, or even lead to flow reversal for high salt concentration.

The dissipative particle dynamics (DPD) is applied to explore the dynamics of electric-driven translocation of homopolymer through a nanopore, in which the homopolymer is modeled as a worm-like chain (WLC). The DPD simulations show that the polymer chain undergoes conformation changes during the translocation process. The different structures of polymer in the translocation process, i.e., single-file, double folded, and partially folded, are analyzed in the present investigation, as well as the current blockades induced. These current blockades are found to have the different magnitude resulted from the polymer molecules traversing the pore with different folding conformations. We also examine the nanoscale vortices caused by the concentration polarization layers (CPL) in the vicinity of the sheet. Results indicate that the translocation of polymer might have the effect of eliminating these vortices in polyelectrolyte solution. These findings are expected to provide theoretical guide for improving the technique of nanopore sequencing.

[6] **Dmitry A. Fedosov**, Institute of Complex Systems, Research Center Juelich, Germany.

Title: From single cells to intricate multi-cell interactions in blood flow.

Abstract: Blood flow plays an important role in many physiological processes and pathologies in the organism. To understand these processes, detailed investigation of blood flow is required under realistic conditions including cell deformability, hydrodynamic interactions, and complex geometries. We employ the smoothed dissipative particle dynamics method, a mesoscopic hydrodynamic simulation technique, to model blood as a suspension of deformable cells represented by a viscoelastic spring-network which incorporates appropriate mechanical and rheological cell-membrane properties. Blood flow in idealized micro-channel geometries will be investigated. We will discuss the physical mechanisms which govern migration of micro- and nano-carriers toward the walls in micro-vessels. Moreover,

we will present the flow behavior of blood cells in a microfluidic device which offers great opportunities for cell sorting. We will illustrate the use of complex flow geometries to separate cells of different sizes and the application of realistic blood flow simulations to optimize the device performance.

[7] **Marco Ellero**, Zienkiewicz Centre for Computational Engineering, Swansea University, United Kingdom.

Title: Smoothed Dissipative Particle Dynamics: theory and applications to complex fluids.

Abstract: Dissipative Particle Dynamics (DPD) [1,2] as a model of fluid particles suffers from the problem that it has no thermodynamic scale associated with the particles. Therefore, a DPD simulation requires an ambiguous fine-tuning of the model parameters with the physical parameters, i.e. to specify the fluid transport coefficients one needs to rely on kinetic theory [3,4] or to map and calibrate the parameters in ways that are not always systematic [5,6].

A corrected version of DPD that does not suffer from this problem is Smoothed Dissipative Particle Dynamics (SDPD) [7,8] SDPD is, in fact, a version of the well-known Smoothed Particle Hydrodynamics method (SPH), albeit with the proper inclusion of thermal fluctuations. The SDPD model is entirely embedded in the GENERIC framework, therefore it maintains the thermodynamic consistency of the original DPD method, but in addition allows for a direct specification of the transport coefficients as input parameters.

Another remarkable advantage of the method is that the application of GENERIC lead directly to a size-dependent thermal noise which satisfies the Fluctuation Dissipation Theorem [8]. In other words, whenever the fluid particle size is large enough, no thermal noise will be present in the hydrodynamic variables, whereas it will show up only when the fluid description needs to be miniaturized, e.g. under microflow conditions. This property allows to formally unify the Lagrangian description of fluid flow based on a stochastic mesoscopic approach (SDPD) with a fluctuations-free deterministic macro-continuum methods (SPH) [9].

In the first part of this talk I will review the SDPD method, discussing the link with the standard DPD and the macroscopic SPH methods for the modelling of a simple Newtonian solvent. In the second part I will present some applications of SDPD for the modelling of complex fluids, i.e. in the context of viscoelastic polymeric solutions [10,11,12] and colloidal dispersions [13,14] based on a hierarchical description of the fluid microstructure.

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[8] **Yu-Hang Tang**, Division of Applied Mathematics, Brown University, USA.

Title: *In Silico* Investigation on the Self-Assembly Dynamics of Thermo-Responsive Smart Material.

Abstract: In this talk I will present mesoscopic simulation study on thermoresponsive block copolymers, reveiling unexpected molecular behaviors and proving experimental hypotheses. By explicitly modeling internal energy as a degree of freedom of coarse-grained particles, we simulated thermally induced self-assembly process triggered by unsteady evolution of temperature over time and space using energy-conserving Dissipative Particle Dynamics (eDPD). We identified two dominant molecular movement modes, namely flip and slip, in thermoresponsive bilayer membranes during the inversion of composition. In addition, our simulation observations support the hypotheses that vesicle inversion proceeds by diffusion. We further show that both kinetic and thermodynamic factors can alter the assembly pathway of thermoresponsive micelles and hence regulate final aggregate morphology. It was also found that thermoresponsive micelles exhibit distinctive hydrodynamic behaviors when flowing between regions whose temperature spans across the inversion temperature of the aggregate.

[9] **Ting Ye**, School & Institute of Mathematics, Jilin University, China.

Title: Numerical modeling of a file of red blood cells in tube flow using dissipative particle dynamics.

Abstract: Red blood cell (RBC) is the main important component in whole blood, at 40%∼45% in volume concentration, and plays an essential role in the microcirculation. Early studies on RBCs mainly focused on the measurement of their physical properties, such as viscosity and membrane shear modulus, and the rheology of blood flow. Recent studies mainly concentrated on the dynamic behaviors of a suspension of RBCs in either Couette or Poiseuille flow. In particular, intensive simulations had been carried out via different numerical methods thanks to advances in computational hardware/software. This paper focuses on the 3D simulation of rheology of a file of RBCs in a Poiseuille flow using the dissipative particle dynamics (DPD) method. The theoretical models consist of a spring model to describe the RBC deformation, a Morse potential model to characterize the RBC-RBC interaction, and a DPD model to provide all the relevant information on the suspension flow. Three important features of the suspension flow are simulated and analyzed, (i) the effect of the tube hematocrit, (ii) the effect of the cell spacing, and (iii) the effect of the flow velocity. The results show that the cell deformation decreases with increasing tube hematocrit, and a good agreement between the simulation and available experiments is found for the discharge hematocrit and relative apparent viscosity of RBC suspension. The non-uniform cell spacing has a slight effect on the cell deformation, and almost has no effect on the rheology of suspension. A typical plug-flow velocity profile is observed. With increasing flow velocity, the cell deformation increases, and the discharge hematocrit also increases, but the relative apparent viscosity decreases.

[10] **Jian-Hua Huang**, Department of Chemistry, Zhejiang Sci-Tech university, China.

Title: Dissipative particle dynamics simulations on the self-assembly of confined rod-coil block copolymers.

Abstract: Self-assemblies of rod-coil (RC) diblock copolymers and rod-coil-rod (RCR) triblock copolymers confined within a rod-selective nanoslit are investigated by using dissipative particle dynamics simulations. The self-assembled structure of confined copolymers is sensitively dependent on the rigidity and fraction of rod blocks and the slit height. For the confined RC diblock copolymer-

s, four main structures, including disordered cylinder structure, hexagonally packed cylinders (HPC) perpendicular to the slit surfaces, and lamellar structures parallel and perpendicular to surfaces, are observed. And copolymers with longer rod block favor to form perpendicular lamellae with the increase in the rod rigidity. For the confined RCR triblock copolymers, we sequentially observe HPC of rod blocks, parallel wavy lamellae, orderly packed alternating cylinders, a mixture structure of HPC near surfaces and perpendicular lamellae in the interior region, and parallel lamellae with the increase in the slit thickness. Our results suggest an effective way to control the ordering of rod-coil block copolymers under nanoscale confinement.

[11] **Hong-Xia Guo**, State-key Lab. of Polymer Physics and Chemistry, Institute of Chemistry, Chinese Academy of Sciences, China.

Title: The application of dissipative particle dynamics simulation techniques to complex fluids.

Abstract: Recently, a relatively new particle-based mesoscopic simulation technique known as dissipative particle dynamics (DPD) has been developed for the study of various complex fluids including polymers, liquid crystals, lipid membranes, and amphiphiles. In DPD simulations, individual particle represents a cluster of atoms or molecules, interacts via soft potentials, and is subjected to dissipative and random forces that act together as a momentum conserving thermostat. As such, the use of soft potential and the reduced number of interaction sites make DPD simulations a valuable tool to access the large-scale collective phenomena at a reasonable computational cost. Besides, DPD has established itself as a useful thermostat for molecular simulations. In this talk, I not only describe the current progresses of my group on DPD simulations of several typical complex fluids including ternary polymer blend, Janus nanoparticles filled polymer system, polymer liquid-crystal, lipid membrane, and T-shaped ternary amphiphiles, but also reexamine DPD thermostats in molecular simulations and extend DPD thermostat to Gay-Berne Fluids. I hope that this talk may be helpful to provide a deep understanding of the algorithms and advantages of DPD simulation techniques.

[12] **Alexander Alexeev**, Georgia Institute of Technology, USA.

Title: Mesoscale simulations of stimuli-sensitive polymer networks.

Abstract: Using dissipative particle dynamics, we examine transport properties, swelling kinetics, and applications of stimuli-sensitive polymer networks. Such networks are common in various biological and synthetic systems. Our model employs a bond-bending bead-spring approach to capture the micromechanics of random elastic networks. First we demonstrate that our model can properly describe transport properties of random networks and examine how the transport changes when a network undergoes mechanical deformation. We then employ our model to study the dynamics of responsive microgels during swelling volume transition and probe how hollow microgel capsules can be harnessed in controlled release applications. Finally, we probe how a bi-layered microgel sheet can be used to design a microscopic self-propelling swimmer.

[13] **Ikuya Kinefuchi**, The University of Tokyo, Japan.

Title: New formulation of dissipative particle dynamics: Non-Markovian models.

Abstract: In the present study, we derive the equation of motion for non-Markovian dissipative particle dynamics (NMDPD) by introducing the history effects on the time evolution of the system [Y. Yoshimoto et al., Phys. Rev. E 88, 043305 (2013)]. Our formulation is based on the generalized Langevin equation, which describes the motions of the centers of mass of clusters comprising microscopic particles. The mean, friction, and fluctuating forces in the NMDPD model are directly constructed

from an underlying MD system without any scaling procedure. For the validation of our formulation, we construct NMDPD models from high-density Lennard-Jones systems, in which the typical time scales of the coarse-grained particle motions and the fluctuating forces are not fully separable. The NMDPD models reproduce the temperatures, diffusion coefficients, and viscosities of the corresponding MD systems more accurately than the DPD models based on a Markovian approximation.

[14] **Ming-Ge Deng**, Division of Applied Mathematics, Brown University, USA.

Title: Modeling of mesoscopic electrokinetic phenomena using charged dissipative particle dynamics.

Abstract: We propose a charged dissipative particle dynamics (cDPD) model for investigation of mesoscopic electrokinetic phenomena. In particular, this particle-based method was designed to simulate micro- or nano- flows which governing by Poisson-Nernst-Planck (PNP) equation coupled with Naiver-Stokes (NS equation. For cDPD simulations of wall-bounded fluid systems, a methodology for imposing correct Dirichlet and Neumann boundary conditions for both PNP and NS equations is developed. To validate the present cDPD model and the corresponding boundary method, we perform cDPD simulations of electrostatic double layer (EDL) in the vicinity of a charged wall, and the results show good agreement with the mean-field theoretical solutions. The capacity density of a parallel plate capacitor in salt solution is also investigated with different salt concentration. Moreover, we utilize the proposed methodology to study the electroosmotic and electroosmotic/pressure-driven flow in a microchannel. In the last, we simulate the dilute polyelectrolytes solution both in bulk and micro-channel, which show the flexibility and capability of this method in studying complex fluids.

[15] **Yu-Xiang Wang**, Tongji University, China.

Title: Mesoscopic study on droplet by using Many-body dissipative particle dynamics.

Abstract: We present our recent research work about droplet dynamics by using MDPD, including the impact of droplets on microtextured surfaces and the sliding across these surfaces.

[16] **Xian-Ren Zhang**, State key laboratory of organic-inorganic composites, Beijing University of Chemical Technology, China.

Title: The interaction between nanoparticles and membranes: from cytotoxicity to drug delivery.

Abstract: Nanoparticles are widely used in biomedical fields, such as gene and drug delivery, nanoparticle-based sensing and imaging etc. In these applications, the efficient uptake of nanoparticles (NPs) into cells becomes a critical issue, because NPs are required to be capable of transporting through cell membranes. On the other hand, nanoparticles adhering on cells may cause damage to cell membranes and induce adverse biological effects, with the potential to create cytotoxicity. In this regard, understanding of the mechanism of NP uptake is essential to bio-applications of nanoparticles. In this talk, our recent simulation works on the interaction between cell membrane and nanoparticles are addressed. The dependence of the internalization pathways of nanoparticles, including endocytosis and penetration, on size, shape and rigidness of nanoparticles is also presented. In addition, the membrane response to nanoparticle adsorption is discussed.

[17] **Changho Kim**, Division of Applied Mathematics, Brown University, USA.

Title: Quantifying uncertainties in equilibrium particle dynamics simulations.

Abstract: Material properties of a system can be calculated through either equilibrium or non-equilibrium simulation. While the non-equilibrium approach is conceptually more direct, the equilib-

rium dynamics simulation method is theoretically and computationally more reliable. In this talk, I will review the latter method and discuss two types of intrinsic uncertainties in equilibrium particle dynamics simulation: statistical errors and finite-system-size effects. Although the suppression of the level of these uncertainties is crucial for reliable estimation of material properties and higher-level uncertainty quantification analysis, until now, they have not been systematically investigated. I will present a theoretical and computational analysis based on large-ensemble simulation technique.

[18] **Dmitrii Azarnykh**, Technische Universität München, Germany.

Title: Measurement technique of macroscopic parameters in DPD solvent.

Abstract: The work is devoted to the measurement of macroscopic parameters: shear viscosity, isothermal speed of sound and bulk viscosity in simulations of Dissipative Particle Dynamics solvent. For this purpose we analyse Fourier transform of velocity autocorrelation function (FTVACF). We introduce a new function that gives a good approximation for the modes of FTVACF in DPD solvent and allows to measure shear viscosity with reasonably high accuracy from FTVACF for a wide range of parameters. We observe that macroscopic parameters of DPD solvent depend on lengthscale. Bulk viscosity and shear viscosity measured in simulations are compared with analytical predictions, that were derived by Marsh for DPD solvent without repulsive potential.

[19] **Qing-Lin Hu**, Institute of Mechanics, Chinese Academy of Sciences, China.

Title: Impacts of Graphene Oxide Nanosheets on Structure and Bio-physical Properties of Pulmonary Surfactant Film.

Abstract: Graphene oxide (GO) is the most common derivative of graphene and has been used in a large range of biomedical applications. Despite considerable progress in understanding its cytotoxicity, its potential inhalation toxicity is still largely unknown. As the pulmonary surfactant (PS) film is the first line of host defense, interaction with the PS film determines the fate of inhaled nanomaterials and their potential toxicity. Using molecular dynamics simulation, we found that upon depositing, GO nanosheets induce pores in the PS film and thus have adverse effects on the ultrastructure and biophysical properties of the PS film. Notably, the pore induced by GO nanosheets results in increasing compressibility of the PS film, which is an important indication of surfactant inhibition. In vitro experiments have also been conducted to study interactions between GO and animal-derived natural PS films, qualitatively confirming the simulation results.

[20] **Wu-Ming Li**, Northwestern Polytechnical University, China.

Title: 3D dissipative particle dynamics simulations of microstructure of ferromagnetic fluids.

Abstract: Three-dimensional (3D) microstructure of ferromagnetic fluids is simulated using a dissipative particle dynamics (DPD)-based method. Here magnetic fluids are regarded as being composed of various nanosized ferromagnetic particles distributed in a DPD solvent. Three important factors affecting the microstructure of magnetic fluids are investigated in detail, that is, magnetic particle-particle interaction, particle-field interaction and volume fraction of magnetic particles. Various aggregate structures of magnetic particles are obtained, which agree well with those shown in the literature obtained using other simulation methods.

[21] **Alexandre Tartakovsky**, Pacific Northwest National Laboratory (PNNL), USA.

Title: Stochastic Smoothed Particle Hydrodynamics and its applications for multiphase flow and reactive transport in porous media.

Abstract: Smoothed Particle Hydrodynamics (SPH) is a Lagrangian method based on a meshless discretization of partial differential equations. I will present SPH discretization of the stochastic and deterministic Navier-Stokes and Advection-Diffusion-Reaction equations, implementation of various boundary conditions, and time integration of the SPH equations, and discuss applications of the SPH method for modeling multiphase flows and reactive transport in domains with complex geometries.

[22] **Zhong-Yuan Lu**, Institute of Theoretical Chemistry, Jilin University, China.

Title: Multiscale Simulation Study of Polymer Systems Based on Dissipative Particle Dynamics.

Abstract: Due to large molecular size and slow relaxation of polymer chains, a great amount of issues related to long-distance chain displacement, such as phase separation and self-assembly, can not be tackled easily with conventional molecular dynamic simulations. We need to use generic polymer models based on dissipative particle dynamics (DPD) to solve problems commonly encountered in polymer phase separation and self-assembly. A soft patchy particle model originated from DPD, which is suitable to describe "soft" particle formed by star-like polymers and dendrimers, has been proposed to study their self-assembly structures. A stochastic reaction model in DPD simulations has been used to cope with the problems related to the coupling between polymerization and chain diffusion. We have also developed a GPU-accellerated molecular simulation toolkit for use in coarse-grained simulations of polymer systems with several unique simulation tools implemented.

[23] **Tutorial Session**

Instructor 1: **Yu-Hang Tang**, Division of Applied Mathematics, Brown University, USA.
Title: Practicing Dissipative Particle Dynamics.
Content: This tutorial will be focused on using the LAMMPS software to conduct and post-process DPD simulations. Techniques for constructing initial configuration of particle systems will be demonstrated, followed by basic scripting for enabling various integration schemes and custom functionalities. Compiling and configuring LAMMPS for parallel execution will also be covered. No previous experience with LAMMPS is required.

Instructor 2: **Changho Kim**, Division of Applied Mathematics, Brown University, USA.
Title: Calculating material properties from LAMMPS.
Content: For various ways of calculating transport coefficients, including the non-equilibrium simulation approach and the Green-Kubo method, the actual implementations on LAMMPS are demonstrated. The underlying principles from statistical mechanics are also reviewed and possible computational issues are discussed. In addition, it is discussed how the sampling uncertainties and the finite-system-size effects are quantified in particle dynamics simulations.