

# International Workshop on Soft Matter Analysis, Computation, and Applications

Jilin University • Changchun Tianyuan Mathematical Center in Northeast China 2019.6.15 – 6.16



国家自然科学基金数学天元基金资助



吉林大学资助

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#### **Goal of the Workshop**

Soft Matter includes liquid crystals, polymers, colloids, emulsions, foams, surfactant solutions, gels, granular materials, and a number of biological materials. Soft materials are important in a wide range of technological applications, for example, liquid crystal display devices. Studying soft matter is a typical cross-disciplinary subject. An improved level of engagement and understanding between researchers in different areas will bring great benefits to our understanding of soft matter. The central aim of this workshop is to bring together different research communities to facilitate an exchange of ideas, the exploration of different approaches and the sharing of knowledge. Another important goal is the identification of key scientific and mathematical problems arising from experiment, computer simulations and industrial applications.

The workshop will capitalize on recent progress on soft matter by giving leading researchers a forum to discuss how different approaches can be most effectively combined to tackle and solve the big open problems in the field.

## **Scientific Committee**

Jeff Z.Y. Chen	University of Waterloo
An-Chang Shi	McMaster University
Pingwen Zhang	Peking University

## **Organizing Committee**

Kai JiangXiangtan UniversityTing YeJilin UniversityLei ZhangPeking UniversityRan ZhangJilin University

## **Workshop Sponsors**

This workshop is sponsored by:

\*National Natural Science Foundation Mathematics Tianyuan Fund

**※**Jilin University.



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## Information

#### 1、Registration

Registration Opens: 14:00pm to 20:00pm on June 14, at June Hotel

8:00am to 11:30am on June 15, at the Lecture Hall of the Math Building

For other time registration, please contact us.

#### 2、Venue

The Second Lecture Hall, School of Mathematics of Jilin University



The Math Building



The Lecture Hall

#### 3、Dining

	Breakfast	Lunch	Dinner
	6:30-9:00	12:00-14:00	18:00-20:00
June 14			June Hotel
June 15	June Hotel	June Hotel	Banquet
June 16	June Hotel	June Hotel	June Hotel

\*The Banquet will be held on June 15, starting at 6:00pm.

#### 4、Contact us

Xiuping Gao	13596117968
Xingwu Sun	13504468895

#### 5、Tips

#### **※**June Hotel

Address: No.811 Xiuzheng Road, Changchun City, Jilin Province, China

Tel: +86-431-87058888

**※**Taking taxi

Please do not take a taxi in the night.

If you need, Please contact Mr. Lv for picking up service before you come to Changchun , Tel:13624465812.

# **Invited Speakers**

No.	Name	Institute	
1	Jeff Z.Y. Chen	University of Waterloo, Canada	
2	Tomonari Dotera	Kindai University, Japan	
3	Yucheng Hu	Tsinghua University, China	
4	Kai Jiang	Xiangtan University, China	
5	Ying Jiang	Beihang University, China	
6	Qin Liang	Xiangtan University, China	
7	Yuyuan Lu	Changchun Institute of Applied Chemistry Chinese Academy of Sciences, China	
8	Xingkun Man	Beihang University, China	
9	Bing Miao	University of Chinese Academy of Sciences, China	
10	Rudi Podgornik	Institute of Physics, Chinese Academy of Sciences, China	
11	Igor I. Potemkin	Moscow State University, Russia	
12	Alastair Rucklidge	University of Leeds, UK	
13	An-Chang Shi	Mcmaster University, Canada	
14	Wei Wang	Zhejiang University, China	
15	Zhen-Gang Wang	California Institute of Technology, USA	
16	Ning Xu	University of Science and Technology of China, China	
17	Ting Ye	Jilin University, China	
18	Hui Zhang	Beijing Normal University, China	
19	Lei Zhang(张磊)	Beijing International Center for Mathematical Research, Peking University, China	
20	Lei Zhang(张镭)	Shanghai Jiao Tong University, China	

## Schedule

## International Workshop on Soft Matter: Analysis, Computation, and Applications

Venue: The Second Lecture Hall, School of Mathematics of Jilin University

Date	Time	Schedule
June 14	14:00 - 20:00	Registration: June Hotel
	08:30 - 09:00	Opening Ceremony and Group Photo
	09:00 - 10:05	Chair: Zhen-Gang Wang
	09:00 - 09:30	An-Chang Shi: The Packing of Soft Spheres
	09:35 - 10:05	Rudi Podgornik: Continuity Condition(s) in Continuum Description of Polymer Nematics
	10:10 - 10:30	Tea Break
	10:30 - 12:10	Chair: Rudi Podgornik
	10:30 - 11:00	Zhen-Gang Wang: Improved Local Lattice Monte Carlo Simulation for Charged Systems
	11:05 - 11:35	Yucheng Hu: Vector and Tensor Models for Liquid Crystal Dynamics
	11:40 - 12:10	Lei Zhang (张磊): Construct the Solution Landscape beyond the Energy Landscape
June 15	12:15 - 14:00	Lunch
(Saturday)	14:00 - 16:00	Chair: An-Chang Shi
	14:00 - 14:30	Alastair Rucklidge: Quasicrystals in Density Functional Theory
	14:35 - 15:05	Tomonari Dotera: Metallic-mean Quasicrystals: Sequences of Quasicrystals that Approach Crystals
	15:10 - 15:40	Ning Xu: A New Approach to Realize Auxetic Materials
	15:45 - 16:00	Tea Break
	16:00 - 17:40	Chair: Hui Zhang
	16:00 - 16:30	Xingkun Man: Evaporation-induced Droplet Motion
	16:35 - 17:05	Wei Wang: Sharp Interface Limit of the Isotropic-nematic Interface Problem for Liquid Crystals
	17:10 - 17:40	Kai Jiang: An Adaptive Dccelerated Proximal Gradient Method for Computing Stationary States of Phase Field crystal models
	18:10 -	Dinner

Date	Time	Schedule
	09:00 - 10:40	Chair: Igor I. Petemkin
	09:00 - 09:30	Jeff Z. Y. Chen: Statistical Physics of a Wormlike Chain in Confinement
	09:35 - 10:05	Ying Jiang: Stratification of Colloidal Particles by Evaporation
	10:10 - 10:40	Lei Zhang (张镭): Modeling and Simulation of an Active Swimmer in Nematic Liquid Crystal
	10:45 - 11:05	Tea Break
	11:05 - 12:10	Chair: Jeff Z. Y. Chen
	11:05 - 11:35	Igor I. Petemkin: Polymer Microgels Adsorbed at Liquid Interfaces and Solid Surfaces
	11:40 - 12:10	Hui Zhang: A Model for the Phase Transition of the Freely Swelling Hydrogel with Chain Detachment based on Energy Density Functional
June 16	12:15 - 14:30	Lunch
(Sunday)	14:30 - 15:40	Chair: Alastair Rucklidge
	14:30 - 15:00	Yuyuan Lu: Mechanism of Nonmonotonic Increase in Polymer Size: Comparison between Linear and Ring Chains at High Shear Rates
	15:05 - 15:35	Qin Liang: Ordered Pattern of Liquid Crystals in Spherical Cavity
	15:40 - 16:05	Tea Break
	16:05 - 17:15	Chair: Yucheng Hu
	16:05 - 16:35	Ting Ye: Parallel Modeling of Cell Suspension Flow in Complex Micro-networks with Inflow/Outflow Boundary Conditions
	16:40 - 17:10	Bin Miao: Casimir Forces in Gaussian Fluctuating Media
	18:00 -	Dinner

#### Abstracts

#### Statistical Physics of a Wormlike Chain in Confinement

Jeff Z.Y. Chen

jeffchen@uwaterloo.ca, University of Waterloo, Canada

**Abstract**: Within a finite confinement geometry, the multi-threads of a strongly confined polymer exert the excluded-volume repulsions on each other and produce physical properties that are very different from those of a confined ideal chain. The conformational properties of a such confined wormlike chain are of fundamental interest and are also practically useful in understanding the DNA confinement problems. The excluded-volume effects can be added to the standard wormlike-chain model by a self-consistent field theory. Here I review the recent progress in understanding this problem.

#### Metallic-mean Quasicrystals: Sequences of Quasicrystals that Approach Crystals

Tomonari Dotera

dotera@phys.kindai.ac.jp, Kindai University, Japan

**Abstract**: Ever since the discovery of quasicrystals, crystalline approximants of these aperiodic structures constitute a very useful experimental and theoretical device. Characterized by packing motifs typical for quasicrystals but arranged in large unit cells, approximants are often seen in similar conditions as quasicrystals and they bridge the conceptual gap between periodic and aperiodic translational order.

In this talk, we propose a class of sequences of 2D quasicrystals that consist of increasingly larger crystalline domains and are marked by an ever more pronounced periodicity, thereby representing aperiodic approximants of a crystal lattice. The sequences are based on metallic means of multiples of 3, have a 6-fold rotational symmetry, and can be viewed as extensions of the bronze-mean quasicrystal, which have been obtained from Monte Carlo simulations of hardcore-softshell particles [1, 2], motivated by soft-matter quasicrystals [3].

- [1] T. Dotera, S. Bekku, P. Ziherl, Nat. Mater. 16, (2017) 987.
- [2] T. Dotera, T. Oshiro & P. Ziherl, Nature. 506, (2014) 208.
- [3] T. Dotera, Isr. J. Chem. 51, (2011) 1197.

#### Vector and Tensor Models for Liquid Crystal Dynamics

Yucheng Hu

huyc@tsinghua.edu.cn, Tsinghua University, China

**Abstract**: Two commonly used continuous models for liquid crystals are the Oseen-Frank model and the Landau-de Gennes model. In this talk we will first show that, for confined liquid crystals, the phase transition processes predicted by the two models may be quite different. This phenomenon provides evidence that the Oseen-Frank model is inadequate to describe the dynamics of nematic liquid crystals. Then we will discuss how to restore the head-to-tail symmetry in vector-based models.

#### An Adaptive Accelerated Proximal Gradient Method for Computing Stationary States of Phase Field Crystal Models

#### Kai Jiang kaijiang@xtu.edu.cn, Xiangtan University

Abstract: In this talk, we will present an adaptive accelerated proximal gradient (APG) method for computing stationary states of phase field crystal models, which can be formulated as an energy minimization problem. The energy functional is discretized by different discretization schemes dependent on the physical problem. For periodic crystals, the Fourier pseudospectral method is applied, while for quasicrystals, the projection method is adopted. Thus the original infinite nonconvex minimization problem is approximated by a finite dimensional nonconvex minimization problem. The convergence of the adaptive APG method is established. Extensive numerical experiments, including several three dimensional periodic crystals in Landau-Brazovskii model and two dimensional quasicrystals in Lifshitz-Petrich model, demonstrate that our method is efficient, fast and robust.

#### **Stratification of Colloidal Particles by Evaporation**

Ying Jiang

vjiang@buaa.edu.cn, Beihang University, China

**Abstract**: When a liquid film of a colloidal solution consisting of particles of different sizes is dried on a substrate, the colloids often stratify, where smaller colloids are laid upon larger colloids. This phenomenon is counterintuitive because larger colloids which have a smaller diffusion constant, are expected to remain near the surface during the drying process, leaving a layer of larger colloids on top of smaller colloids. Here we show that the phenomenon is caused by the interaction between the colloids, and can be explained by a diffusion model accounting for the interaction between the colloids. By studying the evolution equations both numerically and analytically, we derive the condition at which the stratified structures are obtained.

#### **Ordered Pattern of Liquid Crystals in Spherical Cavity**

Qin Liang

liangqin1997@xtu.edu.cn, Xiangtan University, China

**Abstract**: When confined in a spherical cavity, liquid crystals will be organized in an orientationally ordered pattern. In this work, we simulated this confined system and found six distinct patterns, which include bipolar, twisted bipolar, Hopf fibration, concentric spool, tennis ball and cut-and-rotate. The corresponding simulated cross polarizer images were given for experiment comparison. Both twisted bipolar and Hopf fibration can be regarded as some twisted version of the bipolar configuration. The difference is their twist angles. Here we show the impact of physical parameters on the twist angle. We conclude that increase the molecule length or decrease the molecule rigidity will trigger a bipolar/twisted bipolar/Hopf fibration. For long molecule case, the only stable configuration is the Hopf fibration. Moreover, by decreasing the density below the I-N point, a condensed/biaxial/uniaxial transition is detected for bipolar and tennis ball structures.

## Mechanism of Nonmonotonic Increase in Polymer Size: Comparison Between Linear and Ring Chains at High Shear Rates

#### Yuyuan Lu

#### yylu@ciac.ac.cn

Changchun Institute of Applied Chemistry Chinese Academy of Sciences, China

Abstract: The static and dynamic behaviors of linear and ring polymers under shear flow over a wide range of shear rates are studied using a hybrid simulation method that couples multiple-particle collision dynamics with molecular dynamics. The results reveal that the polymer size increases monotonically with increasing shear rate when hydrodynamic interactions are ignored, in agreement with classic theoretical predictions. However, for the cases with hydrodynamic interactions, the size of both linear and ring chains exhibits a nonmonotonic dependence on the shear rate. This counterintuitive behavior could be divided into 3 regimes for linear chains and 4 regimes for the ring polymers. At specific shear rates, linear polymers exhibit a relatively stable stretched state and a rapidly rotating collapsed state, which correspond to the maximum and minimum sizes, respectively. While the rings behave similarly to the linear polymers, there exist two different relatively stable stretched states: one with an oval-shaped conformation and the other with an S-shaped conformation. For the oval-shaped state, the tumbling motion almost disappears but the tank-treading motion persists, while for the S-shaped state, both tumbling and tank-treading motions are greatly suppressed. Moreover, contrary to previous theoretical predictions, a noticeable bulge is observed for the polymer size in the gradient direction and the alignment angle deviates considerably from theoretical prediction, indicating the existence of relatively stable collapsed conformations at large shear rates for both linear and ring polymers. These results shed new light on the understanding of the dynamic response of linear and ring polymers in ultrahigh shear flows.

#### **Evaporation-induced Droplet Motion**

#### Xingkun Man

manxk@buaa.edu.cn, Beihang University, China

**Abstract**: Motion of evaporating droplets on surfaces has long held a special fascination; the Leidenfrost phenomena of water droplet on hot skillet was observed as early as the 18th century. Equally complex motions of evaporating droplets have been provided by a number of recent papers. Conventionally, such complex motions have been interpreted as the Marangoni effect: flow induced by the gradient of surface tension, but it is still a conjecture and no quantitative theory has been given. In fact, the Marangoni effect cannot explain the phenomena that a pair of pure liquid droplets approach each other since there should be no Marangoni effect in this case. We show that the droplet motion can be induced even in the absence of the Marangoni effect due to the gradient of evaporation rate. We derive an equation for the velocity of a droplet subject to non-uniform evaporation rate and non-uniform surface tension. This theory explains previously observed attraction-repulsion-chasing motions of evaporating droplets. Experimental tests have been done and confirmed this prediction.

#### **Casimir Forces in Gaussian Fluctuating Media**

Bing Miao1(bmiao@ucas.ac.cn), David S. Dean2, Rudolf Podgornik1

1. University of Chinese Academy of Sciences, Beijing 100049, China

 Laboratoire Ondes et Mati`ere d'Aquitaine (LOMA), CNRS, UMR 5798, Universit´e de Bordeaux, F-33400 Talence, France

Abstract: Confining a fluctuating medium with long range, power law correlation leads to Casimir forces. Depending on the nature of fluctuations, Casimir forces cover a wide spectrum of topics in physics, including both quantum and thermal, equilibrium and non-equilibrium Casimir effects. In this talk, within the Gaussian field theory of different types of kernels, I will discuss the field theoretic calculation schemes of thermal Casimir forces in several different confinement set-ups, such as, confining geometries, boundary conditions, etc.

#### **Continuity Condition(s) in Continuum Description of Polymer Nematics**

Rudi Podgornik

podgornik@mac.com, Institute of Physics, Chinese Academy of Sciences, China

**Abstract**: Ordered states of long semi-flexible polyelectrolytes in hard enclosures, e.g., DNA in a bacteriophage capsid, can be described on various levels: polymer physics formulation, molecular simulations and finally the Landau - de Gennes (LdG) description. The LdG description cannot be straightforwardly transplanted into the world of polymer nematogens as additional "continuity equations" for continuous polymer chains need to be satisfied. These equations can be derived in the framework of a vectorial and a tensorial description of polymer nematics and they lead to different constraints on the nematic configurations of confined semiflexible polymers.

#### Polymer Microgels Adsorbed at Liquid Interfaces and Solid Surfaces

Igor I. Potemkin

igor@polly.phys.msu.ru

<sup>1</sup>Physics Department, Lomonosov Moscow State University, Moscow 119991, Russian Federation <sup>2</sup>DWI-Leibniz Institute for Interactive Materials, Aachen 52056, Germany

Abstract: Recently, it was proposed to use soft, adaptive polymer microgels for the emulsion stabilization. As compared to the rigid colloids, polymer microgels possess the ability to swell/collapse and the penetrability for low-molecular-weight substances. Being responsive to pH, temperature, and solution ionic strength, these particles can serve as a tool controlling droplet size and emulsion stability. Alternation of external condition affecting microgel charge and degree of swelling may result in breaking of emulsions on demand. The sensitivity to external stimuli as well as microgel permeability makes the microgel-stabilized emulsions promising for many applications including biocatalysis. In this study we demonstrate a number of new effects. The microgels can serve as compatibilizers of immiscible molecules.1,2 In particular, we demonstrate that two initially immiscible liquids, A and B (oil and water), can partially or fully be mixed within the microgel adsorbed at their interface. If the incompatibility of the liquids is relatively low, they form a homogeneous mixture within the whole microgel particle being segregated outside. As the incompatibility grows, separation into two (micro)phases within the microgel occurs. We demonstrate this effect for homopolymer1,2 and amphiphilic3 (AB-copolymer) microgels. Adsorption of the microgels on a solid surface leads to their flattening: the shape of the microgel is determined by a balance between the gain in the energy of adsorbed monomer units and the penalty in the elastic free energy of the subchains subjected to lateral stretching. Despite a strong interaction with the surface, the adsorbed microgels are able to swell and collapse in response to environmental changes (pH and temperature) varying the size on the surface. We have demonstrated a peculiar behavior of the microgels adsorbed on a patterned surface (planar surface with cylindrical holes or pores).4 It turns out that a microgel can enter and exit a narrow cylindrical pore under external stimuli leading to collapse and swelling of the microgel. Attractive interactions between the microgel and the pore surface stimulate the microgel entering upon its collapse. The entering is driven by a gain in the surface energy: the area of the microgel-pore contacts is maximized within the pore. Swelling of the microgel within the pore of a finite size is thermodynamically favorable if the pore thickness exceeds a certain threshold value. Otherwise, the swelling leads to the microgel exit. The physical reason for this is a gain in the elastic free energy of the subchains which are less stretched outside the pore. We systematically study swelling and collapse of the microgel within the pore. Both longitudinal size and radial concentration profiles are calculated for different strength of interactions of the beads with each other and the pore surface. We predict an intramicrogel "phase" coexistence leading to the formation of a dense adsorbed layer near the pore surface and highly swollen central part of the microgel. Furthermore, the permeation of nanoparticles, whose size is smaller than the mesh-size of the microgels was simulated under different swelling and adsorption degrees. It is demonstrated that the microgel can slow down and completely stop the permeation of nanoparticles through the pore.

Acknowledgement. Financial support of the Russian Science Foundation, project # 15-13-00124 is gratefully acknowledged.

#### **References:**

<sup>1</sup>A. M. Rumyantsev, R. A. Gumerov, I. I. Potemkin, *Soft Matter* 2016, *12*, 6799—6811.
<sup>2</sup>R. A. Gumerov, A. M. Rumyantsev, A. A. Rudov, A. Pich, W. Richtering, M. Moeller, I. I. Potemkin, *ACS Macro Letters* 2016, *5*, 612-616.

<sup>3</sup>R. A. Gumerov, S. A. Filippov, W. Richtering, A. Pich, I. I. Potemkin, *Soft Matter* 2019.
<sup>4</sup>I. V. Portnov, M. Moeller, W. Richtering, I. I. Potemkin, *Macromolecules* 2018, *51*, 8147–8155.

#### **Quasicrystals in Density Functional Theory**

Alastair Rucklidge

A.M.Rucklidge@leeds.ac.uk, University of Leeds, UK

**Abstract**: Phase field crystal (PFC) theory is extensively used for modelling the phase behaviour, structure and thermodynamics of solids. PFC theory can be derived from dynamical density functional theory (DDFT) via a sequence of approximations. We show that these approximations lead to substantial quantitative and qualitative differences between the two theories, with agreement only for unstable crystals very close to the transition from liquid to solid. We propose an alternative formulation in terms of the logarithm of the density, and show how this can be used to construct accurately crystals and quasicrystals in density functional theory.

#### **The Packing of Soft Spheres**

#### An-Chang Shi

#### shi@mcmaster.ca, Mcmaster University, Canada

**Abstract**: The packing of spheres is an interesting problem in mathematics and physics with a long history dated back to the work of Kepler and Lord Kelvin. In recent years, intricate periodic and aperiodic spherical packing phases have emerged in a host of soft matter systems including supramolecular assemblies, surfactants and block copolymers, underscoring the universality of emergent order in condensed matter. In particular, the rich phase behavior of block copolymers provides an ideal model system to study the origin and stability of order phases in soft matter. Our recent study of block copolymer systems using the self-consistent field theory reveals that one key mechanism of forming complex spherical phases is the conformational asymmetry of the blocks. Furthermore, we have predicted that the segregation of different polymeric species in block copolymer blends provides another mechanism to stabilize spherical packing phases with very different sized-spherical domains. I will summarize recent progresses on this fascinating topic and discuss possible future research directions.

## Sharp Interface Limit of the Isotropic-nematic Interface Problem for Liquid Crystals

Wei Wang

wangw07@zju.edu.cn, Zhejiang University, China

**Abstract**: We will discuss the Laudau-de Gennes Q-tensor model at the critical phase transition temperature, which can model the isotropic-nematic interface for liquid crystals. In particular, we will talk about stabilities/instabilities of profile solutions for the corresponding Euler-Lagrange equation as well as the sharp interface limit of the dynamic equation.

#### **Improved Local Lattice Monte Carlo Simulation for Charged Systems**

Zhen-Gang Wang

zgw@cheme.caltech.edu, California Institute of Technology, USA

**Abstract**: We propose two improvements on the local Monte Carlo simulation algorithm proposed by Maggs and Rossetto [A. C. Maggs and V. Rossetto, Phys. Rev. Lett. 88, 196402 (2002)]. By making use of the linear supposition principle for the electric field, we suggest a new particle move by the construct of a "ghost" charge. This improved particle move significantly enhances the acceptance rate associated with moving a charged particle in the system. We also show that the original Maggs and Rossetto algorithm did not guarantee full ergodicity in systems with periodic boundary conditions and introduce an additional updating step for the field, named ``open-circuit update", to ensure that the system is fully ergodic. We illustrate the application of our improved algorithm by applying it to an ionic solution confined between two parallel plates having lower dielectric constant than the intervening solution. The simulation results are in excellent agreement with previous theoretical work. We further use this method to study the adsorption of a polyelectrolyte chain near an dielectric surface and find that the image charge repulsion results in a significant shift in the adsorption threshold as well as the adsorbed chain conformation.

#### A New Approach to Realize Auxetic Materials

#### Ning Xu

ningxu@ustc.edu.cn, University of Science and Technology of China, China

Abstract: Previously, auxetic materials have been realized by either designing specific local geometries or playing with the topology to achieve a negative Poisson's ratio. Here we report another approach by properly introducing disorder to a spring network. Starting with an unstressed spring network with a perfect close-packed geometry, e.g., triangular lattice in two dimensions and face centered cubic lattice in three dimensions, we successively distort the network by randomly displacing the nodes, while maintaining zero stress and the network topology. Interestingly, the Poisson's ratio decreases with the increase of the structural disorder and eventually drops below zero. We find that such a simple network distortion results in a correlation between bond length and bond contribution to the global elastic moduli: Longer springs tend to contribute more to the shear modulus but less to the bulk modulus. Inspired by such a correlation, we achieve auxetic networks with smaller network distortion by making longer springs stiffer and shorter ones softer. More interestingly, by manipulating the spring stiffness according to a virtual network distortion, we realize isotropic auxeticity in triangular lattice without changing the site locations and topology.

### Parallel Modeling of Cell Suspension Flow in Complex Micro-networks with Inflow/Outflow Boundary Conditions

Ting Ye yeting@jlu.edu.cn, Jilin University, China

**Abstract**: In biofluid flow systems, often the flow problems of fluids in complex structures, such as the flow of red blood cells (RBCs) through complex capillary vessels and the separation of circulating tumor cells (CTCs) by a microfluidic device, need to be considered. The smoothed dissipative particle dynamics (SDPD), a particle-based method, is one of the easy and flexible methods to model such complex structure fluids. The immersed boundary method (IBM), a preferred method for handling fluid-structure interaction problems, has been widely used to handle the fluid-RBC interaction in RBC simulations. Therefore, it is believed that the combination of SDPD and IBM will have special advantages to solve biofluidic problems, especially those with complex structure interaction. In this talk, a parallel framework is introduced for the hybrid SDPD-IBM approach with inflow/outflow boundary conditions, which is applied to simulate the cell suspension flow in complex networks.

## A Model for the Phase Transition of the Freely Swelling Hydrogel with Chain Detachment based on Energy Density Functional

Hui Zhang

hzhang@bnu.edu.cn, Beijing Normal University, China

**Abstract**: Here we use the Time-Dependent Ginzburg-Landau (TDGL) mesoscopic model to simulate the phase transition process of the freely swelling hydrogel. We propose a free energy consisting of the stretching energy and the mixing energy based on Flory's mean theory. We combine the traditional stretching energy with sequential chain detachment to describe the process of chains detaching from cross-links. Since the hydrogel has polymer chains of different lengths, we divide the length into different types. A stabilized semi-implicit difference scheme is used to numerically solve the TDGL equation. Numerical results show the influence of chain detachment and some parameters.

#### Construct the Solution Landscape beyond the Energy Landscape

#### Lei Zhang (张磊)

zhangl@math.pku.edu.cn

Beijing International Center for Mathematical Research, Peking University, China

Abstract: In mathematics, physics, and chemistry, an energy landscape is a map of the energy function across the configuration space of the system, which can provide the information such as local minima. In this talk, we propose an efficient algorithm to construct the solution landscape, which is a directed graph consisting of all critical points of the energy function. The solution landscape shows a global and intrinsic properties of the system that is beyond the energy landscape. As an illustration, we apply the Landau-de Gennes theory to study the defects in nematic liquid crystal. We show how to build the complete solution landscape of nematic liquid crystals in a 2D square to advance our understanding on the mathematical models. The joint work with Pingwen Zhang (PKU), Jianyuan Yin (PKU).

#### Modeling and Simulation of an Active Swimmer in Nematic Liquid Crystal

Lei Zhang (张镭)

lzhang2012@sjtu.edu.cn, Shanghai Jiao Tong University, China

**Abstract**: Living liquid crystal (LLC) is a class of active matter that combines active particles such as swimming bacteria with a lyotropic liquid crystal. The interaction of active motion with orientation order of liquid crystal (LC) leads to striking optical, hydrodynamical, and electrical properties of LLC, as well as collective behavior and emergence of intriguing patterns. In this work, we aim to understand how the orientation order of liquid crystal affects the motion of a single swimmer. We study a nonlinearly coupled PDE model which combines the well-known Edwards-Beris model for liquid crystal hydrodynamics with a squirmer model describing active swimmer. Numerical results show how the anchoring and force dipole strengths affect the stable squirming direction. This is a joint work with Hai Chi, Leonid Berlyand, and Igor Aronson.

## Workshop Participants

No.	Name	Institute	Email
1	Pingwen Zhang	Peking University	pzhang@pku.edu.cn
2	Jeff Z. Y. Chen	University of Waterloo	jeffchen@uwaterloo.ca
3	Tomonari Dotera	Kindai University	dotera@phys.kindai.ac.jp
4	Lidong Fang	Shanghai Jiao Tong University	
5	Yucen Han	Peking University	
6	Yucheng Hu	Tsinghua University	huyc@tsinghua.edu.cn
7	Kai Jiang	Xiangtan University	kaijiang@xtu.edu.cn
8	Ying Jiang	Beihang University	<u>yjiang@buaa.edu.cn</u>
9	Qin Liang	Xiangtan University	liangqin1997@xtu.edu.cn
10	Yuyuan Lu	Changchun Institute of Applied Chemistry Chinese Academy of Sciences	yylu@ciac.ac.cn
11	Zhongyuan Lv	Jilin University	luzhy@jlu.edu.cn
12	Xingkun Man	Beihang University	manxk@buaa.edu.cn
13	Bing Miao	University of Chinese Academy of Sciences	bmiao@ucas.ac.cn
14	Rudi Podgornik	Institute of Physics, Chinese Academy of Sciences	podgornik@mac.com
15	Igor I. Potemkin	Moscow State University	igor@polly.phys.msu.ru
16	Alastair Rucklidge	University of Leeds	a.m.rucklidge@leeds.ac.uk
17	An-Chang Shi	Mcmaster University	shi@mcmaster.ca
18	Kuan Tao	Peking University	
19	Tian Tian	Peking University	
20	Wei Wang	Zhejiang University	wangw07@zju.edu.cn
21	Zhen-Gang Wang	California Institute of Technology	zgw@cheme.caltech.edu

22	Zuobing Wu	State Key Laboratory of Nonlinear Mechanics Institute of Mechanics Chinese Academy of Sciences	wuzb@lnm.imech.ac.cn
23	Di Xie	Peking University	
24	Ning Xu	University of Science and Technology of China	ningxu@ustc.edu.cn
25	Zhen Xu	Beijing Normal University	
26	Ting Ye	Jilin University	yeting@jlu.edu.cn
27	Jianyuan Yin	Peking University	
28	Bing Yu	Peking University	
29	Hui Zhang	Beijing Normal University	hzhang@bnu.edu.cn
30	Lei Zhang (张磊)	Peking University	zhangl@math.pku.edu.cn
31	Lei Zhang (张镭)	Shanghai Jiao Tong University	lzhang2012@sjtu.edu.cn

# Introduction to Tianyuan Mathematical Center in Northeast China

Tianyuan Mathematical Fund, administrated by the Natural Science Foundation of China, was founded to advance mathematics in China to the internationally competitive level. Supported by the Tianyuan Mathematical Fund, the National Tianyuan Mathematical Center in Northeastern China (TM-NE) is managed by Jilin University, with the participation of other universities in the northeast region of China, including Northeast Normal University, Harbin Institute of Technology, and Dalian University of Science and Technology. The mission of the center is to serve as a platform for mathematicians from China and around the world to collaborate on cutting edge mathematical research, especially in computational mathematics and related interdisciplinary areas, and to serve as a station for training and developing China's next generation of high caliber mathematicians.