Workshop on Multiscale Modeling: Complex Fluids and Microfluidics

9 — 13 January 2006

Hong Kong University of Science and Technology (HKUST)

Tremendous progress has been made in recent years on multi-scale modeling and simulation of microfluidics with complex fluids. In this workshop several leading experts (plenary speakers) will keep us abreast of the latest development in this exciting emerging field, which is at the interdisciplinary boundary of applied mathematics, physics, biology, and material science. Hosted in Hong Kong, this workshop will also serve to present the leading results of East Asian scientists in this area.

Plenary speakers

Stephen H. Davis	Northwestern University
Masao Doi	University of Tokyo
Weinan E	Princeton University
Kurt Kremer	Max Planck Institute for Polymer Research
David A. Weitz	Harvard University

Invited speakers

Weizhu Bao	National University of Singapore
Emily Ching	Chinese University of Hong Kong
Qiang Du	Penn State University
Haiping Fang	Shanghai Institute of Applied Physics, CAS
Guowei He	Institute of Mechanics, CAS
Tiejun Li	Peking University
Ping Lin	National University of Singapore
Chun Liu	Penn State University
Yuqiang Ma	Nanjing University
Tiezheng Qian	Hong Kong University of Science and Technology
Penger Tong	Hong Kong University of Science and Technology
Jinchao Xu	Penn State University
Dadong Yan	Institute of Chemistry, CAS
Xingye Yue	Suzhou University
Hui Zhang	Beijing Normal University
Pingwen Zhang	Peking University
Haijun Zhou	Institute of Theoretical Physics, CAS

Organizing committee

Weinan E	Princeton University
Tiezheng Qian	HKUST
Ping Sheng (Co-Chair)	HKUST
Penger Tong	HKUST
Xiao-Ping Wang (Co-Chair)	HKUST
Zhou-Ping Xin	Chinese University of Hong Kong

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Hong Kong Mathematical Society
K. C. Wong Education Foundation

Workshop on Multiscale Modeling: Complex Fluids and Microfluidics

Registration (Lecture Theatre G, 8:45—9:15, Monday, 9 January 2006)

Opening ceremony (Lecture Theatre G, 9:15—9:30, Monday, 9 January 2006)

Session 1 (Lecture Theatre G, 09:30—12:20, Monday, 9 January 2006)

(Chair: Ping Sheng)

09:30—10:30 Stephen H. Davis
Dynamics and Solidification of Metallic Foams

10:30—10:50 Coffee Break

10:50—11:50 David A. Weitz
Dripping, Jetting, Drops and Wetting: The Magic of Microfluidics

11:50—12:20 Jinchao Xu
New numerical techniques for complex fluids models and a solution to the high Weissenberg number problem

Session 2 (Lecture Theatre G, 14:00—16:20, Monday, 9 January 2006)

(Chair: Xiao-Ping Wang)

14:00—15:00 Masao Doi
Challenge of Multiscale Modeling

15:00—15:20 Coffee Break

15:20—15:50 Qiang Du
From vesicle membrane deformation to cell aggregation

15:50—16:20 Hui Zhang
On the multiscale models of polymeric fluids: FENE-dumbbell model and rodlike model

Reception at University Center (18:00—21:00)

Session 3 (Lecture Theatre G, 09:30—12:20, Tuesday, 10 January 2006)

(Chair: Tiezheng Qian)

09:30—10:30 Weinan E
Multiscale Modeling of Complex Fluids

10:30—10:50 Coffee Break

10:50—11:50 Masao Doi
Motion of micro-particles of complex shape

11:50—12:20 Guowei He
A constrained particle dynamics for the hybrid atomistic-continuum computation of micro-flows

Session 4 (Lecture Theatre G, 14:00—16:20, Tuesday, 10 January 2006)

(Chair: Penger Tong)

14:00—15:00 Stephen H. Davis
Evolution of Quantum Dots

15:00—15:20 Coffee Break

15:20—15:50 Emily Ching
A model study of turbulent drag reduction by polymers

15:50—16:20 Tiejun Li
Numerical analysis of stochastic methods for dumbbell models in polymeric liquids

Session 5 (Lecture Theatre G, 09:30—12:20, Wednesday, 11 January 2006)

(Chair: Weinan E)

09:30—10:30 Kurt Kremer
Multiscale Simulations of Soft Matter (Part I)

10:30—10:50 Coffee Break

10:50—11:20 Yuqiang Ma
Self-assembly of colloid-polymer mixtures confined by soft walls

11:20—11:50 Haiping Fang
Dynamics of the single hydrogen-bonded chain of water molecules in channels on the nanometer scale

11:50—12:20 Penger Tong
Attractions between charged colloidal particles at aqueous interfaces

Session 6 (Lecture Theatre G, 14:00—16:20, Wednesday, 11 January 2006)

(Chair: Xiao-Ping Wang)

14:00—15:00 David A. Weitz
Microfluidic Nanoreactors: NanoMolar in Femtoliters

15:00—15:20 Coffee Break

15:20—15:50 Pingwen Zhang
The structure of solutions for Doi-Onsager equation and applications

15:50—16:20 Ping Lin
Simulation of Singularity Dynamics for Liquid Crystal Flows: A C^0 Finite Element Method

Session 7 (Lecture Theatre G, 09:30—12:20, Thursday, 12 January 2006)

(Chair: Zhou-Ping Xin)

09:30—10:30 Weinan E
The Moving Contact Line Problem

10:30—10:50 Coffee Break

10:50—11:20 Tiezheng Qian
A variational approach to the moving contact line hydrodynamics

11:20—11:50 Chun Liu
Micro-Macro Models for Viscoelastic Fluids: An Energetic Variational Approach

11:50—12:20 Xingye Yue
A Percolation Network Model for the Thermal-Hydro Processes associated with Nuclear Waste Repositories

Thursday afternoon for a local trip

Banquet starting at 7:00 pm

Session 8 (Lecture Theatre G, 09:30—12:20, Friday, 13 January 2006)

(Chair: Tiezheng Qian)

09:30—10:30 Kurt Kremer
Multiscale Simulations of Soft Matter (Part II)

10:30—10:50 Coffee Break

10:50—11:20 Dadong Yan
Effects of confinement on the order-disorder transition in diblock copolymer melts and crystallization

11:20—11:50 Haijun Zhou
Elasticity Models for Biopolymers: DNA and Spider Capture Silk

11:50—12:20 Weizhu Bao
Numerical simulation of quantized vortex dynamics in superconductivity and superfluidity

Appendix A: Abstracts from plenary speakers

Stephen H. Davis	Northwestern University
Masao Doi	University of Tokyo
Weinan E	Princeton University
Kurt Kremer	Max Planck Institute for Polymer Research
David A. Weitz	Harvard University

Dynamics and Solidification of Metallic Foams

Stephen H. Davis
Northwestern University

High-porosity solids, solid foams, are extremely useful in construction projects in which high strength and light weight are both essential. Many of these properties fit the needs of vehicles and armaments where weight considerations are directly related to fuel consumption or carrying weight. For some applications one would want an extremely regular array of pores while in others prescribed variations in space may be required.

Most of the efforts of modern researchers focuses on aqueous systems and hence surfactant dynamics. The analogous problem of freezing of metallic foams has received less attention. The characterization of solid foams is well studied but the solidification process itself is not well understood. We examine the case in which bubbles are numerous enough that they crowd each other and so have polygonal boundaries, but one in which the liquid channels drain and control the dynamics of the foam as a whole. Here, the liquid fraction is roughly in the 5%-15% range.

The microscale processes involve the liquid flows in channels. There are gravitational draining, capillary effects, as well as van der Waals attractions that could accelerate the film rupture that could cause the foam to collapse. There is also the freezing of such channels, which involves a solid-liquid front progressing into a channel with free boundaries and flowing liquid. In being able to study such effects one needs to examine the response of the liquid in channels to the imposition of temperature gradients. In the isothermal case there is a gravitational/capillary draining. In a temperature gradient, thermocapillary effects are superposed on this and one must determine the flow dynamics here. Given such dynamics, phase transformation is induced in a channel in which there is a complex fluid flow is present. The character and speed of freezing, and the microstructure created are strongly affected by the fluid flows. The mesoscale processes link together the dynamics of whole bubbles with that of the channels of a fluid network. In this talk we shall discuss new thinning models and rupture instabilities that generate coarsening, in both cases utilizing the “thin” nature of a lamella to develop approximations.

Evolution of Quantum Dots

Stephen H. Davis
Northwestern University

New methods of computing may be possible using islands of dimension tens of nanometers whose electrical properties a quantized. Rather than trying to deposit such dots individually on substrates, one can take advantage of the instabilities of thin solid films that form islands, coarsen, and ultimately produce the desired scale and pattern.

In this talk we shall examine such processes by deriving evolution equations governing the surface contours, including the effects of surface energy and its anisotropy, surface diffusion, elasticity, wetting layers, and surface stress. Predictions are made of coarsening rates and pathways as well as transitions from coarsening to roughening.

Challenge of Multiscale Modeling

Masao Doi
University of Tokyo

Multi-scale modeling is a simulation method which models a large, complex system by combining various simulation models each dedicated to certain physical aspects characterized by a certain length scale. There is a strong expectation for such method, but there is a also a big challenge in the method.

There are two ingredients which are needed to construct such system. One ingredient is the simulation programs which can handle the phenomena of the intermediate length scale between molecular level and macroscopic level. These are called mesoscopic models. The other ingredient is the mechanism of bridging these simulation programs. This involves many problems: how to combine simulation programs based on different physical models, how to pass information, how to prove the consistency of different models, and how to validate the system as a whole.

I this talk, I will discuss the challenge of the multiscale modeling.

Motion of micro-particles of complex shape

Masao Doi
University of Tokyo

Motion of a particle suspending in a Newtonian fluid subject to an external force and flow becomes complex if the particle shape is not simple. For example, a propeller like particle rotates as it settles down, and a helical particle migrates normal to the ambient fluid velocity in shear flow. These properties are important in separating and manipulating micro-particles. To analyze the motion, we constructed a simulator which calculates the Brownian motion of a particle of general shape subject to force, torque and external flow.

Here we discuss two problems (a) separation of chiral particles in shear flow, (b) electrophoresis of particles of non-uniform charge distribution.

Multiscale Modeling of Complex Fluids

Weinan E
Princeton University

This is a general introduction to multiscale modeling of complex fluids, particularly polymeric fluids and liquid crystal polymer flows. Topics that we will discuss include molecular dynamics, Brownian dynamics, kinetic theory and hydrodynamic theory. In each case, we will discuss the current status and the challenges that remain. We will also discuss how to couple these different methodologies together to formulate multiscale models.

The Moving Contact Line Problem

Weinan E
Princeton University

We will discuss the microscale and macroscale physics of the moving contact line problem. We will review the results obtained using continuum theory, molecular dynamics and the more recent multiscale techniques. We will also discuss how these techniques can be combined to give us a better understanding of the fundamental physics of the moving contact line problem and formulate simpler and more effective models.

Dripping, Jetting, Drops and Wetting: The Magic of Microfluidics

David A. Weitz
Harvard University

In this talk, I explore the instabilities responsible for droplet formation in fluid flow in thing capillaries. I also examine the use of these flows to create new structures.

Microfluidic Nanoreactors: NanoMolar in Femtoliters

David A. Weitz
Harvard University

Drops in microfluidics can be manipulated very precisely on a drop-by-drop basis. I will demonstrate methods that can be used to accomplish this, and will describe potential applications of this to high throughput bio-assays.

Appendix B: Abstracts from invited speakers

Weizhu Bao	National University of Singapore
Emily Ching	Chinese University of Hong Kong
Qiang Du	Penn State University
Haiping Fang	Shanghai Institute of Applied Physics, CAS
Guowei He	Institute of Mechanics, CAS
Tiejun Li	Peking University
Ping Lin	National University of Singapore
Chun Liu	Penn State University
Yuqiang Ma	Nanjing University
Tiezheng Qian	Hong Kong University of Science and Technology
Penger Tong	Hong Kong University of Science and Technology
Jinchao Xu	Penn State University
Dadong Yan	Institute of Chemistry, CAS
Xingye Yue	Suzhou University
Hui Zhang	Beijing Normal University
Pingwen Zhang	Peking University
Haijun Zhou	Institute of Theoretical Physics, CAS

A model study of turbulent drag reduction by polymers

Emily Ching
Chinese University of Hong Kong

The addition of long-chain polymers to turbulent flows can result in a significant reduction of the friction drag. This intriguing phenomenon was discovered more than fifty years ago but many fundamental aspects remain poorly understood. In this talk, I shall present our study of this problem using a simple dynamical model of viscoelastic flows. Using this model, we are able to understand two main features observed in experiments, namely, the onset of drag reduction and the maximum drag reduction asymptote. Moreover, we find that the essence of the phenomenon of drag reduction can be recaptured by replacing the polymers by an effective scale-dependent viscosity.

From vesicle membrane deformation to cell aggregation

Qiang Du
Department of Mathematics
Penn State University

In this talk, some joint works with colleagues at Penn State on the modeling and simulations of vesicle membrane deformations are presented. In particular, we report on recent studies on membranes interacting with background fluid flow. In addition, We also discuss some mathematical and numerical analysis of coagulation models for cell aggregation.

Dynamics of the single hydrogen-bonded chain of water molecules in channels on the nanometer scale

Haiping Fang[1*] *, Rongzheng Wan*[1]*, Jingyuan Li*[2]*, Hangjun Lu*[1]

[1] Shanghai Institute of Applied Physics, Chinese Academy of Sciences

[2] Department of Physics, Zhejiang University

The importance of the studies of water molecules in channels of nanometer dimensions is not only the observation that the confinement of matter on the nanometer scale can induce phase transition not seen in bulk system, but also the structure similarity with the biological water channels that primary characteristics can usually be exploited in simple systems. A most remarkable common behavior of the water molecules in those channels on the nanometer scale is inside the channels. In this paper, the dynamics of water molecules forming single hydrogen-bonded chains in a single-walled carbon nanotube (SWNT) with under continuous deformations was studied with molecular dynamics simulations. It is found that the water distribution in the channel has a wave-like pattern for integer rings of the SWNTs along the channel. The phase of the wave-like pattern will change to accommodate the deformation of the SWNT due to the external force. Consequently, the number of molecules inside the SWNTs and the water conduction across the water channel can be keep almost fixed for a considerable deformation. For large enough deformation, the phase change of the wave-like pattern can not accommodate the deformation to keep an almost same wave-like water distribution, the number of molecules inside the SWNTs decreases very quickly and the channel will sharply closed. The observation has biological significance since similar wavelike water distributions have been found in biological water channels. The mechanics can be helpful to understand the single molecular mysteries in biological systems such as available signals can be effectively transferred in a high noise environment.

Reference: Rongzheng Wan, Jingyuan Li, Hangjun Lu, Haiping Fang, Controllable water channel gating of nanometer dimensions， J. Am. Chem. Soc. 127, 7166 (2005)

A constrained particle dynamics for the hybrid atomistic-continuum computation of micro-flows

Jia Cui[1] and Guo-wei He[1,2*]

[1]LNM, Institute of Mechanics,
Chinese Academy of Sciences, Beijing, 100080, China,
[2]Department of Aerospace Engineering,
Iowa State University, Ames, IA 50011-2271

Abstract: The hybrid methods of atomistic-continuum computation are being developed for the numerical simulation of micro-flows. In the hybrid methods, fluids are described as amount of particles in one domain that is solved by molecular dynamics and as continuum hydrodynamics in another domain that is solved by the Navier-Stokes equations. These two solutions are coupled in the overlap region by constrained particle dynamics. The computational expense of the hybrid method is expected to be less than full molecular dynamics method in the whole domain, since in most of the computational region the Navier-Stokes equations is used. The challenge is how to construct a constrained particle dynamics, which is used to couple the continuum dynamics and molecular dynamics for the continuity of the physical quantities. In this paper, a constrained particle dynamics is developed by introducing a virtual damping force and an additional mass force to particle dynamics. The sudden-start Couette flows with non-slip and slip boundary conditions are used to test the hybrid method respectively. It is shown that the results obtained are quantitatively in agreement with analytical solutions under the non-slip boundary condition and full molecular dynamics simulations under the slip boundary conditions.

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Simulation of Singularity Dynamics for Liquid Crystal Flows: A C^0 Finite Element Method

Ping Lin
Department of Mathematics
National University of Singapore

Liquid crystal flow model is a coupling between orientation (director field) of liquid crystal molecules and a flow field. The model is also related to a phase field model of multiphase flows and to microfluidics device. It is crucial to preserve the energy laws of the hydrodynamical system in numerical simulation of liquid crystal flows, especially when orientation singularities are involved. We shall use a C^0 finite element method which is simpler than existing C^1 element methods and mixed element formulation and the energy law is formally derived as well. The formulation is verified by comparing its results with those obtained by C^1 elements and by mixed formulation. A characteristic finite element method combined with operator splitting and a very few fixed point iterations for the penalty term of the director field reduces the size of the stiffness matrix and keeps the stiffness matrix time-independent. The latter avoids solving a linear system at every time step and largely reduces the computational time, especially when direct linear system solvers are used. We will consider both both liquid crystal molecule cases. Through numerical experiments of a few splitting strategies and explicit-implicit schemes we recommend a fast and reliable algorithm for this model. A number of examples are computed to demonstrate the algorithm.

Numerical analysis of stochastic methods for dumbbell models in polymeric liquids

Tiejun Li
School of Mathematics
Peking University

As a multiscale coupling method, Brownian Configuration Fields (BCF) is quite popular in polymer field recent years. But the rigorous analysis of the BCF is still at the very early stage. In the talk I will give a review on the numerical analysis of BCF for dumbbell models.

Micro-Macro Models for Viscoelastic Fluids: An Energetic Variational Approach

Chun Liu
Department of Mathematics
Penn State University

The distinguished hydrodynamical and rheological properties of viscoelastical materials can be viewed as the consequences of the competition between the kinetic energy and various elastic energies. Such coupling is in turn through specific transport of the internal elastic variables. In this talk, I will look at several micro-macro models of polymeric materials in order to demonstrate such interactions between different energy functionals. This common feature of the problems also provides the guideline in achieving various well-posedness of the systems under an unified energetic variational formulation.

Self-assembly of Colloid-Polymer Mixtures Confined by Soft Walls

Yu-qiang Ma
National Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China

Abstract

In this talk, I first present a simple review of self-organizing behaviors in soft materials, and then discuss how to design and control self-assembled ordering structures in colloid-polymer systems confined by soft walls. We find that with varying the colloidal concentration, the colloidal self-assembly undergoes a series of symmetry-changing transitions between disordered liquid, square, hexagonal, and cylindric structures, due to the competition between the elastic entropy effect of soft walls and steric packing effect of colloidal particles. The results may provide a helpful guide for fabricating the functionally useful microstructures in materials science of complex liquids.

A variational approach to the moving contact line hydrodynamics

Tiezheng Qian and Xiao-Ping Wang
Department of Mathematics
The Hong Kong University of Science and Technology

Ping Sheng
Department of Physics and Institute of Nano Science and Technology
The Hong Kong University of Science and Technology

In immiscible two-phase flows, contact line denotes the intersection of the fluid-fluid interface with the solid wall. When one fluid displaces the other, the contact line moves along the wall. A classical problem in continuum hydrodynamics is the incompatibility between the moving contact line and the no-slip boundary condition, as the latter leads to a non-integrable singularity. The recently discovered generalized Navier boundary condition (GNBC) offers an alternative to the no-slip boundary condition which can resolve the moving contact line conundrum [1]. We present a variational derivation of the GNBC through the principle of minimum dissipation (entropy generation), supplemented with general considerations of dissipative linear response for small perturbations away from the equilibrium. Through numerical implementation of a continuum hydrodynamic model, it is demonstrated that the GNBC can quantitatively reproduce the moving contact line slip velocity profiles obtained from molecular dynamics simulations [1,2].

[1] T. Z. Qian, X. P. Wang, and P. Sheng, Phys. Rev. E **68**, 016306 (2003).
[2] T. Z. Qian, X. P. Wang, and P. Sheng, Phys. Rev. Lett. **93**, 094501 (2004).

Attractions between charged colloidal particles at aqueous interfaces

Penger Tong*
Hong Kong University of Science and Technology, Hong Kong

Charged colloidal particles at aqueous interfaces are found to experience attractive interactions but the origin of such attraction is not well understood. Because of its fundamental interest and important implications in colloid science and biology, the paradox of like-charge attractions has been under intensive theoretical scrutiny for many years. Here we report our recent experimental results of an optical and atomic force microscopic (AFM) study of attractive interactions between charged polystyrene spheres at the water-air interface [1]. Optical observations of bonded particle clusters and formation of circular chain-like structures at the interface demonstrate that the interaction potential is of dipole origin. AFM phase images show patchy domains on the colloidal surface, indicating that the surface charge distribution is not uniform as is commonly believed. Such surface heterogeneity introduces in-plane dipoles, leading to an attraction at short inter-particle distances.
*Work supported by the Research Grants Council of Hong Kong SAR.
[1] "Long-ranged attraction between charged polystyrene spheres at aqueous interfaces," W. Chen, S.-S. Tan, T. K. Ng, W. T. Ford, and P. Tong, *Phys. Rev. Lett.* **95**, 218301 (2005).

New numerical techniques for complex fluids models and a solution to the high Weissenberg number problem

Jinchao Xu
Penn State University

Effects of confinement on the order-disorder transition in diblock copolymer melts and crystallization

Dadong Yan
Institute of Chemistry, Chinese Academy of Sciences
Beijing 100080, China

The effects of confinement, in terms of size and geometry, on the order-disorder transition (ODT) in diblock copolymer melts are studied theoretically. Within the frame of self-consistent field theory and random phase approximation, the second-order fluctuation of free energy functional is studied by calculating the correlation function in appropriate geometries and sizes of confinement. This leads to a size-dependent correlation function, and the minimum of it determines the spinodal point of the homogeneous phase. As modeling systems, confinements are applied by restricting diblock copolymers in two slabs, cylinder and sphere, respectively. For the slabs and cylinder cases the spinodal point $(\chi N)_s$ of the homogeneous phase is independent of the confinement, indicating that the confinement has no effect in these cases. However, in sphere case $(\chi N)_s$ is increased except some suitable radius of the sphere, indicating that the confinement makes the ODT more difficult to happen. Employing the Landau-Brazovskii model, all the results can be well understood. In addition, using the idea that before nucleation there is the fluctuation of the orientation of polymer chains, the puzzling direction of lamellae in the crystallization under confinement can be well explained.

A Percolation Network Model for the Thermal-hydro Processes associated with Nuclear Waste Repositories

Xingye YUE
Department of Math., Suzhou Univ.

We present a percolation network model to simulate the heterogeneous porous media around the nuclear waste repositories. Main attention is paid to the thermal effect from the waste, which will induce convective flow in the network. So the waste is transported not only by the diffusion but also by the dispersion. The first passage time is investigated by numerical simulation. This is a joint work with Weinan E.

On the multiscale models of polymeric fluids: FENE-dumbbell model and rodlike model

Hui Zhang
Department of Mathematics
Beijing Normal University

We study the well-posedness of a multi-scale model of polymeric fluids. The microscopic model is the kinetic theory of the finitely extensible nonlinear elastic (FENE) dumbbell model. The macroscopic model is the in- compressible non-Newton fluids with polymer stress computed via the Kramers expression. The boundary condition of the FENE-type Fokker-Planck equation is proved to be unnecessary by the singularity on the boundary. Other main results are the local existence, uniqueness and regularity theorems for the FENE model in certain parameter range. For rodlike model we show the contrbution and structure of the transport terms to the rodlike Fokker-Planck equation. In particular, we also prove that there exist classical solutions globally in time.

The Structure of Solutions for Doi-Onsager Equation and Applications

Pingwen Zhang

LMAM and School of Mathematical Sciences
Peking University, Beijing, 100871.

Abstract. We study the structure and stability of stationary solutions to the Doi-Onsager equation with Maier-Saupe potential on the sphere, which arises in the modelling of rigid rod-like molecules of polymers. The stationary solutions are shown to be necessarily a set of axially symmetric functions, and a complete classification of parameters for phase transitions to these stationary solutions is obtained. It is shown that the number of stationary solutions hinges on whether the potential intensity crosses two critical values $\alpha_1 \approx 6.731393$ and $\alpha_2 = 7.5$. Furthermore, we present explicit formulas and linearized stabilities for all stationary solutions.

The Doi kinetic theory for homogeneous flows of rodlike liquid crystalline polymers (LCPs) is extended to inhomogeneous flows through introducing a nonlocal intermolecular potential. An extra term in the form of an elastic body force comes out as a result of this extension. Systematic asympototic analysis in the small Deborah number limit is carried out, and the classical Ericksen-Leslie equations are derived in this limit. The Leslie coefficients are derived in terms of molecular parameters, and the Ericksen stress emerges from the body force.

Elasticity Models for Biopolymers: DNA and Spider Capture Silk

Haijun Zhou
Institute of Theoretical Physics, Chinese Academy of Sciences
Beijing 100080, China

In this presentation, I first review the characteristics of three most widely used polymer models: the Gaussian chain model, the freely-jointed chain model, and the worm-like chain model. Then I will introduce two semi-microscopic models for real biopolymers DNA and spider capture silk, whose elastic properties could not be understood by the above-mentioned simple polymer models.

In the double-stranded stacking chain model of DNA, base-pair stacking potential is considered, and a folding angle parameter is defined to describe the local twisting behavior of DNA helix. It turns out that the short-ranged base-pair stacking interaction is the key contributor both for DNA's stability and for its capability to deform cooperatively under large external perturbations.

Spider capture silk is a bio-material with perfect combination of strength and extensibility, whose force-extension response shows a peculiar exponential form. The structural organization principle of spider capture silk is, however, largely unknown. As a working hypothesis, we suggested that the spider capture silk is a system with hierarchically organized modules. Simple calculations based on this hierarchical chain model lead to predictions that are compatible with known experimental observations.