Special Session 27: Multiscale Modeling and Simulations in Materials Science

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The mini-symposium will focus on analytical and computational aspects for problems involving multiple temporal and spatial scales in a wide variety of systems such as liquid crystals, polymers, ferromagnetic and superconducting materials, and magnetic fluids, among others.

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Three-dimensional shear flow dynamics of a model for liquid crystalline polymers

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Liquid crystalline polymers (LCPs) have found a multitude of applications in the form of fibers, and applications that take advantage of the low thermal expansion coefficient and relatively low viscosity of LCPs such as small-scale precision molded parts. In spite of these successes, however, there are other potentially more important applications that have not been realized, among which the greatest loss is the inability to produce high-strength, lightweight engineering materials with mechanical properties that derive from the spontaneous ordering LCPs display in the liquid state. The difficulty lies in the fact that, although the spinning process used to produce fibers enhances this tendency for ordering, other forms of polymer processing, such as injection molding, involve either shear flows or combinations of shear and extensional flows. For LCPs that "tumble" in shear flows–which include all lyotropic and, apparently, many commercially interesting thermotropic LCPs–these flows seriously degrade or even destroy the orientational order.

The question, then, is whether the degradation of orientational order can be controlled sufficiently by some modification of the processing procedure (i.e., modest changes in the flow geometry). A necessary first step is to elucidate the structure-flow interaction and the dependence of the structural evolution on the flow type, and to develop a predictive capability that reproduces experimental observations. Accounting for the coupling between the microscopic structure and macroscopic stress using a molecular-based continuum model, we have analyzed the three-dimensional flow that occurs in a linear shear cell. In this talk, I will give an overview of our results, with an emphasis placed upon the strong correlations between our findings and relevant experimental observations reported in the literature.

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Stochastic Mode Reduction with Metastability in Biomolecular Modeling

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One approach to accelerating biomolecular simulations is to simulate explicitly only certain slow degrees of freedom of interest, incorporating the effects of the remaining "fast" variables through effective stochastic models. A prevalent feature in these biomolecular systems is metastability – a high potential energy barrier separating different conformational states. We illustrate a systematic multi-scale stochastic mode reduction procedure on a simple model problem of a particle undergoing overdamped Smoluchowski dynamics in a metastable potential with one slow variable and one fast variable. We show how the metastability can lead to various effective stochastic equations for the slow degree of freedom depending on the relations between the physical parameters and properties of the potential energy landscape.

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Numerical analysis for micro-macro models of polymeric fluids

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Micro-macro models for polymeric fluids couple a stochastic differential equation describing the dynamics of the polymer chain in the fluid, with a partial differential equation, namely the classical conservation of momentum and mass of continuum mechanics. I will present such

models, their discretization and some results concerning the numerical analysis of these discretizations.

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Stochastic modeling and multiscale computation of biochemical networks

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We present some recent progress on the stochastic modeling and multiscale computation of mesoscopic chemical kinetic systems, with applications to Genetic Regulatory Networks (GRN). We first discuss the motivations for the stochastic modeling of genetic networks and demonstrate the approach through simple examples. On different time and concentration scales, the dynamics of chemical kinetic systems are governed by different stochastic dynamical systems driven by Poisson noise, Brownian noise, or both. The standard Stochastic Simulation Algorithm (SSA) for chemical kinetic systems is usually limited by the multiscale nature of the genetic networks. We finally discuss the recent advances on overcoming the numerical stiffness induced by disparate reaction rates and metastability of the stochastic systems. The methods are illustrated through numerical examples.

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Mesoscopic dynamics of copolymer thin films with dispersed nanoparticles

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We present a mesoscopic model for the analysis of the electroactive and flow-related properties of P(VDF-TrFE) copolymer thin films with dispersed nanoparticles for electromechanical tunability. Very large recoverable strain with tunable semiconductive and electrostrictive properties in such flexible and large-area thin films are of practical importance in micro-electronics, mechanical and bio-medical industries. Since in such a tunable copolymer film the coupled nonlinear deformation and the electrical mechanisms act over nano to macrosopic length scales, we develop a mesoscopic modeling approach. First, we derive a homogenized constitutive model that takes into account the local transport of cations in polymer, electrostriction and anhysteretic polarization. Then, based on the developed model of coupled partial differential equations, we provide a finite strain description accounting for the mesoscopic dispersion of copolymer chains. This and other key characteristics (electrical field distribution and conductivity properties) are obtained by the finite element methodology under different electromechanical loading conditions. Finally, changes in the deformation pattern of the film as a function of the copolymer volume fraction are analyzed.

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A variational approach to the moving contact line hydrodynamics

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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. We present a variational derivation of the GNBC through the principle of minimum energy dissipation (entropy production), as formulated by Onsager 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. In particular, the transition from complete slip at the moving contact line to near-zero slip far away is shown to be governed by a power-law partial slip regime, extending to mesoscopic length scales.

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Dynamic theory and applications in smectic A liquid crystals

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A novel dynamic continuum theory is presented for smectic A liquid crystals in which the usual director **n** and unit layer normal **a** do not always necessarily coincide. Most previous dynamic continuum theories equate **n** with **a**;

the theory developed here allows **n** and **a** to differ in non-equilibrium situations, work that has been motivated by the recent investigations by Auernhammer *et al.*, Soddemann *et al.* and Weinan E. The usual Oseen constraint for smectics is not imposed upon the unit normal **a**. Permeation effects are also included. After a summary of the complete dynamic equations, an application is given which shows that planar aligned layers of smectic A subjected to an arbitrary periodic disturbance are linearly stable. Boundary layer effects will also be discussed.

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Dislocation dynamics in thin films using the level set method

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The control of the density and location of dislocations (line defects) in heteroepitaxial thin-film is very important in designing semiconductor-based electronic devices. We have developed a level set method based, three dimensional dislocation dynamics simulation method to describe the motion of dislocations in thin films. This method is based on the level set method for dislocation dynamics in bulk materials proposed by Xiang et al. (Acta Materialia, 51, 5499-5518, 2003). The dislocation location is given by the intersection of the zero level sets of a pair of level set functions. This representation does not require discretization and tracking of the dislocation and therefore handles topological changes naturally. The simulation method incorporates the elastic interactions of the dislocations and the stress fields throughout the film and substrate. Using the above approach, various dislocations interactions within a thin film are simulated.

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