Ecole des Ponts - Peking University joint workshop Rheology of complex fluids: modeling and numerics.

List of abstracts

David Andelman (Tel Aviv University)

Title: *Modulated Phases in Complex Fluids: from Ferrofluids to Organic Films and Polymeric Melts*

Abstract:

Self-assembling domains in the nano scales are observed in a wide variety of complex fluid systems. I will review the phenomenology behind these patterns and shapes as seen in ferrofluids, organic films and block copolymeriv melts. I will discuss, in particular, several recent advances in thin films of block copolymers. Chemically patterned surfaces induces complex film morphology, while the substrate roughness affects the orientation of the copolymers. A second topic is the behavior of thin films in presence of external electric fields in the range of 1-100V/micron. Such fields can re-orientate phases of block copolymers, and even cause morphological phase transitions.

John W. Barrett (Imperial College London)

Title: *Existence and Approximation of Global Weak Solutions to some Regularized Dumbbell Models for Dilute Polymers*

Abstract:

We consider the existence of global-in-time weak solutions to a coupled macroscopic-microscopic bead-spring model with microscopic cut-off, which arises from the kinetic theory of dilute solutions of polymeric liquids with noninteracting polymer chains. The model consists of the unsteady incompressible Navier-Stokes equations in a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 2or3$, for the velocity and the pressure of the fluid, with an elastic extra-stress tensor as the right-hand side in the momentum equation. The extra-stress tensor stems from the random movement of the polymer chains and is defined through the associated probability density function ψ that satisfies a Fokker-Planck-type parabolic equation, crucial features of which are the presence of a center-of-mass diffusion term and a cut-off function $\beta^L(\cdot) := \min(\cdot, L)$ in the drag term, where $L \gg 1$. We establish the existence of global-in-time weak solutions to this model for a general class of spring-force potentials including, in particular, the widely used finitely extensible nonlinear elastic (FENE) potential.

We construct a fully discrete Galerkin finite element method for the numerical approximation of this model, which mimics the energy law in the continuous case. We show that a (sub)sequence of numerical solutions converges to a weak solution of this coupled Navier-Stokes-Fokker-Planck system as the spatial and temporal discretization parameters tend to zero.

We prove similar existence and approximation results for a corresponding regularized Oldroyd-B model.

The work on the regularized macroscopic/microscopic model is joint with Endre Süli, OUCL, University of Oxford, Parks Road, Oxford OX1 3QD, UK.

The work on the regularized Oldroyd-B model is joint with Sébastien Boyaval, CERMICS, Ecole Nationale des Ponts et Chaussées (ParisTech/Université Paris-Est), 77455 Marne-la-Vallée Cedex 2, France.

Andrew Belmonte (Penn State University)

Title: *Reactive Hydrodynamics and Interfacial Instabilities of Micellar Systems*

Abstract: While many fluid instabilities involving free surfaces are governed by interfacial forces - the classic example being surface tension - real materials often have surface forces produced by physical processes not present in the bulk. A striking example of this is a viscoelastic micellar fluid, in which the long tubelike aggregates form at low concentrations due to the presence of an organic salt/cosurfactant, without which the micelles are spherical and the fluid is completely Newtonian. I will present some of our recent experimental observations and modeling of the instabilities occurring when two such Newtonian fluids react to produce a fragile elastic micellar material, either during impact splashes or viscous fingering.

Mireille Bossy (INRIA Sophia Antipolis)

Title: *Stochastic Lagrangian models for turbulent flows. Application to a downscaling method for wind forecast at small scales.*

Abstract: We propose a new downscaling method for the simulation of wind at small scales. Based on an existing numerical weather prediction model, we introduce a Langevin system as a local Lagrangian model aimed to estimate the distribution of the wind at small scales. We borrow and adapt stochastic models proposed by Stephen B. Pope that have been widely used in the framework of multiphasic fluids.

After a brief description of the Pope models, we present our adaptation to the meteorological downscaling problem, the associated numerical algorithm and some numerical results (joint work with F. Bernardin, C. Chauvin, P. Drobinski, A. Rousseau, T. Salameh).

The last part of this talk will be devoted to the study of the well-posedness of a simplified Lagrangian model and its confined version in a spatial sub-domain which is used in the downscaling problem (joint work with J.F. Jabir).

Sébastien Boyaval (Ecole des Ponts)

Title: *A Variance Reduction Method for Parametrized Stochastic Differential Equations using the Reduced Basis Paradigm*

Abstract: We develop a reduced-basis approach for the efficient computation of a large number of expected values using the control variate method to reduce the variance. Two algorithms are proposed to compute online, through a cheap reduced-basis approximation, the numerous (parametrized) control variates for a large number of expectations of a functional of a parametrized Itô stochastic process (solution to a parametrized stochastic differential equation). For each algorithm, a reduced basis is pre-computed offline, following a Greedy procedure, which minimizes the variance among a trial sample of expectations. Numerical results in situations relevant to practical applications (the calibration of volatility in option pricing, and the velocity-gradient-driven evolution of a vector field of FENE dumbbells) illustrate the efficiency of the method.

Didier Bresch (Université de Savoie)

Title: *Visco-plastic fluids and free-surface*

Abstract: Avalanches are natural phenomena that occur in mountainous regions such as Alps in France. As usually in complex phenomena, it is very difficult to postulate a constitutive relation for the stress tensor in terms of a deformation measure that correctly descrives avalanches behavior. During the last few year, more and more efforts have been devoted to the physical understanding of avalanche formation. In this talk, we will derive an example of compressible visco-plastic model occuring as a depth averaged system. Then we present a generalization to compressible flows of the Augmented Lagrangian method for incompressible Bingham visco-plastic flow initiated by R. Glowinski. We will see on several numerical tests that there exists a real interaction between the finite volume scheme and the Augmented Lagrangian procedure. We will also present some other models sometimes used in Avalanches and the mathematical difficulties encountoured for instance to establish the existence of global weak solutions. Part of this talk is a joint work with E. Fernandez-Nieto, I. Ionescu, P. Vigneaux.

Jean-Pierre Eckmann (Université de Genève)

Title: *Heat Conduction as a Non-Equilibrium Problem*

Abstract: In this talk I will discuss a Boltzmann-like method to analyze a deterministic model of heat conduction. I will show both analytical and numerical studies of a simple 1-dimensional model of a row of scatterers coupled at each end to a heat bath. This model has both energy and mass transport, and can be rigorously discussed. My talk is based on work with Pierre Collet and Carlos Mejia-Monasterio.

M. Gregory Forest (University of North Carolina)

Title: *The interplay between hydrodynamic feedback and defects in sheared nematic liquids*

Abstract: There is a rich history of defects in liquid crystals and liquid crystal polymers, which has focused almost exclusively on static morphologies, the topology of the nematic director field, followed by regularization by a blow-up of the core of the defect. We show a tensorial or probability distribution description of a defect core provides accelerated detection and tracking strategies of defects, and applies more generally than topological defect metrics. In the past decade or so, there has been a great deal of attention to shear banding in flows of anisotropic viscoelastic liquids such as wormlike micelles. In this lecture we show strong correlations between dynamic defect morphology and strong flow feedback in benchmark non-equilibrium shear flows. This lecture is based on joint work with several collaborators, especially the algorithms and simulations of X. Yang at North Carolina, recent projects with S. Heidenreich from the Hess group in Berlin and R. Zhou from Old Dominion University, and longstanding work with Q. Wang, now at U. South Carolina.

Colette Guillopé (Université Paris XII)

Title: *Review of existence results for slightly compressible viscoelastic fluids*

Raz Kupferman (Hebrew University of Jerusalem)

Title: *Progress and challenges in the high Weissenberg number problem*

Abstract: Since the early 1970s the field of computational rheology has been haunted by the so-called high-Weissenberg number problem—the breakdown of all computational methods at frustratingly low values of the elasticity parameter. Even the very nature of this phenomenon has been a matter of great controversy. Despite the fact that this field has evolved in many new directions, the original difficulties have remained to a large extent unanswered. In my talk I will review (relatively) recent progress such as the log-c formulation, and re-examine from both numerical and anaytical points of view the remaining difficulties.

François Lequeux (ESPCI Paris)

Title: *Pasty fluids modeling : a physicist point of view*

Abstract: Many complex fluids exhibit a yield stress : below some stress, they are solid like, while above the flow. This plastic behavior is complex, because the state in the absence of shear is not unique. In addition and as a consequence, the yield stress fluids that are sensitive to themral motions exhibit aging. I will describe how it is possible to write simple models that take into accounts these coupled phenomena.

Hervé Le Meur (Université Paris Sud)

Title: *Small-time existence for a viscoelastic model with free bounday and a free surface.*

Abstract : We prove the small-time existence of the solution of a Johnson-Segalmann-type viscoelastic fluid for any initial data and a free boundary. We take into account the surface tension. To that purpose, we split the Navier-Stokes part of the equations, which is solved in G. Allain Appl. Math. Optim. 16 (1987), no. 1, 37–50, and the purely viscoelastic constitutive equation. In the Lagrangian coordinates, the constitutive equation improves the time regularity. This enables to have continuity constants depending on the final time in a convenient way. Then we estimate all the error terms and then prove the result with a fixed point theorem.

Ruo Li (Peking University)

Title: *Dynamic Depletion of Vortex Stretching and Non-Blowup of the 3-D Incompressible Euler Equations*

Abstract: We study the interplay between the local geometric properties and the non-blowup of the 3D incompressible Euler equations. We consider the interaction of two perturbed antiparallel vortex tubes [Phys. Fluids 5 (1993), 1725]. We use a pseudo-spectral method with very high resolution to resolve the nearly singular behavior of the Euler equations. Our numerical results demonstrate that the maximum vorticity does not grow faster than double exponential in time until the solution is numerically resolved. The velocity, the enstrophy and enstrophy production rate remain bounded throughout the computations. As the flow evolves, the vortex tubes are flattened severely and turned into thin vortex sheets, which roll up subsequently. The vortex lines near the region of the maximum vorticity are relatively straight. This local geometric regularity of vortex lines seems to be responsible for the dynamic depletion of vortex stretching.

Tiejun Li (Peking University)

Title: *Highly accurate tau-leaping methods for simulating chemical reaction systems*

Abstract: The tau-leaping algorithm is proposed by D.T. Gillespie in 2001 for accelerating the simulation for chemical reaction systems. It is faster than the traditional stochastic simulation algorithm (SSA), which is an exact simulation algorithm. In this lecture, I will report some recent advances of tau-leaping algorithms, which is called RC-tau-leaping by us. This algorithm is highly accurate than the primitive tau-leaping algorithms. The brief history is also reviewed in this talk.

Alexei Lozinski (Université Paul Sabatier)

Title: *On discretization schemes for stochastic differential equations with unbounded drift in the kinetic theory of polymer solutions.*

Claude Mangoubi (Hebrew University of Jerusalem)

Title: *Numerical Stability of the method of Brownian configuration fields*

Abstract: The computation of viscoelastic flow using macroscopic models is known to be problematic when the Weissenberg number (the ratio of the typical relaxation time of the fluid considered to a typical flow time) reaches a value of O(1).

In the last decade, kinetic (or micro-macro) models have been introduced in the simulation of viscoelastic fluids. While they seem to have better stability properties than their macroscopic counterparts, this has not been clearly shown.

In this talk, we investigate the numerical stability of the Brownian configuration fields method as the Weissenberg (Wi) number increases. We do not encounter the typical numerical blow-up known in macroscopic models. However, solutions become mesh-dependent as Wi is large.

This lecture is based on joint work with Martien Hulsen and Raz Kupferman.

Bertrand Maury (Université Paris Sud)

Title: *Modeling of dense suspensions*

Abstract: We present some issues related to the numerical modeling of dense suspensions of rigid bodies in a viscous fluid, for which close range lubrication forces may play a significant role. In the context of direct numerical simulations, thoses forces are supposed to be accounted for in the equations for the fluid. Yet, as interparticle distances may be very small compared to other characteristic lengths, most solvers are likely to fail in giving an accurate description of the interstitial flow. For this reason, different approaches have been proposed, and we will describe some of them in terms of numerical efficiency, respect of the underlying physics, and influence upon the global behaviour of the suspension.

Pingbing Ming (Chinese Academy of Sciences)

Title: *A Linear Scaling Algorithm for Molecular Mechanics Model*

Abstract: In this talk, I will introduce a linear scaling algorithm for models arising from the molecular mechanics models. Numerical results will be reported for the homogeneous

deformation as well as the inhomogeneous deformation. The tests for the homogeneous deformation include one-dimensional tension, tension and shear tests for Aluminum. The tests for the inhomogeneous deformation include tension for Aluminum with vacancy and the nanoindentation.

This is a joint work of Jingrun Chen in AMSS and Weinan E in Princeton University.

Marco Picasso (Ecole Polytechnique Fédérale de Lausanne)

Title: *Numerical simulation of Rhone's glacier from 1874 to 2100*

Abstract: The numerical simulation of the motion of Rhone's glacier in the Swiss Alps is performed from 1874 to 2007, and then from 2007 to 2100. Given the shape of the glacier, the velocity of ice is obtained by solving a 3D nonlinear Stokes problem with a nonlinear sliding law along the bedrock-ice interface. Then, the shape of the glacier is updated by computing the volume fraction of ice which satisfies a transport equation. A source term acting only on the ice-air interface accounts for the accumulation or ablation of ice due to snow falls or melting.

A decoupling algorithm allows the two above problems to be solved using different numerical techniques. The nonlinear Stokes problem is solved on a fixed, unstructured finite element mesh made of tetrahedrons. The transport equation is solved using a fixed, structured grid made of smaller cells.

The numerical simulation between 1874 and 2007 is compared to measurements. Then, three different climatic scenario are considered in order to predict the shape of the glacier from 2007 until 2100.

Alejandro Rey (McGill University)

Title: *Computational Rheology of Carbonaceous Mesophases*

Abstract: A review of flow and texture modeling of liquid crystalline materials with emphasis on carbonaceous mesophases is presented. Two models of nematodynamics are presented and discussed in terms of their ability to resolve time and length scales likely to arise in typical rheological and processing flows. Defect physics and rheophysics are integrated with nematodynamics and specific mechanisms of defect nucleation and annihilation are used to derive texture scale power laws. The integrated nematodynamics models specialized to carbonaceous mesophases are used to analyze: (i) linear and nonlinear viscoelasticity, (ii) rheological flows, and (iii) carbon fiber and flow-induced textures. The linear and nonlinear viscoelasticity reveals the essential nature of these materials : coupling between flow-induced orientation and orientation-induced flow , elastic storage through orientation gradients, and anisotropy. The rheological flow simulations, shown to be in excellent agreement with experimental data, reveal several liquid crystal specific rheological characteristics including shear thinning due to anisotropic viscosities and flow-induced orientation, and negative first normal stress difference due to orientation nonlinearities in the shear stress. Nematodynamic predictions are shown to follows a Carreau-Yasuda liquid crystal equation. Nematodynamics predictions rationalize shear-induced texture refinement in terms of defect nucleation and coarsening mechanisms and are used to derive texture scaling relations in terms of macroscopic, molecular, and flow time scales. This knowledge is then condensed into a generic texture-flow diagram that specifies the required temperature and Deborah number required to produce well oriented monodomain materials. The fine details of mesophase structuring by flow through screens are shown to be

captured by nematostatic simulations. Finally the mechanisms behind the carbon fiber textures produced by melt spinning of carbonaceous mesophases are elucidated. The proven range and predictive accuracy of nematodynamics to simulate flows of textured mesophases and the ever-growing industrial interest in lower cost high performance super-fibers and functional materials will fuel the evolution of liquid crystal rheology and processing science for years to come.

Yossi Shamai (Hebrew University of Jerusalem)

Title: *Spatial correlations and variance reduction in Brownian simulations.*

Abstract: Brownian simulation methods have become very popular in the context of complex fluids since the 1990's. We start with a motivational background to polymeric fluid models and introduce the notions of Hilbert space-valued Brownian motions and spatial correlation operators. We then give a general formulation for Brownian simulation methods which differ in different choices of noise correlation.

We present a variance minimization problem in Brownian simulations with respect to an optimal choice of noise correlations.

Huazhong Tang (Peking University)

Title: *An Adaptive Phase Field Method for the Mixture of Two Incompressible Fluids*

Abstract: We present an adaptive moving mesh method to solve a phase field model for the mixture of two incompressible fluids.The projection method is implemented on a half-staggered, moving quadrilateral mesh to keep the velocity field divergence-free, and the conjugate gradient or multigrid method is employed to solve the discrete Poisson equations. The current algorithm is composed by two independent parts: evolution of the governing equations and mesh-redistribution. In the first part, the incompressible Navier-Stokes equations are solved on a fixed half-staggered mesh by the rotational incremental pressure-correction scheme, and the Allen-Cahn type of phase equation is approximated by a conservative, second-order accurate central difference scheme, where the Lagrangian multiplier is used to preserve the mass-conservation of the phase field. The second part is an iteration procedure. During the mesh redistribution, the phase field is remapped onto the newly resulted meshes by the high-resolution conservative interpolation, while the non-conservative interpolation algorithm is applied to the velocity field. The projection technique is used to obtain a divergence-free velocity field at the end of this part. The resultant numerical scheme is stable, mass conservative, highly efficient and fast, and capable of handling variable density and viscosity. Several numerical experiments are presented to demonstrate the efficiency and robustness of the proposed algorithm.

Giuseppe Toscani (University of Pavia)

Title: *A kinetic model for flocking*

Abstract: The description of emerging collective behaviors and self-organization in multi- agent interactions has gained increasing interest from various research commu- nities in biology, ecology, robotics and control theory, as well as sociology and economics. In the biological context, the emergent behavior of bird flocks, fish schools or bacteria aggregations, among others, is a ma jor research topic in population and behavioral biology and ecology. In this talk [1], we introduce and analyze a continuous version of the

flocking model of Cucker and Smale [2], which describes the state of a population of birds. Within the same idea that a bird adjusts its velocity towards the average of neighbors' velocities, we construct a spatially dependent Boltzmann-type equation which describes the behavior of the flock in terms of a density $f = f(x, v, t)$. The large-time behavior of f is subsequently studied by means of mass transportation techniques. In particular, a continuous analogue of the theorems of [2] is shown to hold for the solution. These results generalize the approach by Ha and Tadmor [3], who investigated the large-time behavior of the solution by different techniques.

References:

[1] J.A. Carrillo, M. Fornasier, G. Toscani: A kinetic model for flocking (preprint) (2008).
[2] F. Cucker, S. Smale: IEEE Trans. Automat. Control 52 (2007) 852-862.
[3] Seung-Yeal Ha, E. Tadmor: Kinetic and Related Models 1(3) (2008) 415-435.

Noel J. Walkington (Carnegie Mellon University)

Title: *Numerical Schemes for Complex Fluids*

Abstract: Models of complex fluids typically couple the momentum equation to an equation governing the evolution of the microstructure. Examples include liquid crystals, fluids containing elastic particles, and polymer fluids. These systems posses a Hamiltonian structure which reveals the subtle structure of the terms coupling of the two equations, and a delicate balance between inertia, transport, and dissipation.

This talk will focus on the development and analysis of numerical schemes which inherit the Hamiltonian structure, and hence stability, of the continuous problem. Compactness properties of the discrete solutions will then be presented to establish convergence of these schemes.

Hui Zhang (Beijing Normal University)

Title: *Long-time asymptotic behaviour of a multiscale rod-like model of polymeric fluids*

Abstract: We investigate the long-time asymptotic behaviour of some multiscale rod-like models for polymeric fluids in various settings which include no flow, shear flow, general bounded domain with homogeneous and non-homogeneous Dirichlet boundary conditions on the velocity. We use entropy approach to obtain the decay rates of dynamic states converging to the equilibrium in some norms in virtue of the Csiszar-Kullback inequality.

Pingwen Zhang (Peking University)

Title: *Nucleation and Boundary Layer in Diblock Copolymer SCFT Model*

Abstract: The phase diagram of the equilibrium states and the stability of the possible microstructures are both important for polymer scientists. The phase behavior of a diblock copolymer system could be studied through self-consistent mean field theory (SCFT). We extensively study the boundary layer of a diblock copolymer melt confined system using compressible self-consistent mean-field theory. We discover the boundary layer profile and its thickness are only determined by boundary potential and compressible parameter. We have also investigated several effects due to the confinement of polymer melts by impenetrable hard surfaces in the self-consistent field calculations.

We will also introduce a numerical method to study the nucleation in copolymer melts. Nucleation is the decay of a metastable state via the thermally activated formation and

subsequent growth of droplets of the equilibrium phase. We will consider the nucleation in diblock copolymer melts, whose equilibrium phases are well understood. We apply a new numerical method, called the string method, to compute the minimum energy path (MEP). Then from the MEP, we find the size and shape of the critical droplet and the free-energy barrier to nucleation.