Name of 5-day Workshop
Date of 5-day Workshop

MEALS

Breakfast (Continental): 7:00 – 9:00 am, 2nd floor lounge, Corbett Hall, Sunday – Thursday
*Lunch (Buffet): 11:30 am – 1:30 pm, Donald Cameron Hall, Sunday – Thursday
*Dinner (Buffet): 5:30 – 7:30 pm, Donald Cameron Hall, Saturday – Wednesday
Coffee Breaks: As per daily schedule, 2nd floor lounge, Corbett Hall
***Please remember to scan your meal card at the host/hostess station in the dining room for each lunch and dinner.**

MEETING ROOMS

All lectures will be held in Max Bell 159 (Max Bell Building accessible by bridge on 2nd floor of Corbett Hall). Hours: 6 am – 12 midnight. LCD projector, overhead projectors and blackboards are available for presentations. *Please note that the meeting space designated for BIRS is the lower level of Max Bell, Rooms 155-159. Please respect that all other space has been contracted to other Banff Centre guests, including any Food and Beverage in those areas.*

SCHEDULE

Saturday

16:00 Check-in begins (Front Desk – Professional Development Centre - open 24 hours)
Lecture rooms available after 18:00 (if desired)

17:30-19:30 Buffet Dinner, Donald Cameron Hall

20:00 Informal gathering in 2nd floor lounge, Corbett Hall (if desired)
Beverages and small assortment of snacks available on a cash honour-system basis.

Sunday

7:00-8:45 Breakfast
8:45-9:00 Welcome by Jimmy Feng, Chun Liu and Brenda Shakotko, BIRS Station Manager, Max Bell 159

Moderator: Jimmy Feng

9:00-9:25 Yuriko Renardy: *Numerical simulations of drop deformation for viscoelastic liquid-liquid systems*
9:25-9:50 Gary Leal: *Theoretical studies of flow-induced coalescence*
9:50-10:15 Jie Shen: *A phase-field model for the mixtures of two incompressible fluids: applications to drop formation*

10:15-10:35 Coffee Break, 2nd floor lounge, Corbett Hall

10:35-11:00 Jianjun Xu: *A level-set method for interfacial flows with surfactant*
11:00-11:25 Chunfeng Zhou: *Simulation of neutrophil transit in capillaries using simple and compound drop models*

11:30-13:30 Lunch

Moderator: Chun Liu

13:30-13:55 Sanjoy Banerjee: *Computational approaches to complex fluid formulation design*
13:55-14:20 Eliot Fried: *Sharp-interface theory for solvent, momentum, and energy transfer between a surfactant solution and a vapor atmosphere*

14:20-14:40 Coffee Break, 2nd floor lounge, Corbett Hall

14:40-15:05 Roger Khayat: *Thin-film flow of viscoelastic fluids*
15:05-15:30 Juan Lopez: *Couplings between bulk flows with inertia and monolayer mesoscale structure*
15:30-15:55 Greg Forest: *Orientational gradients, shear bands & stored stresses in plane Couette flow of rigid-rod suspensions*

17:30-19:30 Dinner

Monday

7:00-9:00 Breakfast

Moderator: Ellen Longmire

9:00-9:25 Qiang Du: *Diffusive interface modeling and numerical simulation of lipid membranes*
9:25-9:50 Elaine Zhu: *Fluids moving past smooth hydrophilic surfaces – slip?*
9:50-10:15 Len Pismen: *Droplets propelled by surface forces*

10:15-10:35 Coffee Break, 2nd floor lounge, Corbett Hall

10:35-11:00 Kerstin Wielage: *Immiscible displacement flow along a plane channel*
11:00-11:25 Boris Stoeber: *Visco-thermal flow instabilities of thermally responsive fluids*

11:30-12:30 Lunch
12:30-13:20 Guided Tour of the Banff Centre; meet on front steps of Corbett Hall
13:20-13:30 Group Photo on the front steps of Corbett Hall

Moderator: Boris Stoeber

13:30-13:55 Ellen Longmire: *Experiments on coalescence in liquid/liquid mixtures*
13:55-14:20 Jimmy Feng: *Experiments and simulation of partial coalescence in Newtonian and polymeric fluids*
14:20-14:45 Wei Yu: *The effect of interfacial viscosity on the droplet dynamics under flow field*

14:45-15:05 Coffee Break, 2nd floor lounge, Corbett Hall

15:05-15:30 Amy Shen: *Effects of surface property and geometric confinement on the droplet formation and deposition inside microfluidic devices*
15:30-15:55 Shelley Anna: *Thread formation and tipstreaming in a microfluidic flow focusing device*
15:55-16:20 David Jacqmin: *Phase-field calculations of wetting failure and instabilities*

17:30-19:30 Dinner

Tuesday

7:00-9:00 Breakfast

Moderator: Howard Hu

9:00-9:25 Carme Calderer**:** *Nonlocal electrostatic effects in spontaneously polarized liquid crystals*
9:25-9:50 Qi Wang: *Numerical and analytic study of nematic polymer flows coupled with external fields*
9:50-10:15 Pam Cook: *Wormlike micellar solutions: A model and its predictions*

10:15-10:35 Coffee Break, 2nd floor lounge, Corbett Hall

10:35-11:00 Pingwen Zhang: *Numerical method of the equilibrium states and the nucleation in copolymer melts*
11:00-11:25 An-Chang Shi: *Phases, phase transitions and self-assembly in block copolymers*

11:30-13:30 Lunch

Free Afternoon!

17:30-19:30 Dinner

Wednesday

7:00-9:00 Breakfast

Moderator: Becca Thomases

9:00-9:25 Peter Minev: *A compromise between the Eulerian and ALE approach to free boundary problems*
9:25-9:50 Howard Hu: *Simulation of motion and deformation of elastic objects in flows*
9:50-10:15 Pengtao Yue: *Simulation of bubble growth in polymer foaming*

10:15-10:35 Coffee Break, 2nd floor lounge, Corbett Hall

10:35-11:00 Simon Tavener: *Rayleigh-Bénard-Marangoni convection with a deformable interface*
11:00-11:25 David Trebotich: *The critical Mach number problem and well-posed viscoelastic flows*

11:30-13:30 Lunch

Moderator: Simon Tavener

13:30-13:55 Tiejun Li: *Path integral analysis for the heteropolymer*
13:55-14:20 Jorge Vinals: *Mesoscopic hydrodynamics of lamellar phases, and orientation selection under shear*

14:20-14:45 Mike Shelley: *Transport in visco-elastic flows*

14:45-15:05 Coffee Break, 2nd floor lounge, Corbett Hall

15:05-15:30 Chun Liu: *New closure approximation for FENE models*
15:30-15:55 Becca Thomases: *Analysis and numerics for Oldroyd-B fluids*

17:30-19:30 Dinner

Thursday

7:00-9:00 Breakfast

Moderator: Chun Liu

9:00-9:25 Alejandro Rey: *A model of membrane flexoelectricity*
9:25-9:50 Rolf Ryham: *Deformation of charge selective vesicles*
9:50-10:15 Noel Walkington: *Phase field/level set methods for problems involving elastic membranes*

10:15-10:35 Coffee Break, 2nd floor lounge, Corbett Hall

11:30-13:30 Lunch

Checkout by 12 noon.

** 5-day workshops are welcome to use the BIRS facilities (2nd Floor Lounge, Max Bell Meeting Rooms, Reading Room) until 4 pm on Thursday, although participants are still required to checkout of the guest rooms by 12 noon. **

(Abstracts in alphabetical order by last name of speaker)

Speaker: S. L. Anna

Thread formation and tipstreaming in a microfluidic flow focusing device

Hans C. Mayer and Shelley L. Anna
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Microfluidic devices have recently emerged as an effective method of generating monodisperse emulsion droplets. However, in these and other methods, the drop size produced is typically limited by the size of the orifice from which the droplet grows. In microfluidic devices, this limits the minimum achievable drop size to around 5 to 10 microns. The ability to reduce the drop size still further, into the submicron range, is of interest in a range of applications including drug and gene delivery, medical imaging and nanoparticle synthesis.

We present a novel microfluidic method of synthesizing micron-scale and smaller droplets. Our method utilizes surfactants at the liquid-liquid interface, combined with elongational flow in a microfluidic flow focusing device, to promote a phenomenon called tipstreaming. Tipstreaming occurs when a parent drop forms a highly pointed tip, and daughter drops up to two orders of magnitude smaller are ejected from that tip. Recent numerical simulations have shown that tipstreaming occurs in a specific range of surfactant concentration and capillary number [1]. We present experiments to test this prediction by systematically varying surfactant concentration, capillary number, and flow rate ratio. We observe that in a particular range of surfactant concentration, large drops are followed by the formation of long thin threads. As the flow rate ratio increases, the threads grow longer, eventually exhibiting sustained tipstreaming at very large flow rate ratios. This behavior occurs in a range of capillary numbers between $0.4 < Ca < 1.0$ with a peak in the thread length at $Ca \sim 0.5$, consistent with conditions at which tipstreaming is observed in classic drop breakup experiments. We characterize the thread length and diameter as a function of the above dimensionless parameters, and we interpret the observed results in terms of induced surface tension gradients. To aid our understanding we utilize a physical model of the tipstreaming process similar to that recently presented by Krechetnikov and Homsy [2].

References

[1] C. D. Eggleton, T. M. Tsai, and K. J. Stebe, Tip streaming from a drop in the presence of surfactants, Phys. Rev. Lett. 87, 048302, 2001.
[2] R. Krechetnikov and G. M. Homsy, On physical mechanisms in chemical reaction-driven tip-streaming, Phys. Fluids 16, 2556-2566, 2004.

Speaker: Sanjoy Banerjee

Computational Approaches to Complex Fluid Formulation Design

Dept. of Chemical Engineering, UCSB

Complex fluid formulations, such as paints, polymeric liquids, cosmetics, personal care and some pharmaceutical products, are usually mixtures characterized by many components, multiple coexisting phases, and structural heterogeneities spanning a wide range of length scales. The nano- and micro-structure of such formulations are significantly affected by processing, which determines their macroscopic behavior and properties. The design of new formulations typically proceeds by trial and error, perhaps using historical recipes as a starting point. Theory and computation could potentially speed the design process, but direct use of inter-atom potentials in molecular dynamics or Monte Carlo simulations have not yet been able to resolve the structural scales of interest, which are much

larger than atomic dimensions. An alternative approach based on statistical field theory models is discussed, where atomic coordinates are replaced by one or more fluctuating chemical potential fields. Such models can be coarse grained to length scales corresponding to those that appear in materials of interest and results in a framework of coupled field equations for flow and structure that captures, in principle, the realistic dynamics out of equilibrium.

This scheme has been applied to dense systems in which mean field theory is accurate, and fluctuations in all fields have been removed. This leads to a two- (or multi-) fluid model for coupled structure-flow problems that incorporates an effective Hamiltonian in terms of the local chemical potential and strain fields. Phase-ordering kinetics models and self-consistent (mean-) field theory models for equilibrium structure arise as special cases. Simulations, based on the two-fluid model, will be presented to demonstrate that shear-induced effects on formulation structure can be successfully captured. In particular, different structures can be obtained for specified compositions of phase separating or self-assembling systems by changing processing conditions. These can take one, or some combination, of a variety of forms such as necklaces of drops, cylindrical strings, lamellae or more complex bi-continuous structures, from which the desired configuration for a specific product can be selected.

Speaker: Maria-Carme T. Calderer
Nonlocal electrostatic effects in spontaneously polarized liquid crystals
University of Minnesota

This presentation deals with modeling of nonlocal electrostatic effects in liquid crystals. While many of the liquid crystals found in applications are dielectric, the synthesis of new materials, such as the bent-core molecule type, motivate studies of ferroelectric phases. The spontaneous polarization of the liquid crystal creates an electrostatic energy that may be felt in the whole space. Molecular and shape rearrangement take place in order to prevent energetically costly configurations. We will discuss bulk rearrangements in terms of undulation and periodicity. Likewise, we argue that the development of telephone cord shapes observed in bent-core molecule liquid crystal filaments is also the result of an optimization mechanism. We will discuss the formation of helical filaments from the point of view of nonlinear elasticity.

Another consequence of the nonlocal effects due to polarization become apparent near the phase transition temperature from smectic~C to nematic. The model that we propose, indeed, predicts long range fluctuations of the smectic parameters near the transition temperature. We show consistentcy of such predictions with experimental observations of Casimir forces. We will end the presentation addressing related flow phenomena.

Speaker: P. Cook
Wormlike micellar solutions: A model and its predictions
Pam Cook (University of Delaware), Gareth McKinley (MIT), Paula Vasquez (University of Delaware), Lin Zhou (University of Delaware)

Wormlike micellar fluids, also known as "living polymers", continuously break and reform their structure in solution thus exhibiting a characteristic breakage time in addition to the (network) relaxation time. Experimental observations reveal that these wormlike micellar solutions exhibit a plateau in the steady state "flow curve" of shear stress vs shear-rate, and microscopic observations show that is accompanied by the development of spatial inhomogeneities in the flow. This "shear-rate-banding" results in regions of localized intense birefringence in which the micelles are locally oriented and elongated. The transient response to the start-up of steady shear within this plateau region, shows a stress overshoot followed by an undershoot before reaching steady state. In transient extensional flow, these solutions exhibit pronounced strain-hardening at moderate strains followed by

a decrease in the extensional viscosity (rate-thinning) at a critical extension rate.

We outline the development of a network-based constitutive model that incorporates the breaking and reforming of the micelles (similar to the original theory of Cates & coworkers). In this model we assume, for simplicity, a finite number of lengths/species, as opposed to the continuous length distribution described in the original Cates theory. Each micellar species is modeled as a nonlinear bead-spring dumbbell.

Predictions of the model in transient and steady state shear and in extension will be presented and compared with experiment.

Speaker: Q. Du

Diffusive interface modeling and numerical simulation of lipid membranes

Department of Mathematics, Penn State University

Lipid membranes are becoming a major focus of biological, biophysical and biochemical studies in recent years. In this talk, we present a series of works done by the Penn State group on the phase field modeling and simulations of vesicle membrane deformations under the elastic bending energy. These include studies of full three dimensional energy minimizing configurations, effect of spontaneous curvature, interaction with background fluid flows, multicomponent and open membranes. Convergence analysis and the effectiveness of various numerical methods developed for these models are discussed. In addition, we also demonstrate how to effectively retrieve topological information within the diffusive interface framework which may have broad applications.

Speaker: J. Feng

Experiments and simulation of partial coalescence in Newtonian and polymeric fluids

Department of Mathematics and Department of Chemical and Biological Engineering
University of British Columbia

A drop falling onto a fluid-fluid interface may not merge with it at once but undergo a so-called partial coalescence cascade. I will discuss our recent experimental observations and numerical simulations of this phenomenon for Newtonian as well as polymeric fluids. In Newtonian fluids, the partial coalescence takes place for an intermediate range of drop sizes and consists of viscous, inertio-capillary and gravity regimes. Viscoelasticity in either the drop or the ambient fluid tends to delay the pinch-off of the secondary drop, and may even suppress partial coalescence altogether. The underlying mechanism is large tensile polymer stresses resisting the stretching and thinning of the fluid neck. The numerical results are in qualitative, and in some cases quantitative, agreement with experiments.

Speaker: G. Forest

Orientational gradients, shear bands & stored stresses in plane Couette flow of rigid-rod suspensions

University of North Carolina-Chapel Hill

Experimentalists have observed intriguing phenomena in sheared "anisotropic" suspensions, where the anisotropy may arise from rigid macromolecules or even malleable micelles. The phenomena range from rheo-oscillators (tumbling and more esoteric limit cycle responses to steady shear conditions), to sign changes in normal stress differences, to evidence of shear banding, to nearly solid-like linear viscoelasticity, and secondary flow instabilities. Several research groups have made progress in modeling of these observations, including those of Larson, Leal, Feng, Rey, and others. Our group has also worked toward descriptions of and correlations among these observations, choosing the model system of rigid nano-rods in viscous solvents. I will report some of our findings in the time allotted. The group includes students (E. Choate, J. Lee, X. Zheng), Z. Cui (postdoc), along with collaborators

Q. Wang, H. Zhou & R. Zhou.

Speaker: E. Fried

Sharp-interface theory for solvent, momentum, and energy transfer between a surfactant solution and a vapor atmosphere

Department of Mechanical and Aerospace Engineering
Washington University in St. Louis
St. Louis, MO 63130-4899, USA

We develop a complete set of equations governing the evolution of a sharp interface separating a volatile-solvent/nonvolatile-surfactant solution from a vapor atmosphere. In addition to a sorption isotherm equation and the conventional balances for mass, linear momentum, and energy, these equations include an alternative to the Hertz--Knudsen--Langmuir equation familiar from conventional theories of evaporation-condensation. This additional equation arises from a consideration of configurational forces within a thermodynamical framework. While the notion of configurational forces is well-developed and understood for the description of materials, like crystalline solids, that possess natural reference configurations, very little has been done regarding their role in materials, such as viscous fluids, that do not possess preferred reference states. We therefore provide comprehensive developments of configurational forces, the balance of configurational momentum, and configurational thermodynamics. Our treatment does not require a choice of reference configuration. The general evolution equations arising from our theory account for the thermodynamic structure of the solution and the interface and for sources of dissipation related to the transport of surfactant, momentum, and heat in the solution and within the interface along with the transport of solute, momentum, kinetic energy, and heat across the interface. Moreover, the equations account for the Soret and Dufour effects in the solution and on the interface and for observed discontinuities of the temperature and chemical potential across the interface. Due to the complexity of these equations, we provide approximate equations which we compare to equations pre-existent in the literature. Finally, we consider the influence of the additional terms entering our approximate equations on the stability of an evaporating film. We find that these terms are particularly important for films with thicknesses of one or two monolayers.

Speaker: Howard H. Hu

Simulation of Motion and Deformation of Elastic Objects in Flows

Department of Mechanical Engineering and Applied Mechanics
University of Pennsylvania
229 Towne, 220 S. 33rd Street
Philadelphia, PA 19104-6315

In this work, we present a numerical technique that simulates the dynamics of flexible bodies in moving fluids. The current implementation is only in two dimensions. We are interested in studying the motion and deformation of elastic particles, for example biological cells, which are flexible and liable to undergo large deformations along with translations and rotations. Our numerical technique uses the moving mesh finite element method to solve the initial value problem of moving particles. The movement and the deformation of the particles are handled with an Arbitrary Lagrangian Eulerian (ALE) scheme. The numerical scheme solves the equations of motion for an incompressible elastic solid (with non-linear strain tensor) inside the particles, and those for Newtonian and/or viscoelastic fluids for the liquid phase. The coupling between the solid and liquid phase is enforced by assuming that the material velocity and the stress are continuous across the interface between the solid and the liquid. In addition, the displacement field inside the particles is solved, and its gradient in the form of Almansi strain tensor is used to evaluate the stress inside the particles. This numerical scheme is demonstrated to be stable and is capable to resolve large deformations of the particles.

Speaker: David Jacqmin

Phase-field calculations of wetting failure and instabilities

NASA Glenn Research Center, Cleveland, OH 44135, USA

Wetting phenomena are important in industrial coating, in oil extraction and in hydrology. Wetting is a form of molecular bonding. This takes place at the nano-scale and the details of it vary considerably depending on the wetting liquid and the solid being wetted. Nevertheless, the visible hydrodynamics of wetting can often be approximately predicted by the Navier-Stokes equations supplemented by slip-length models for the flow against the solid and/or diffuse interface (phase-field) thermodynamically-based models of the meniscus. These models eliminate an apparent singularity at the wetting line and the phase-field model also captures the gross energetics of wetting.

This talk will discuss surface-tension-driven flows with an emphasis on wetting and coating. Methods for calculating wetting flows using phase-field models will be briefly described and some two- and three-dimensional phase-field-Navier-Stokes calculations of surface-tension-driven flows will be discussed.

Next, some model problems are considered in order to investigate wetting failure in liquid-liquid systems. Three methods of analysis are used for the equiviscous case, an essentially exact Fourier series method, a quasi-parallel approximation and a phase-field model. The Fourier series validates the phase-field method in that they both give nearly identical results for onset of instability.

Three-dimensional phase-field calculations are then discussed that show wetting failure through tipstreaming and splitting instabilities. Spot checks indicate that the onset points of two- and three-dimensional instabilities are very close. It is hypothesized that tipstreaming can be understood in part as a quasi-two-dimensional phenomenon.

Speaker: Roger E. Khayat

Thin-film flow of viscoelastic fluids

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The interplay between inertia and elasticity is examined for transient flow of a thin film. The fluid is assumed to emerge from an annulus, as it is driven by axial pressure gradient and/or gravity. The substrate is assumed to be stationary and of arbitrary shape. The boundary-layer equations are generalized for a viscoelastic film obeying the Oldroyd-B constitutive model. These equations are solved by expanding the flow field in terms of orthonormal shape functions in the radial direction and using the Galerkin projection, combined with a time-stepping implicit scheme, and integration along the flow direction. It is found that the viscosity ratio and fluid elasticity can have a significant effect on steady state as well as transient behavior. It is also found that low-inertia and/or highly elastic fluids tend to accumulate near the annulus, exhibiting a standing wave that grows with time. This behavior clearly illustrates the difficulty associated with coating viscoelastic high-viscosity fluids. A criterion for film rupture is also established, which is based on the steepening of flow and stress gradients. The topography of the substrate has a drastic effect on the flow as well.

Speaker: L. G. Leal

Theoretical Studies of Flow-Induced Coalescence

Y. Yoon, F. Baldessari and L. G. Leal
Dept of Chemical Engineering
University of California, Santa Barbara

We report on recent boundary integral simulations of the flow induced coalescence of a pair of drops in the creeping flow limit. These calculations are based upon a classical sharp interface model, with "retarded" van der Waals forces included via disjoining pressure approximation using Lifschitz theory to determine the appropriate value of the Hamaker constant corresponding to PBd drops and a PDMS suspending fluid. The results show that a local film thickness of the order 100 angstroms (or less) is required for film rupture. We compare predictions of the drainage time for head-on collisions with experimentally measured values, as well as predictions and experimental data for the critical capillary number and the coalescence angle as a function of the capillary number corresponding to different non-head-on trajectories.

Speaker: T. Li

Path integral analysis for the heteropolymer

Department of Scientific & Engineering Computing
School of Mathematical Sciences
Peking University, Beijing, China

It is well known that the bending rigidity of DNA is base pair dependent. There are two major theoretical analysis concerning this random heterogeneity with different results. We give a new path integral analysis for the random rod like chain which corresponds to a random walk on SO(3) group.

Speaker: Chun Liu

New closure approximation for FENE models

Mathematics Department, Penn State University

I will present a new closure approximation for FENE nonlinear viscoelastic models. The closure incorporate the information of the microequilibrium distribution (in particular, the presence of the singularities) and also preserves the overall energy laws.

Speaker: Ellen K. Longmire

Experiments on Coalescence in Liquid/Liquid Mixtures

Department of Aerospace Engineering & Mechanics
University of Minnesota

Coalescence transitions in mixtures of oil- and water-based fluids are investigated experimentally with the goal of understanding the underlying dynamics and of eventually developing accurate numerical models for practical applications such as transport, mixing, and separation of petroleum, chemical, and waste streams. Two geometries have been examined: drops impacting and eventually coalescing at a quiescent interface and coalescing drop pairs. Refractive index matching and laser induced fluorescence are employed to obtain clear images of the interfaces and interior volumes within each flow. Real-time flow sequences of planar fields are acquired using a high-frequency laser and camera system, and the resulting images are analyzed to determine interfacial behavior as well as two- and three-component velocity fields. In the drop/interface case, coalescence occurs after buoyancy-driven film thinning. In the drop/drop case, coalescence is associated with significant deformation and vortex-driven induction. The effects of viscosity ratio, impact Weber number and impact angle will be discussed.

Speaker: J. M. Lopez

Couplings between bulk flows with inertia and monolayer mesoscale structure

Juan M. Lopez, Amir. H. Hirsa and Michael J. Vogel

Monolayer hydrodynamics are usually described in terms of a Newtonian constitutive relationship. However, this macroscopic view fails to account for small-scale co-existing phase domains, which are generally present in the monolayer and appear to have profound macroscopic effects. In this talk we

shall consider two flow situations. First, in a flow where the monolayer is being periodically compressed and dilated, we provide direct evidence of these effects, consisting of Brewster angle microscopy images of the monolayer, space and time resolved interfacial velocity measurements and comparisons with predictions based on the Navier-Stokes equations together with the classic model for a Newtonian interface. In a second flow system, we impart a well controlled shear-rate distribution with inertia to a monolayer consisting of coexisting phases, and study the resulting phase morphology and domain fragmentation. These evolve on distinct time scales: the viscous time associated with the viscosity in the bulk and the Marangoni stress, and the fragmentation/relaxation time associated with the phase morphology. A relationship between microstructure (line tension) and macroflow (shear rate) determining the meso length scale of the coexisting phase domains has been deduced from dimensional analysis and found to correlate well with the quantitative experimental observations.

Speaker: P. D. Minev

A compromise between the Eulerian and ALE approach to free boundary problems

B. Bejanov and P.D. Minev
Department of Mathematical & Statistical Sciences
University of Alberta, Edmonton, Canada T6G 2G1

This study is an attempt to produce a scheme that comprises the advantages of the two main approaches for discretization of free boundary problems in fluid dynamics: the Eulerian and the Arbitrary Lagrangian-Eulerian (ALE) approaches. In our opinion, a good algorithm for discretization of such problems should posses the following features. 1. The spatial approximation of both, velocity and pressure should be optimal. 2. The method should be easy for a parallel implementation which typically means that the grid should be fixed or at least the domain should not be re-meshed very often. 3. The method should conserve mass. This is a problem for most of the Eulerian methods and to some extend it affects the ALE methods too. The present scheme can be considered as an ALE scheme because at each time step we align the free boundary with finite element faces. On the other hand the structure of the grid remains unchanged. We developed an algorithm, which uses a fixed background grid, but at each time step it finds the closest to the free boundary grid points and projects them onto the boundary without changing the structure of the grid. Of course it requires recomputation of part of the matrices, but their structure remains unchanged (this recomputation is unavoidable if an optimal approximation is to be achieved). The time discretization is done by means of a velocity correction scheme which utilizes non-conforming elements for the projection step. The mass conservation is guaranteed by means of one Lagrange multiplier per each distributed phase which imposes the condition that the mass of this phase is preserved. The scheme is validated on several well known free boundary flows.

Speaker: Len Pismen

Droplets propelled by surface forces

Department of Chemical Engineering Technion,
Israel Institute of Technology
Haifa 32000, Israel

A fluid droplet may exhibit self-propelled motion by modifying wetting properties of the substrate, resulting in asymmetry in the contact angles. This motion, fueled by either chemical reactions or phase transitions, has been observed experimentally in various systems. Another source of motion is interaction mediated by the substrate or precursor layer. Droplet velocities can be computed analytically in lubrication approximation using an integral solvability condition. A logarithm of the ratio of the macroscopic to molecular scales appearing in the expression for effective mobility is a telltale sign of the notorious contact line singularity resolved on the molecular scale. The velocity computed in this way is in a very good agreement with straightforward numerical computations. Long-time dynamics in particular systems may lead, depending on relative time scales of motion and

substrate modification, to coarsening, pattern formation or persistent wandering of droplets.

Speaker: Yuriko Renardy
Numerical simulations of drop deformation for viscoelastic liquid-liquid systems.
Department of Mathematics
Virginia Polytechnic Institute and State University

We implement a volume-of-fluid algorithm with a parabolic re-construction of the interface for the calculation of the surface tension force (VOF-PROST). This achieves higher accuracy for drop deformation simulations in comparison with existing VOF methods based on a piecewise linear interface re-construction. The algorithm is formulated for the Giesekus constitutive law. The evolution of a drop suspended in a second liquid and undergoing simple shear is simulated. Numerical results are first checked against two cases in the literature: the small deformation theory for second-order liquids, and an Oldroyd-B extensional flow simulation. We then address the experimental data of Guido, Simeone and Greco (Deformation of a Newtonian drop in a viscoelastic matrix under steady shear flow. Experimental validation of slow flow theory. J. Non-Newtonian Fluid Mech., 114:65--82, 2003) The data deviate from existing theories as the capillary number increases, and reasons for this are explored with numerical simulations.

Speaker: A. D. Rey
A Model of Membrane Flexoelectricity
Department of Chemical Engineering and McGill Institute of Advanced Materials
McGill University, Montreal, Quebec Canada H3A 2B2

An interfacial electro-elastic model is used to formulate a membrane shape equation that takes into account mechanical and flexoelectric pressures. Interfacial flexoelectricity incorporates electric field-curvature couplings and is of relevance to the study and characterization of biological membranes. While the better known interfacial piezoelectric effect couples electric fields to interfacial strain, interfacial flexoelectircity introduces an energy contribution that depends on surface curvature (H) and the surface unit normal (k). This model shows how the energy dependence on k and H leads to a renormalization of the membrane mechanical tension, shear, and bending effects, and hence it offers diverse pathways to manipulate the membrane's shape and extract biomechanical information. The electro-elastic shape equation shows that for classical membrane energies the average curvature scales with the imposed field. Dynamic extensions of the model are presented.

Speaker: R. Ryham
Deformation of Charge Selective Vesicles.
Department of Mathematics, Pennsylvania State University

We present a model of a charged fluid/interface system where diffuse charges are selectively encapsulated by vesicles. The model is derived from energetic variational principles. We emphasize the dynamic coupling between interfacial and electric forces. We highlight the energetic consistency of the numerical methods, some analysis and finally, simulation.

Speaker: Michael Shelley
Transport in Visco-Elastic Flows
Courant Institute

I will discuss two fundamental problems in complex fluid dynamics. The first concerns pumping. The pumping of complex fluids – whether peristaltic or pressure driven -- is important in many biological processes, such as reproduction. In joint work with J. Teran and L. Fauci, we have developed an immersed boundary method for studying the pumping of an Oldroyd-B fluid at low Reynolds number.

Through simulation we explore some of the ways in which pumping of an elastic fluid -- such as by loss of flow reversibility -- differs from a Newtonian one. We also study the effects of channel geometry. The second problem is motivated by experimental work by V. Steinberg and his collaborators on "low Reynolds turbulence" in elastic flows, in which they use fluorescent DNA molecules to investigate stretch-coil transitions in strongly mixing elastic flows. In joint work with Y. Young we consider the much simpler problem of an elastic fiber moving in a background cellular flow. The fiber acts as a spatially extended test particle whose internal dynamics, particularly buckling at hyperbolic points, leads to complex transport properties across space. We also investigate the associated extra stress fields produced by a test particle.

Speaker: A. Shen

Effects of surface property and geometric confinement on the droplet formation and deposition inside microfluidic devices

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Micro-fluidic devices offer a unique method of creating and controlling droplets on small length scales. A microfluidic device is used to study the effects of surface properties and geometric confinement on droplet formation of a 2-phase flow system. Four phase diagrams are generated to compare the dynamics of the 2 immiscible fluid system (silicone oil and water) inside microchannels with different surface properties. Results show that the channel surface plays an important role in determining the flow patterns and the droplet formation of the 2-phase fluid system. The surface effect and length scale factor on the droplet deposition inside microchannels will also be discussed. Secondly, we investigate the effects of geometric confinement on the polymer chains in a polyethylene oxide solution during droplet formation. The molecular weights, as well as the channel dimensions, are varied while the droplet pinch-off dynamics and polymer contribution to the solution viscosity are examined. Results show that as the length scale of the polymer chains approaches that of the channels, the elastic effects of the polymers become more pronounced.

Speaker: J. Shen

A phase-field model for the mixtures of two incompressible fluids: applications to drop formation

Department of Mathematics, Purdue University

A phase field model is proposed to describe the motion of mixtures of two incompressible fluids, and is used to the study of contraction and pinch-off phenomena of a liquid filament. An efficient and accurate numerical scheme is presented and implemented for the coupled nonlinear system of Navier-Stokes equations and Allen-Cahn phase equation. Detailed numerical simulations for a Newtonian fluid filament falling into another ambient Newtonian fluid are carried out. The dynamical scaling behavior and the pinch-off behavior, as well as the formation of the consequent satellite droplets are investigated.

Speaker: A.-C. Shi

Phases, Phase Transitions and Self-Assembly in Block Copolymers

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Nature often assembles simple molecular building blocks, such as polymers, lipids and colloids, into complex mesophases. Among these self-assembling soft materials, block copolymers are unique in that the advances in synthetic chemistry have resulted in well-controlled molecular architectures to produce structured materials with tailored mechanical, optical, electrical and other physical properties. Block

copolymers are macromolecules composed of chemically different blocks tethered together, which spontaneously form a variety of ordered phases with domain sizes in nanometer range (1-100nm). These materials are widely used industrially, and they also provide an ideal model system for studying self-assembly principles. Understanding the structures and phase transitions in block copolymers has been one of the most active research areas in polymer science in the past two decades. I will review of the physics of block copolymers by addressing the following questions: What are block copolymers? Why do they self-assemble? What determined the self-assembled structure? What are the physical properties of the mesophases?

Speaker: B. Stoeber

Visco-Thermal Flow Instabilities of Thermally Responsive Fluids

Boris Stoeber (University of British Columbia), Dorian Liepmann (UC Berkeley), Susan J. Muller (UC Berkeley)

Aqueous solutions of Pluronics, which are (polyethylene oxide)x–(polypropylene oxide)y–(polyethylene oxide)x triblock copolymers, undergo gelation at elevated temperatures. Rheological characterization of these materials reveals their thermo-thickening and shear-thinning behavior. The scaling of viscous heating in microchannels under constant flow rate and constant pressure drop conditions explains the complex behavior of these fluids in microchannels. In the case of pressure-driven flow through a microchannel, it will be demonstrated that viscous heating can cause periodic gel formation leading to flow instabilities. Velocity fields above and below the gel temperature were mapped using digital particle image velocimetry; above the gel temperature flow fluctuations may be caused by the competing mechanisms of thermo-thickening and shear-thinning.

The reversible phase change of these thermally responsive fluids and their particular rheological behavior has promise for various microflow control applications including active valving and passive microflow control based on viscous heating within the flow.

Speaker: S. Tavener

Rayleigh-Bénard-Marangoni convection with a deformable interface

Simon Tavener and K. Andrew Cliffe
Colorado State University and University of Nottingham

The convective motions that arise when a fluid layer is heated from below were most famously studied by Bénard and Rayleigh in the early part of this century and have attracted numerous theoretical, experimental and numerical investigations in the intervening years. In an open container, fluid convection is not driven by buoyancy forces alone, but also by surface forces that arise from the temperature-dependent nature of the surface tension. Indeed, thermocapillary forces dominate buoyancy effects in sufficiently shallow layers. Computations of Marangoni-Bénard convection are usually performed in two- or three-dimensional domains with rigid boundaries, and a contact angle of 90 degrees between the fluid and its container is generally assumed. Qualitatively different behavior can occur if the free surface is allowed to deform. Bifurcations arising in a two-dimensional domain with a deformable free surface can be computed using the finite-element method, by combining an orthogonal mapping of the physical domain with extended system techniques for locating singularities. Small deformations of the free surface can result in surprisingly large changes in the critical Marangoni numbers at which convection occurs. Motivated by the Liquid Encapsulated Vertical Bridgeman (LEVB) crystal growth technique, we consider the two-fluid problem, concentrating on instabilities that arise when heating from above.

Speaker: Becca Thomases

Analysis and numerics for Oldroyd-B fluids

Courant Institute of Mathematical Sciences, NYU

Viscoelastic flow modelled by the Oldroyd-B equations will be discussed from an analytical and numerical perspective. First I will present a local energy decay theorem which applies to a large class of hyperbolic systems including the Oldyoryd-B model. This decay theorem is used to prove that global smooth solutions exist for small initial data. While small solutions decay, the problem for large data is much more complicated. I will present some recent numerical work on the Oldroyd-B system which shows that the system develops large stress gradients for certain curvilinear flows. These stress gradients appear to become unbounded for large Weissenberg number.

Speaker: David Trebotich

The Critical Mach Number Problem and Well-Posed Viscoelastic Flows

Lawrence Livermore National Laboratory

The High Weissenberg Number Problem (HWNP) is the benchmark of viscoelastic flows. HWNP is actually a frustratingly low Weissenberg number problem for which stable solutions to flows involving geometric singularities are unobtainable due to a violation in the hyperbolicity condition, or change in mathematical type. However, the dimensionless Weissenberg number parameter does not completely describe the problem as it omits viscous effects. It is more appropriate to identify this problem with criticality in the elastic Mach number, the point at which the onset of wave behavior is admitted in the system, including viscous effects through dependence on the Reynolds number. In the previous work of Trebotich, Colella and Miller, J. Comput. Phys. vol. 205 (2005) it was shown that the system is always hyperbolic by the introduction of the inverse deformation gradient, and stable by recasting Oldroyd-B into a well-posed hyperbolic piece and an elliptic source term using Duhamel's formula. Computations showed that elastic shear waves form and propagate in the sudden contraction flow of a Maxwell fluid; it was also demonstrated that the addition of solvent viscosity leads the solution into a hybrid viscoelastic regime where elastic wave effects are damped as the HWNP parameter space is reached. However, in the latter limit, solutions to the problem do not necessarily converge to steady-state -- a benchmark requirement -- due to persistence in the underlying elastic wave behavior. We present further analysis of this system that relates the condition for well-posedness in the elastic limit to criticality in the elastic Mach number. We also perform grid refinement studies to investigate the convergence of singular behavior in the solution. This work motivates the use of a suitably designed upwind method to address elastic flows.

Speaker: J. Vinals

Mesoscopic hydrodynamics of lamellar phases, and orientation selection under shear

McGill Institute for Advanced Materials and Department of Physics
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We discuss a coarse grained description of monomer diffusion and hydrodynamic flow in lamellar phases of block copolymers. The motion of tilt grain boundaries both with and without imposed shear flows is analyzed, and boundary velocities or instabilities determined. The effect of boundary instabilities on orientation selection under oscillatory shears will be discussed.

Speaker: Noel J. Walkington

Phase Field/Level Set Methods for Problems Involving Elastic Membranes

Carnegie-Mellon University

Models of physical systems often contain implicitly defined surfaces separating different phases, materials, etc. which may evolve over time. Phase field and level set techniques can be used to represent such interfaces without explicitly parameterizing them. When the evolution of the free surfaces can be determined from ``Eulerian" quantities (such as the curvature, flow velocity, etc.) phase field/level set representations have lead to very general robust algorithms and numerical codes to simulate these complex physical systems. In this talk I will discuss how such algorithms may be

extended to model free surfaces, such as elastic membranes, whose evolution depends additionally upon ``Lagrangian'' quantities, e.g. strain.

Speaker: Qi Wang
Numerical and analytic study of nematic polymer flows coupled with external fields
Florida State University

In this talk, I will present a set of results on the solution of the Smoluchowski equation which governs the flow of nematic polymer flows coupled with external fields. Correspondence principles are established between general flows and target ones so that flow types and behavior can be studied on the target one only.

Speaker: K. Wielage
Immiscible displacement flow along a plane channel
Mathematics Department, University of British Columbia

We present results of a numerical study on the displacement of one generalized Newtonian fluid by another in a plane channel. In primary cementing of oil wells, drilling mud is displaced first by a spacer fluid and then by a cement slurry, along a narrow eccentric annulus. Here, the fully 2-dimensional displacement along an radial slice of the annulus is considered. We concentrate on the case of immiscible fluids using the diffuse-interface method. The focus of our investigations is on the potentially beneficial effects of a non-monotonic variation in fluid viscosity as might be caused, for example, by chemical reaction or fluid incompatibility. Results indicate higher displacement efficiencies due to a high-viscosity interfacial layer. In this context, we also examine the effects of model parameters on the contact line motion.

Speaker: Jianjun Xu
A level-set method for interfacial flows with surfactant
Mathematics Dept
UC Irvine

In this talk, I will present a level-set method for the simulation of fluid interfaces with surfactant. The method can be straightforwardly extended to the case of soluble surfactants. The method is based on an Eulerian formulation and couples a semi-implicit discretization of the surfactant equation with the immersed interface method for the flow-solver. Novel techniques are used to accurately conserve component mass and surfactant mass during the evolution. The method is applied in 2D to study the effects of surfactants on single drops, drop-drop interactions and interactions among multiple drops in Stokes flow under an applied shear. A non-monotonic behavior of the minimum distance between approaching drops versus capillary number is observed. Accordingly, a critical capillary number Ca* measuring the tendency to coalescence is determined as a function of the surfactant coverage. A transition in behavior is observed to occur at a critical coverage. This is joint work with J. Lowengrub, Z. Li and H.-K. Zhao.

Speaker: W. Yu
The effect of interfacial viscosity on the droplet dynamics under flow field
Wei Yu and Chixing Zhou
Department of Polymer Science and Engineering, Shanghai Jiao Tong University, P. R. China

Interfacial properties are very important in the dynamical evolution of interface under flow field. The interfacial tension is the first, and in most cases the only interfacial property that considered in theoretical model and numerical simulations. However, the interfacial properties are more than the interfacial tension in the concept of diffuse interface model. The viscoelastic properties also affect the

droplet dynamics. Usually the viscosity in the interfacial regime is assumed to be a linear function of the concentration profile of components. However, it is possible for the interfacial viscosity to be much lower or higher than the linear profile, which corresponds to the interfacial slip in immiscible blends or the interface with copolymer formed from the reaction between two components. The effects of interfacial viscosity on the droplet dynamics under different flow fields are investigated and discussed in this work.

Speaker: P. Yue

Simulation of bubble growth in polymer foaming

Department of Mathematics and Department of Chemical and Biological Engineering
University of British Columbia

Bubble growth plays an important role in determining the cell size distribution in thermoplastic foams. In this work, the diffusion-driven bubble growth in a polymer melt is computed by direct numerical simulation. The pressure and mass inside each bubble follow the equation of state for an ideal gas. A finite element method is used to calculate the gas concentration and flow variables in the polymer melt. Henry's law is employed to relate the bubble pressure and the gas concentration at the bubble surface. An Arbitrary Lagrangian-Eulerian (ALE) technique is used to handle the moving boundary. Within each time step, the whole system is solved iteratively. By modeling the polymer melts as Oldroyd-B fluids, we will study the influence of rheology on single bubble growth and interactions between multiple bubbles.

Speaker: Pingwen Zhang

Numerical Method of the Equilibrium States and the Nucleation in Copolymer Melts

School of Mathematical Sciences
Peking University, Beijing, China

We introduce new numerical methods to study the equilibrium states and the nucleation in copolymer melts. We propose a new numerical method which can adjust the periodical region of the equilibrium states automatically. The main idea is to treat the shape of the simulation box as a variable, and then transform the region to a unit box. Although the numerical results are achieved under the Landau-Brazovskii model, it is a general method, and the main advantage of our method is that it can be easily planted in any other theoretic frame like self-consistent field theory. The understanding of the equilibrium state provides the foundation to study the nucleation. 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.

Speaker: Chunfeng Zhou

Simulation of neutrophil transit in capillaries using simple and compound drop models

Department of Chemical and Biological Engineering
University of British Columbia

It is well known that neutrophils take much longer time to traverse the pulmonary capillary bed than erythrocytes. This results in their accumulation in the lungs and formation of a reservoir readily recruited when needed. Recent experiment by Yap and Kamm [1] showed neutrophil deformation and activation upon entering a microfluidic channel. We simulate the transit of the neutrophil in a capillary using two models: a simple liquid drop model and a compound drop model with a nucleus, in the framework of a phase-field method. With the pressure drop across the capillary fixed, the entry into the capillary consists of several stages in which flow rate varies in distinct manners. The total entrance

times approximate the experimental measurements. The cell viscosity and viscoelasticity play important roles in the entrance process. Furthermore, a small obstacle at the entrance will greatly increase the transit time. For the compound drop model, the nucleus tends to prolong the transit time since it hampers the inner circulation and thereby subject the cell to higher shear rates near the cortex.

[1] B. Yap and R. D. Kamm, "Mechanical deformation of neutrophils into narrow channels induces pseudopod projection and changes in biomechanical properties," J. Appl. Physiol. **98**, 1930 (2005).

Speaker: Y. Elaine Zhu

Fluids Moving Past Smooth Hydrophilic Surfaces -- Slip?

Department of Chemical and Biomolecular Engineering
University of Notre Dame

Recent experiments challenge the traditional view that fluids satisfy the ``no-slip" boundary condition. While the amount of slip observed differs between research groups, it is now generally accepted that the no-slip boundary condition need not hold strictly -- if the surface is smooth and hydropobic. What happens if the surface is wetted by the moving fluid? This work describes hydrodynamic studies of fluid between two crossed cylinders in a surface forces apparatus, which appears to produce different findings from those obtained from classical methods. Aqueous salt solutions with various ion concentrations were used with mica as the confining surface. We propose a mechanistic theory about air-entrainment that can account for our observations to elucidate the origin of the gas formation at water-solid interface and its consequence on slip motion. Independently, laser spectroscopy is used to directly and non-invasively detect the structure of interfacial layers in flowing water past micro/nano-channels whose surface chemistry and gap spacing are varied.