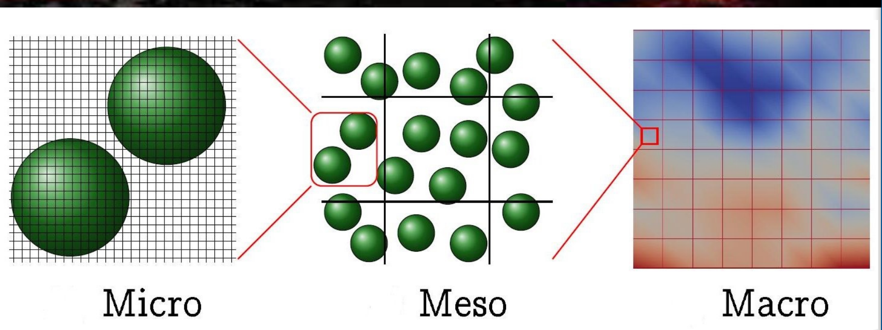
Pacific Institute *for the* Mathematical Sciences



18th International Workshop on Numerical Methods for Non-Newtonian Flows

and

3rd Complex Fluids and Flows in Industry and Nature workshop

12-15 June 2017

University of British Columbia
Vancouver, Canada

UBC

a place of mind

Welcome

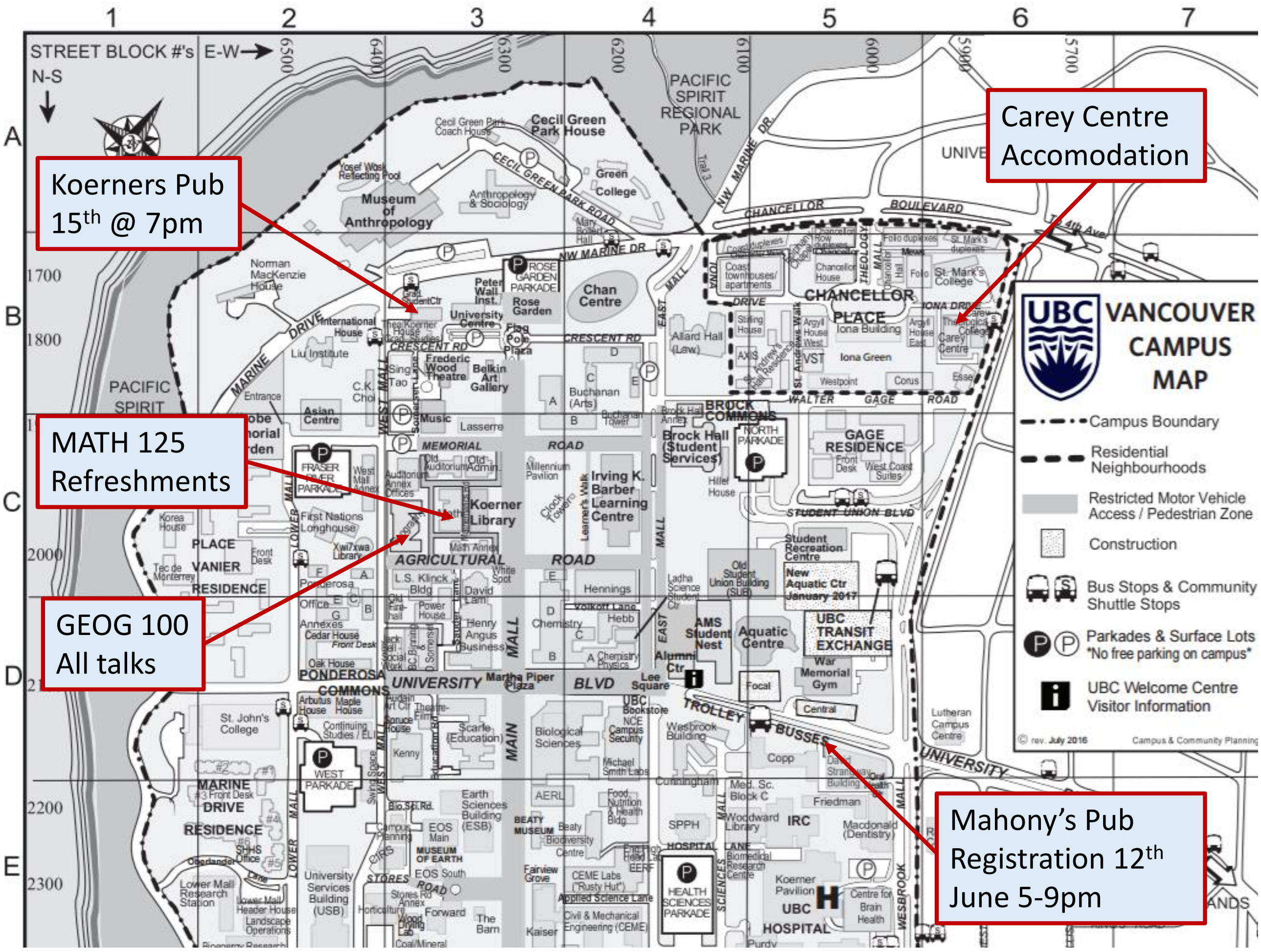
The International Workshops on Numerical Methods in Non-Newtonian Flows (IWNMNNF) have been held roughly biennially, alternating between North America and Europe since 1979. The objective of all workshops over the years has always been to discuss numerical methods for the solution of complex fluid flow problems. While the emphasis was at the start on viscoelastic materials, the workshops have progressively broadened their scope to simulation methods at various scales (Discrete Element Method, Brownian/Stokesian dynamics, dissipative particle dynamics, particle-resolved simulation, volume-of-fluid/level set method, etc), as used in the solution of flow problems involving e.g. granular materials, multiphase mixtures or fluid/fluid interfaces, among others. Equally, the strong links between computation, analytical and experimental methods are emphasized in moving forward to robustly solve practical problems.

The theme of this IWNMNNF is Complex Fluids and Flows in Industry and Nature, and will be the 3rd COFFIN workshop held at UBC. The objective of IWNMNF18 and COFFIN3 is to bring together leading researchers across several disciplines to foster awareness and the transfer of ideas in the field of computational and mathematical non-Newtonian and multiphase fluid mechanics. We aim at discussing challenges, recent progress, future directions and emerging applications of complex fluids and flows. We welcome contributions of computational, analytical or experimental nature, focused at exposing and understanding interesting fluid mechanics problems and phenomena within the workshop theme.

Anthony Wachs
Ian Frigaard
Michael Graham
Jeff Morris
Peter Wapperom

Pacific Institute *for the* Mathematical Sciences

Important Places in UBC



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Things to remember

- Registration is open on Monday 5:30 pm in Mahony and Sons pub and on Tuesday in Geography Building room 100 (Geog 100) from 8:30 to 9:00.
- The scientific program starts everyday at 9:00 and ends at 5:00, except on Wednesday which we end earlier.
- All presentations are given in Geog 100.
- Coffee, refreshments and lunch will be served in Mathematics Building room 125 (Math 125).

Tuesday Sessions at a Glance

Tue-A: Complex fluids/Complex flows I

Geography 100
Chair: A. Beris

9:00-9:20 **Workshop Opening**
I. Frigaard and A. Wachs

9:20-9:40 **Theory of locomotion through complex fluids**
G. Elfring

9:40-10:00 **Convective flow of Andean fruit jellies: numerical simulation and parameter estimation**
S. González-Andrade, A. Jurado and J. Ruales

10:00-10:20 **Two-phase granular fluids**
V. Shelukhin

10:20-10:40 **Deformable bodies in anisotropic fluids**
A. Evans, M. Graham, and S. Spagnolie

Tue-B: Viscoelastic flows I

Chair: L. Xi

11:10-11:30 **On the tails of probability density functions in Newtonian and viscoelastic turbulent channel flows**
A. Beris, G. Samanta, A. Young and K. Housiadas

11:30-11:50 **Paving the Way for Mechanistic Understanding of Shear Banding in Flow of Entangled Polymeric Melts via Detailed Mesoscopic Simulations**
M. Mohagheghi and B. Khomami

11:50-12:10 **Elastic Instability and Secondary Flow of Wormlike Micellar Solutions in Cross-Slot Flow**
M. Cromer, A. Kalb

Tue-C: Suspension flows I

Chair: A. Rahmani

1:30-1:50 **Stability of particle hydrodynamic self-assembly in a channel flow: the effect of confinement, concentration and flow inertia**
M. Abbas, A. Gupta

1:50-2:10 **Understanding Viscoelastic Suspensions via Numerical Simulation**
S. Krishan, M. Yang, W. Murch, G. Iaccarino, E. Shaqfeh

2:10-2:30 **Multi-scale stratagies in improvement of numerical models for the simulation of particle-laden flows**
A. Esteghamatian, A. Wachs

2:30-2:50 **Numerical simulation of elasto-inertial particle migration in square channel flow of viscoelastic fluids**
Z. Yu, P. Wang

2:50-3:10 **Numerical simulation and experimental validation of the evolution of fiber orientation in complex flows**
P. Wapperom, D. Baird, G. Lambert, H. Chen.

Tue-D: Flows at small scale

Chair: A. Taghavi

3:40-4:00 **Numerical simulation of molten metals on nanoscale**
S. Afkhami

4:00-4:20 **Single molecule tracking and modeling of beads-on-a-string structures along viscoelastic membrane nanotubes in live cells**
B. Ovryn and P. Wu

4:20-4:40 **Shear and Extensional Flow Dynamics of Lipid Lamellae and Lamellar Vesicles: A Molecular Dynamics Study**
S. Dhakal, R. Sureshkumar

4:40-5:00 **Stochastic mesoscale modeling of transiently networked fluids**
L. Zhou, L. Cook

Wednesday Sessions at a Glance

Wed-A: Suspension flows II

Geography 100
Chair: M. Abbas

9:00-9:20 **Enhancing shear thickening**
S. Hormozi, Y. Madraki, G. Ovarlez, É. Guazzelli and O Pouliquen

9:20-9:40 **Interface-resolved simulations of rigid and deformable particles in shear flows**
L. Brandt, D. Alghalibi, I. Lashgari and M. Rosti

9:40-10:00 **Rheology and Microstructure of Dense Deformable Colloidal Suspensions: Interplay Between Elasto-hydrodynamic and Frictional Interactions**
S. Khani, A. Boromand, B. Grove and J. Maia

10:00-10:20 **Study of spontaneous structure formation in granular systems using DEM and CFD+DEM framework**
K. Nandakumar, J. Yu, C. Wu, J. Joshi and M. Tyagi

10:20-10:40 **Simulations of suspension flows with a meshless MLS scheme**
A. Howard, M. Maxey

Wed-B: Flows through porous media

Chair: S. Hormozi

11:10-11:30 **Modeling flow and fouling in membrane filters: Insights into filter design**
L. Cummings, P. Sanaei

11:30-11:50 **A multi-scale model for electrokinetic transport in porous networks**
A. Mani and S. Alizadeh

11:50-12:10 **Fluid-solid interactions in a non-convex granular media**
A. Rakotonirina, A. Wachs, M. Rolland, J. Delenne

Thursday Sessions at a Glance

Geography 100

Thur-A: Complex fluids/Complex flows II

Chair: B. Khomami

9:00-9:20 **Analyzing nanofiber formation in centrifugal spinning using a regularized string model**
S. Noroozi, S. Taghavi

9:20-9:40 **A singular perturbation study of the Rolie-Poly model**
M. Renardy and Y. Renardy

9:40-10:00 **Elastic modifications of an inertial instability in a 3D cross-slot**
K. Zografos, N. Burshtein, S. Haward, A. Shen, R. Poole

10:00-10:20 **Quantitative Rheological Model Selection with Bayesian Analysis**
J. Freund and R. Ewoldt

Thur-B: Round Table

Chair: I. Frigaard

11:00-12:20 **Future perspectives for computational complex fluids**
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Thur-C: Free surface flows

Chair: J. Feng

2:00-2:20 **Instability and dewetting of ultra-thin nematic liquid crystal films**
L. Cummings, L. Kondic, M. Lam

2:20-2:40 **Magnetophoretic Interaction of a Pair of Ferrofluid Droplets in a Rotating Magnetic Field**
M. Qiu, S. Afkhami, C. Chen and J. Feng

2:40-3:00 **A new mechanism for the wetting of a surface by the drops of an emulsion**
S. Borkar and A. Ramachandran

3:00-3:20 **Numerical Simulation on Impinging Droplets of Pseudo-Plastic Fluids**
H. Suzuki, R. Hidema, A. Senda, K. Ishihawa, Y. Komoda, K. Suzuki

3:20-3:40 **Numerical and nonlinear dynamic study of melt fracture**
Y. Kwon

Thur-D: Numerical methods

Chair: S. Gonzalez-Andrare

4:20-4:40 **The deformation fields method revisited: stable simulation of viscoelastic fluid flow using integral models**
M. Hulsen, P. Anderson

4:40-5:00 **A new and straightforward stabilization approach to model viscoelastic fluid flows**
C. Fernandes, M. Araújo, L. Ferrás and J. Nóbrega

5:00-5:20 **Numerical Simulation of 'Extreme Fluids' - Some Examples, Challenges and Simulation Techniques for Flow Problems with Complex Rheology**
S. Turek

5:20-5:40 **Practical aspects of implementing dual proximal gradient method for the solution of yield stress flows**
A. Roustaei, T. Treskatis, A. Wachs and I. Frigaard

Friday Sessions at a Glance

Fri-A: Viscoelastic flows II

Geography 100
Chair: P. Wapperom

9:00-9:20	**Mechanistic constitutive model for wormlike micelle solutions with flow-induced structure formation** *S. Dutta and M. Graham*
9:20-9:40	**The Extrudate Swell of HDPE: Experiments and Simulations** *V.K. Konaganti, M. Ansari, E. Mitsoulis and S. Hatzikiriakos*
9:40-10:00	**Viscoelastic Simulations with Integral Models at Extremely High Shear Rates** *E. Mitsoulis*
10:00-10:20	**Polymer effects on the development and bursting of turbulent vortices: implication on high-extent drag reduction** *L. Zhu, X. Bai, L. Xi*
10:20-10:40	**Effects of extensional rheological properties of polymer solutions on vortex deformation in a two-dimensional turbulent flow** *R. Hidema and H. Suzuki*

Fri-B: Yield stress fluids

Chair: G. Elfring

11:20-11:40	**Particles in a yield-stress fluid** *E. Chaparian, A. Wachs and I. Frigaard*
11:30-11:50	**A partially extending strand convection model with Newtonian solvent for modeling thixotropic yield stress fluids: stability of shear-banded flow** *Y. Renardy and M. Renardy*
11:50-12:10	**Computing critical yield numbers in yield stress fluids** *I. Frigaard*

Tue-A: Complex fluids/Complex flows I

Geography 100
Chair: A. Beris

9:00-9:20 **Workshop Opening**
I. Frigaard and A. Wachs

Registration from 8.30 in GEOG 100

9:20-9:40 **Theory of locomotion through complex fluids**
G. Elfring

The vast majority of organisms, because of their small size, live in a regime where their inertia is negligible. Familiar strategies for locomotion through fluids, such as imparting momentum onto the surrounding medium, are ineffective at this scale due to the dominance of viscous dissipation. Instead, these organisms must propel themselves by other means in this restrictive environment. Moreover, microorganisms such as bacteria or spermatozoa often swim in fluid environments that cannot be classified as Newtonian. Many biological fluids contain polymers or other heterogeneities which may yield complex rheology. For a given set of boundary conditions on a moving organism, flows can be substantially different in complex fluids, while non-Newtonian stresses can alter the gait of the microorganisms themselves. In this talk I present a theoretical overview of small-scale locomotion with a focus on recent efforts quantifying the impact of non-Newtonian rheology on the motion of swimming microorganisms.

9:40-10:00 **Convective flow of Andean fruit jellies: numerical simulation and parameter estimation**
S. González-Andrade, A. Jurado and J. Ruales

In this work, we analyze the behavior of jellies of several Andean fruits when subjected to specific temperature changes in a laboratory under controlled conditions. Based on the rheograms obtained, we propose and numerically solve a model for the behavior of these fluids, based on the classic Herschel-Bulkley model. This model leads us to a parameter identification problem currently under study. Finally, we propose an optimal control problem, using the heat source as control variable, to optimize the flow of these jellies in possible industrial applications.

10:00-10:20 **Two-phase granular fluids**
V. Shelukhin

Starting from the basic thermodynamic principles, we develop a new mathematical model which governs dynamics of two-phase granular fluids with non-Newtonian rheology. Applications concern suspensions, coal-water slurry fuels, seepage of animal blood with high value of hematocrit, plastic or fresh concrete flows etc. The model allows to take into account not only particle-fluid interactions but the particle-particle interactions as well. The first phase is a Newtonian viscous fluid. To tackle the second phase as a granular fluid, we apply the notion of the Cosserat continuum, when each fluid point is treated as a rigid body. Such an approach is known as a theory of micropolar fluids (A.C. Eringen, 1999). To meet applications, we make generalizations by passing to a non-Newtonian CosseratBingham fluid which is both a micro-polar medium and a visco-plastic material. On the one hand, such a fluid exhibits microrotational effects and microrotational inertia; the fluid can support the couple stress, the body couples and the nonsymmetric stress tensor. On the other hand, the fluid stiffens if its local stresses and local couple stresses do not exceed some yield stress τ^* and a yield couple-stress τ^n, respectively.

The equations derived are applied to one-dimensional steady flows between two parallel planes. Particularly, we prove that the Ségre-Silberberg tubular pinch effect is due to non-linear Fick's constitutive law for the particle concentration flux. We establish that friction loss is non-linear in a general case because of non-homogeneous distribution of particles. One more result is that the concentration profile is sensitive to pressure gradient.

10:20-10:40 **Deformable bodies in anisotropic fluids**
A. Evans, M. Graham, and S. Spagnolie

Liquid crystals (LCs) are anisotropic, viscoelastic fluids that can be used to direct colloids into organized assemblies with unusual optical, mechanical, and electrical properties. In past studies, the colloids have been sufficiently rigid that their individual shapes and properties have not been strongly coupled to elastic stresses imposed by the environment. We will discuss how soft colloids (micrometer-sized shells) behave in nematic liquid crystals. We reveal a sharing of strain between the LC and shells, resulting in formation of spindle-like shells and other complex shapes. These results hint at previously unidentified designs of reconfigurable soft materials with applications in sensing and biology. Numerical approaches to solving this complex fluid-structure interaction problem and related efforts relevant to biolocomotion will also be discussed.

Tue-B: Viscoelastic flows I

Chair: L. Xi

11:10-11:30 **On the tails of probability density functions in Newtonian and viscoelastic turbulent channel flows**

A. Beris, G. Samanta, A. Young and K. Housiadas

Direct numerical simulations (DNS) of Newtonian and viscoelastic turbulent channel flows generate crucial data to analyze and understand the nature of turbulence modification by viscoelasticity—see, for example, [1] for a recent review. Such an understanding is necessary to enable better drag reduction technologies and has led, among other things, to an expression for the friction factor as modified by low and moderate values of viscoelasticity [2]. Previously, we have shown how viscoelasticity can significantly alter the non-normal character of the probability distributions (PDFs) of many of the turbulent statistics in the flow [3]. In this work, we report another characteristic of those PDFs for the velocity and its derivatives in Newtonian and viscoelastic turbulent channel flows. More specifically, we report the power law index of their tails, as obtained by applying Hills estimator. In particular, fat (or heavy) tails corresponding to an asymptotic power law behavior with low power law exponents have been observed in the PDFs for both Newtonian and viscoelastic cases. In many instances, the power law index is small enough to imply infinite fourth, or even third, moments. We also show that viscoelasticity leads to PDFs with fatter tails than the Newtonian ones. This finding explains why viscoelastic turbulent DNS are much more demanding computationally that Newtonian ones, requiring for proper resolution of the turbulence statistics much longer times and larger computational domain sizes.

References

[1] A.N. Beris and K.D. Housiadas, "Computational Viscoelastic Fluid Mechanics and Numerical Studies of Turbulent Flows of Dilute Polymer Solutions," In: "Modeling and Simulation in Polymers," (P.D. Gujrati and A.I. Leonov, Eds.), Wiley-VCH Verlag, (2010).

[2] K.D. Housiadas, and A.N. Beris, "On the skin friction coefficient in viscoelastic wall-bounded flows", Int. J. Heat Fluid Flow, 42: 49-67, (2013).

[3] G. Samanta, K. D. Housiadas, R. A. Handler, and A. N. Beris, "Effects of viscoelasticity on the probability density functions in turbulent channel flow", Phys. Fluids, 21, 24 pages (2009).

11:30-11:50 **Paving the Way for Mechanistic Understanding of Shear Banding in Flow of Entangled Polymeric Melts via Detailed Mesoscopic Simulations**

M. Mohagheghi and B. Khomami

Quantitative understanding of the influence of physico-chemical parameters on the dynamic evolution of microstructure in polymeric fluids plays a central role in processing of wide variety of micro-structured materials. To this end, robust and accurate simulation models that can quantitatively predict the flow structure and its hydrodynamic stability are essential in knowledge-based design of polymer processing operations and polymer-based products that constitute a significant portion of the U.S. manufacturing economy. In this study, hi-fidelity dissipative particle dynamics (DPD) simulations of flow of entangled polymeric melts have been performed to develop a mechanistic understanding of occurrence of shear banding, where the fluid instead of flowing with a uniform velocity separates into distinct fast and slow flowing regimes, in unidirectional shear flow of this class of fluids. Specifically, a detailed analysis of the simulation results has revealed a new phenomenon, namely, formation of locally inhomogeneous chain deformation and thus entanglement density in the velocity gradient direction. This spatial disparity in the entanglement density results in a considerable jump in normal stress and viscosity, which ultimately leads to shear banding. Overall, a molecular picture for the interrelation between the longest chain orientation and stress relaxation time, local inhomogeneities, and shear banding has been developed and corroborated with extensive analysis.

11:50-12:10 **Elastic Instability and Secondary Flow of Wormlike Micellar Solutions in Cross-Slot Flow**

M. Cromer, A. Kalb

Recently, there has been intense experimental investigations about the development of an asymmetric instability in the flow of viscoelastic liquids in a cross-slot. The instability has been observed in both polymer and wormlike micellar solutions. In addition, a lip vortex upstream of the corners has been observed in experiments of these materials. To date, numerical investigations into the elastic instability have focused on polymeric models. Some of these models predict a constant shear viscosity, while others predict shear thinning. A feature common to the models studied is an increase in extensional viscosity with increasing extension rate. This extensional thickening occurs near the hyperbolic stagnation point in the cross-slot, feeding back on the flow, and causing the symmetric flow to become asymmetric. Unlike polymer chains, wormlike micelles (WLMs) continuously break and reform. This behavior causes a major difference in the extensional rheology. In particular, because of the chain breakage, wormlike micellar solutions typically exhibit strong extensional thinning. Despite this difference with polymers, the elastic instability is still observed. We will discuss this instability in the context of a model, the VCM model, that accurately describes the flow of WLMs.

The VCM constitutive model (Vasquez, McKinley and Cook (2007)) is a two species, microstructural network model, which incorporates breakage and reforming of two micellar chains. The model predicts the typical WLM rheological trends of shear thinning and extensional thinning. Using the open-source CFD library OpenFOAM, we show that the VCM model predicts the formation of an asymmetric elastic instability. In addition, the VCM model predicts the formation of recirculation zones just upstream of where the inlet and outlet channels meet. In this talk, we focus on the role breakage and reforming play on the instability and secondary flow. Finally, the computational results are compared with experimental observations.

Tue-C: Suspension flows I — Chair: A. Rahmani

1:30-1:50 **Stability of particle hydrodynamic self-assembly in a channel flow: the effect of confinement, concentration and flow inertia**
M. Abbas, A. Gupta

Controlling the transport of particles in flowing suspensions at the micro-scale level is of immense interest in numerous contexts such as flow cytometry, single cell encapsulation and cell diagnostics. A commonly used technique for controlling particle positions in microchannel flows is so-called hydrodynamic focusing. It is based on cross-streamline migration of finite-size neutrally buoyant particles, towards specific equilibrium positions in the channel cross-section, due to finite flow inertia at the particle scale. Experiments in different channel geometries show that after reaching equilibrium positions, particles tend to align regularly in the streamwise direction. In this work we investigate this purely hydrodynamic self-assembly mechanism, using particle-resolved numerical simulations and try to rationalize different experimental observations. We carefully explore relative particle trajectories during the stage of streamwise assembly. The computed particle trajectories allow determining the equilibrium distance between aligned particles, which is comparable in average to available experimental data. Particle alignment is connected to the perturbation induced by particles which form spiralling streamlines purely related to the finite flow inertia at the particle scale. The relative trajectories of particle pairs are consequently of spiralling nature, and the trend toward equilibrium is faster when the Reynolds number is increased. The striking result is that the stability of an ensemble of aligned particles depends significantly on the number of particles trying to align and on the particle-to-channel height ratio (the confinement).

1:50-2:10 **Understanding Viscoelastic Suspensions via Numerical Simulation**
S. Krishan, M. Yang, W. Murch, G. Iaccarino, E. Shaqfeh

As is well known, suspensions of rigid particles in viscoelastic fluids play key roles in many energy applications and advanced manufacturing applications. In the present work, we describe the development of an Immersed Boundary Method (IB) to simulate the viscoelastic flow in suspensions of nonBrownian spheres. Since the phenomena of interest occur typically at O(1) values of the flow Weissenberg or Deborah number, we describe the methods necessary to obtain accurate resolution of the stress boundary layers near the particle surface even in the IB framework. Since the code is massively parallel, we demonstrate the simulation of a few hundred particles with the code, and examine in detail two problems where the multi-particle viscoelastic interactions provide unique physical results: 1) The sedimentation of spheres in orthogonal shear in a Taylor Couette Cell and 2) The rheology of a sphere suspension in a viscoelastic fluid in a parallel plate device. We examine these suspensions up to 5% volume fraction and demonstrate that, in each case, the dilute approximation is qualitative, but not quantitative, even at low volume fraction because of the finite Wi wake interactions between particles. In short, the mobility of each particle is a very strong function of Weissenberg number, with elastic effects strongly decreasing mobility. Moreover, rheologically we demonstrate the the suspensions strongly shear thicken because of extensional stresses created in the fluid near the particles. Our work is an important step toward aq comprehensive simulation-based tool for engineering the flows of viscoelastic fluid-particle suspensions in fully three dimensional geometries.

2:10-2:30 **Multi-scale stratagies in improvement of numerical models for the simulation of particle-laden flows**
A. Esteghamatian, A. Wachs

Particle-laden flows are observed in different natural phenomena and industrial applications. Owing to the diversity of temporal and spatial scales, this class of flows exhibit highly nonlinear and rich dynamics. Accordingly, a wide range of numerical models with various levels of complexity/assumptions exists in the literature. In this talk, we first present the state-of-the-art in numerical modeling of dense fluid/particle systems. Next, we focus on one particular class of numerical models which has gained much popularity in simulation of meso-scale systems: Four-way coupled Euler/Lagrange models.

In meso-scale models while the particles motion is handled in a direct fashion, the fluid field remains unresolved at the scale of particles. As compared to Particle Resolved Simulations, we evaluate the performance of meso-scale models in prediction of first- and second-order moment statistics of particles motion in a bi-periodic fluidization configuration. In our previous work [Esteghamatian *et al.* Micro/meso simulation of a fluidized bed in a homogeneous bubbling regime, International Journal of Multiphase Flows, 93:111-91, 2017.], we have shown that while the integral properties of the system is well-predicted by the meso-scale model, particle fluctuations are underestimated particularly in the transverse direction with respect to the mean axial flow. Hence, we propose a novel approach to improve the meso-scale models in a multi-scale framework. Based on a stochastic formulation for the drag law, the proposed model shows promising results in prediction of particles fluctuations particularly in the mean-flow direction.

The model has been tested in both homogeneous and heterogeneous regimes. In both cases, the meso-scale model performs well in prediction of particles statistics particularly in the mean-flow direction. However, we show that in a heterogeneous flow the motion of particles are mostly dominated by already-resolved meso-scale structures and in turn insensitive to the proposed correction. Finally, we explain the limitations of the proposed model and discuss different directions to overcome these limitations.

2:30-2:50 **Numerical simulation of elasto-inertial particle migration in square channel flow of viscoelastic fluids**
Z. Yu, P. Wang

In this paper, the inertia-elasticity-induced migration of a neutrally buoyant spherical particle in a pressure-driven square-shaped channel flow of an Oldroyd-B fluid is numerically investigated with a fictitious domain method. The particle lateral motion trajectories are shown for the bulk Reynolds number ranging from 1 to 100 and the Weissenberg number being up to 1.5. When the inertial effect is negligible, the elastic force acting on the particle determines the particle migration: the particle migrates towards the channel centerline or the closest corner, depending on its initial position. As fluid elasticity is increased, the corner-attractive region is extended, and the migration rate is faster. When the fluid inertial effect is not negligible (the Reynolds number in the range of 10 to 100), the particle migration equilibrium position depends strongly on the elasticity number (the ratio of the Weissenberg number and the Reynolds number) and weakly on the Reynolds number. When the effect of fluid elasticity is negligibly small and the inertia effect dominates, the particle moves towards the channel-centerplane equilibrium positions. Our results reveal a new elasto-inertial equilibrium position located in the channel diagonal plane for the elasticity number in the range of 0.001 to 0.02. When the elasticity number exceeds around 0.02, the particle migrates towards the channel centerline or the closest corner.

2:50-3:10 **Numerical simulation and experimental validation of the evolution of fiber orientation in complex flows**
P. Wapperom, D. Baird, G. Lambert, H. Chen.

Mechanical properties of fiber composites highly depend on the orientation of the fibers in a part. To improve mechanical properties, it is important to predict the complex fiber orientation that develops during processing.

Fiber orientation for concentrated suspensions are traditionally modeled by the Folgar-Tucker model. Although the model accurately predicts the main components of the orientation tensor in steady flow regimes, the model doesn't predict the slow evolution towards the steady state. Recently, two modifications of the Folgar-Tucker model have been proposed. The reduced strain closure model better predicts the slow evolution of fiber orientation, while the anisotropic rotary diffusion model better predicts all components of the orientation tensor.

We discuss the model predictions for fiber orientation in complex and simple flow. Model parameters are obtained from start-up-of-shear experiments in a sliding plate rheometer. These are used to investigate the evolution of the fiber orientation in the entry and frontal region of a center-gated disk. To better understand the fiber evolution in these regions with both shear and extension, the fiber orientation models are assessed in squeeze flow.

Tue-D: Flows at small scale — Chair: A. Taghavi

3:40-4:00 **Numerical simulation of molten metals on nanoscale**
S. Afkhami

Metal nanostructures placed on solid substrates and melted by nanosecond laser irradiation exhibit a rich dynamical behavior, owing to the high surface tension and relatively low viscosity of molten metals. The processes that lead to the final configuration of the solidified particles are of direct relevance to self- and directed-assembly of metal nanoparticles that find their applications in a diverse set of fields. We develop numerical methods based on the Volume-Of-Fluid technique to investigate the fluid dynamics of such systems including their interactions with the supporting solid substrate. We present numerical simulations of various initial metal geometries motivated by experimental observations.

4:00-4:20 **Single molecule tracking and modeling of beads-on-a-string structures along viscoelastic membrane nanotubes in live cells**
B. Ovryn and P. Wu

The modeling of plasma membrane bridges between cells (often called membrane nanotubes) has not, to our knowledge, received adequate treatment as viscoelastic filaments. Indeed, the majority of membrane nanotubes appear as stable liquid cylinder connections between cells, however, we have recently observed from single molecule tracking of glycoproteins in live cells, that membrane nanotubes can manifest stable, large beads-on-a-string structures. Similar behavior has also been observed for so-called "beaded apoptopodia" which are formed in dying cells. Therefore, modeling these nanotubes as Newtonian liquid filaments is incomplete. Although the elastic behavior of plasma membranes have been demonstrated, no one has modeled these beads-on-string as arising from the viscoelastic characteristics which emerge from the polymeric nature of the cell surface glycoproteins. We present data from live cells and propose several mechanisms that could give rise to the viscoelastic behavior and the observed beads-on-a-string in these membrane liquid bridges.

4:20-4:40 **Shear and Extensional Flow Dynamics of Lipid Lamellae and Lamellar Vesicles: A Molecular Dynamics Study**
S. Dhakal, R. Sureshkumar

Mechanics and dynamics of lipid bilayers and vesicles play a crucial role in cellular processes and cell functions that range from cell division to targeted drug delivery. In the past few years, we have developed reliable coarse grained molecular dynamics (CGMD) simulations to probe structure, dynamics and rheology of surfactant micelle solutions and lipid bilayers (e.g. Dhakal and Sureshkumar, J. Chem. Phys., 143, 024905 (2015); ACS Macro Letters, 28, 1766-1771 (2012); Sambasivam et al. PRL, 114, 158302 (2015); Nangia and Sureshkumar, Langmuir, 28, 1766-1771 (2012)). We have also adapted such CGMD simulations to study the influence of shear and extensional flow deformations on vesicle shape and dynamics as well as an experimentally observed shear-induced structure transition from bilayers to multi-lamellar vesicles.

Specifically, we simulate self-assembly of dodecyldimethylammoniumbromide (DDAB) lipids in water using a coarse-grained Martini force field. Large-scale MD simulations are performed using GROMACS and LAMMPS packages on the XSEDE supercomputing platform. MD simulations have revealed various equilibrium morphologies such as micelles, uni-lamellar and multi-lamellar vesicles as well as layered structures with increasing lipid concentration. In this presentation, we will focus on the following points.

Dynamics of vesicles in shear flow: We have developed a numerical method to accurately calculate the reduced volume of a vesicle by expanding the vesicle-water interface topology obtained from MD simulations in terms of spherical harmonics. We then tracked the orientation of non-spherical (ellipsoidal) vesicles by calculating their principal axes from the inertia tensor. Our simulations suggest that the reduced volume of vesicles is a key determinant of their shear flow dynamics. A deflated vesicle shows tumbling dynamics while a nearly spherical vesicle is likely to exhibit tank-treading. We will discuss how the tumbling frequency changes with the applied shear rate.

Lamellar Structures in Shear Flow: We will discuss the mechanical response of lamellar structures in shear flow. As the deformation rate increases, we see a buckling instability leading to a morphology transition from lamellae to vesicles which is accompanied by an increase in the shear viscosity. Our results suggest that the linear dimension of the vesicles thus formed is approximately equal to the wavelength of the primary buckling mode.

Uniaxial Extension of Lamellae: We will discuss the response of lamellar structures under uniaxial extension. We have developed a method to calculate the Poisson's ratio of lamellae. We will discuss the effect of electrostatic screening induced by co-amphiphilic molecules stacked parallel to the lipids on the mechanical properties of the lamella. Specifically, our simulations show that stiffness and Poisson ratio of the lamellae increases and decreases respectively with increasing concentration of co-surfactants. We will discuss the mechanisms underlying this observation.

4:40-5:00 **Stochastic mesoscale modeling of transiently networked fluids**

L. Zhou, L. Cook

Mesoscale modeling of transiently networked fluids avoids the need for a closure approximation that is necessary to upscale such models to the macroscale and thus is particularly useful in modeling complex fluids that may have changes in local properties, such as stretch, orientation, and concentrations. In this talk, we present the modeling and numerical simulation results of a transiently networked fluid which consists of linear chains of Hookean bead-spring dumbbells. The chains break and reform according to prescribed energy functions which are associated with the local chain stretch and hence local stress. The topology of the network is tracked so that the distribution of the lengths of chains and of their stretch can be quantified in time and in space. Model predictions in equilibrium, under step strain, and in steady shearing flow are presented and discussed. Of particular note model simulations predict that, depending on the parameter ranges, step strain relaxation curves are best fit either by an exponential function or a stretched exponential function. In equilibrium chain length distributions are exponential in the length. The steady state flow curves show strong dependence on the functional form of the prescribed energies. Overshoot in the time evolution of the shear stress in steady shearing is also observed.

Wed-A: Suspension flows II

Geography 100
Chair: M. Abbas

9:00-9:20 **Enhancing shear thickening**
S. Hormozi, Y. Madraki, G. Ovarlez, É. Guazzelli and O Pouliquen

A cornstarch suspension is the quintessential particulate system that exhibits shear thickening. We present the results of our experimental study and show that by adding large non-Brownian spheres to a cornstarch suspension, the shear thickening can be significantly enhanced. More precisely, the shear-thickening transition is found to be increasingly shifted to lower critical shear rates. This influence of the large particles on the discontinuous shear thickening transition is shown to be more dramatic than that on the viscosity or the yield stress of the suspension. In addition, we show that how bidisperse suspensions of noncolloidal particles influences the shear thickening, particularly how continuous shear thickening can transition to discontinuous shear thickening.

9:20-9:40 **Interface-resolved simulations of rigid and deformable particles in shear flows**
L. Brandt, D. Alghalibi, I. Lashgari and M. Rosti

We will present interface-resolved numerical simulations of particle suspensions in Newtonian and non-Newtonian fluids. An immersed boundary method is used to couple the fluid and solid phases. We shall first consider a simple shear flow and vary particle volume fraction and particle Reynolds number. We demonstrate that fluid inertia causes a strong microstructure anisotropy that results in the formation of a shadow region with no relative flux of particles. This shear thickening at finite inertia can be explained as an increase of the effective volume fraction when considering the dynamically excluded volume due to these shadow regions. The same configuration is used to study the rheology of suspensions in inelastic non-Newtonian fluids, both shear-thinning and thickening, modelled by the Carreau-Yasuda model. We quantify the distribution of shear stresses in the suspensions and show that it is a strong function of the suspension volume fraction and less of the Reynolds number. We compare our results against the homogenisation theory recently proposed. We also focus on the transition between the inertialess and inertial shear-thickening regimes and report that this occurs at different particle Reynolds numbers when varying the particle concentration for all fluids under investigation. Finally, we present a new Eulerian method to study viscous hyper-elastic materials. Simulations of deformable particle reveal that the viscosity increases with the volume fraction, and decreases with the deformability (shear-thinning). In addition, the particle deformation increases with the volume fraction. We will propose an extension of the Batchelor and Green viscosity ratio model to the case of deformable particles, valid also at relatively high volume fractions.

9:40-10:00 **Rheology and Microstructure of Dense Deformable Colloidal Suspensions: Interplay Between Elasto-hydrodynamic and Frictional Interactions**
S. Khani, A. Boromand, B. Grove and J. Maia

Understanding the physical origin of the rheological response of colloidal suspensions, namely the shear thickening phenomenon, has been the subject of numerous recent studies, with both lubrication hydrodynamic and friction theories having been used to explain the shear rate dependent behavior of these complex fluids. However, neither has been able to replicate by itself the whole range of rheological responses in the continuous and discontinuous shear thickening regimens. Recently, using numerical simulations, our group investigated the role of hydrodynamic and frictional interactions in rheological properties of dense and semi-dense colloidal suspensions and showed that the formation of a frictional percolating network at high stresses is essential for obtaining discontinuous shear thickening behavior and positive N1; however, it is also necessary for hydroclusters to form at low stresses in order to bring particles together and nucleate the frictional contacts. Deformable colloidal particles will change the flow response of colloidal suspensions. Herein we discuss the effect of elasto-hydrodynamic deformation of the particles on the microstructures formed under external shear flows and on the corresponding rheological response, i.e., shear-thickening and normal-stress differences. We will use a mesoscale model that includes lubrication and frictional forces in addition to a contact force developed based on the elasto-hydrodynamic theory. Monitoring the structure and rheology of soft to rigid suspensions, we explore the interplay between the elasto-hydrodynamic and frictional interactions.

10:00-10:20 **Study of spontaneous structure formation in granular systems using DEM and CFD+DEM framework**
K. Nandakumar, J. Yu, C. Wu, J. Joshi and M. Tyagi

Spontaneous cluster and pattern formation can happen in granular systems with multiple particles. Such phenomena have been observed in nature as well as in experiments. Studying these phenomena can help us understand the physics of these systems and build and validate models that can then be used in process equipment design. In this work, we investigate the spontaneous organization of granular particles in a cylindrical vessel by using discrete element method

(DEM) simulations. Two different types of motion of the cylindrical vessel has been studied. In the first type of motion, the cylindrical vessel follows the horizontal circular motion, i.e., the distance between any point in the cylinder and the center of motion is fixed during the entire process. In the second type of motion, the cylindrical vessel follows the motion of an orbital shaker without self-rotation. This type of swirling motion is generated by superposing two sinusoidal vibrations in two perpendicular directions respectively. When the cylinder vessel contains a group of granular particles follows the first type of motion, the particles form a steady, symmetric structure on the side wall of the cylindrical vessel. However, if the cylindrical vessel follows the second type of motion, the particles form an asymmetric structure and becomes dynamic in nature. We examine the results of our simulations and compare to existing published experimental data to gain a better understanding of this phenomenon.

10:20-10:40 **Simulations of suspension flows with a meshless MLS scheme**
A. Howard, M. Maxey

This talk will focus on a meshfree method for simulations of neutrally buoyant, non-Brownian particles in Stokes flow. We will discuss a meshless scheme using Moving Least Squares polynomial reconstructions to provide a computationally efficient method with higher order accuracy for use with general boundary conditions and arbitrary polynomial shapes while maintaining stability. The emphasis will be on applications to dense suspensions of particles, especially particles with polydispersed sizes and non-spherical shapes. Results will be compared to other schemes including the Force Coupling Method.

Wed-B: Flows through porous media

Chair: S. Hormozi

11:10-11:30 **Modeling flow and fouling in membrane filters: Insights into filter design**
L. Cummings, P. Sanaei

We present first-principles models describing flow of particle-laden "feed solution" through a membrane filter. Particles are removed from the feed via a combination of sieving (large particles) and particle adsorption within pores, leading to fouling of the filter. Such fouling increases the membrane resistance, which in turn impacts the flow. In this presentation we will describe some of our recent and ongoing work modeling membrane filtration and fouling. Particular emphasis is paid to how membrane filter design (in particular, permeability gradients across the membrane, and the internal branching structure of pores) can significantly affect filtration efficiency, as measured by (i) total throughput over a filter lifetime, and (ii) proportion of particles removed from the feed.

11:30-11:50 **A multi-scale model for electrokinetic transport in porous networks**
A. Mani and S. Alizadeh

Electrokinetic transport in porous media is relevant to a wide range of applications including electrochemical energy storage and energy conversion, water deionization and purification, soil decontamination and lab-on-a-chip devices. Due to presence of electrostatic charge on surfaces in such systems surface conduction can significantly impact transport of charge, ions, and fluid flow. Additionally, in these systems pore sizes can vary randomly in space, forming a heterogeneous network of micro-scale and nano-scale pores. The nonlinear coupling of surface conduction and domain heterogeneity can provoke complex modes of transport, which are not quantitatively understood in the context of porous networks.

We have developed an efficient model that can accurately capture the aforementioned nonlinearities inside porous media. The computational cost of our model is multiple orders of magnitudes less than that of brute force calculations using direct numerical simulations (DNS). We model a porous medium as a large network of many pores that are coupled at the pore intersections. Our model utilizes equilibrium assumption for variations in scales comparable to the cross sectional dimension of each pore while retaining full equations for variations over pore longitudinal direction. A one-dimensional transport equation is derived for each pore that describes the cross-sectional averaged concentration as a function of time. This approach bridges the gap between traditional homogenization methods, which fail to capture the nonlinearities at small scale, and expensive DNS, which has to resolve complex geometries in multi-dimensions. We present wide range of advantages of this model in terms of physical accuracy, algorithm complexity, and capability of handling numerically stiff limits. Using this model, we demonstrate simulations of large networks of pores. We will discuss how randomness of pore size distribution can impact macroscopic behavior in such systems.

11:50-12:10 **Fluid-solid interactions in a non-convex granular media**
A. Rakotonirina, A. Wachs, M. Rolland, J. Delenne

Non convex granular media are involved in many industrial processes, for instance particle calcination or drying procedure in rotating drums or solid catalyst particles in chemical reactors. So far, optimization of process or particle shape relied on experimental works. In the cases of optimization of catalyst shape, experimental discrimination of new shapes regarding packing density and pressure drop proved to be difficult due to limited control of size distribution and loading procedure. There is an interest in developing numerical tools for predicting the dynamics of granular media made of arbitrary particle shapes and simulating fluid flow around these particles, non-convex particles being much more challenging due to the multiple possible contact points. In this work, we implement these capabilities within our home made high-fidelity parallel numerical tools: GRAINS3D (Powder Tech., 224:373-389, 2012) for granular dynamics of convex particles and PeliGRIFF (Parallel Efficiency Library for Grains In Fluid Flows, Comp. Fluids, 38(8):1608-1628, 2009) for reactive fluid/solid flows. The first part of this work consists in extending the modelling capabilities of Grains3D to non-convex particles based on the decomposition of a non-convex shape into convex ones. Grains3D can now handle any combination of arbitrary convex particles. We validate our numerical model with existing analytical solutions and a rotating drum experiment using "2D cross" particle shapes. We also use our tools to study the loading of fixed reactors with trilobic and quadralobic particles in semi-periodic and small size reactors. The second part of this work consists in extending the modelling capabilities of PeliGRIFF to handle poly-lobed particles for which we use our Particle Resolved Simulation (PRS) method based on Distributed Lagrange Multiplier / Fictitious Domain (DLM/FD) formulation combined with a Finite Volume / Staggered Grid (FV/SG) scheme. Due to the lack of analytical solutions and experimental data, we assess a space convergence to show the accuracy of our PRS method on assorted flow configurations such as flow through periodic arrays of poly-lobed particles and fixed bed reactors. Simulation of flow in fixed beds of poly-lobed particles is consistent with previous experimental work and enable us to decouple optimization parameters and explore repeatability issues stemming from random packing. For illustration purpose, fluidization of few hundred poly-lobed particles is performed as well as reactive flow simulation in a fixed bed of poly-lobed particles.

9:00-9:20 **Analyzing nanofiber formation in centrifugal spinning using a regularized string model**
S. Noroozi, S. Taghavi

We develop a regularized asymptotic method to analyze the thinning of a jet in the centrifugal spinning process, where a polymer solution emerges from a nozzle of a rapidly rotating spinneret to produce nanofibers. We study the steady state trajectory and thinning rate of fiber radius in the presence of centrifugal, Coriolis, inertial, viscous/shear-thinning, surface tension and gravitational forces, forming five important dimensionless groups, namely, the Rossby number (*Rb*), the Reynolds number (*Re*), the Weber number (*We*), the Froude number (Fr) and a power-law index (m), We find that variations in Fr mainly affect the fiber trajectory. We show that for small *Rb* the thinning rate of fiber radius is significant, a feature that is attenuated by decreasing *Re* or increasing m. We also find that a decrease in *We* may cause the fiber to curve towards the spinneret, forming a circular trajectory, where the thinning rate of fiber radius approaches to zero. At large *We*, however, the fiber follows a spiral trajectory. Finally, we map the fiber thinning process regimes for various ranges of *Rb* and *We*, through introducing the *no-thinning*, *intense-thinning*, and *slow*- or *ceased-thinning* regimes.

9:20-9:40 **A singular perturbation study of the Rolie-Poly model**
M. Renardy and Y. Renardy

We study the Rolie-Poly model for entangled polymers, using a singular perturbation analysis for the limit of large relaxation time. In this limit, it is shown that the model displays the characteristic features of thixotropic yield stress fluids, including yield stress hysteresis, delayed yielding and long term persistence of a decreased viscosity after cessation of flow. We focus on the startup and cessation of shear flow. We identify dynamic regimes of fast, slow and yielded dynamics, and show how the combination of these regimes can be used to describe the flow.

9:40-10:00 **Elastic modifications of an inertial instability in a 3D cross-slot**
K. Zografos, N. Burshtein, S. Haward, A. Shen, R. Poole

Recent experimental and numerical studies investigating Newtonian fluid flows in 3D microfluidic cross-slot configurations report the existence of a critical Reynolds number ($\mathrm{Re_c}$) above which an inertial flow instability occurs [1]. When $\mathrm{Re} \geq \mathrm{Re_c}$ the flow is asymmetric, but remains steady with an axially-aligned spiral vortex formed along the two outlet channels of the geometry. Below these critical conditions the flow retains its symmetry.

Experimental investigations over a wide range of viscoelastic fluids characterized by various solvent-to-total viscosity ratios $\beta = \eta_s/(\eta_p + \eta_s)$, where η_s is the solvent viscosity and η_p is the polymer viscosity, show that $\mathrm{Re_c}$ and the subsequent growth of vorticity are noticeably decreased compared to the Newtonian case. Remarkably, even for very low polymer concentrations as low as 3 ppm ($0.90 \leq \beta \leq 0.99$), the flow field is found to be significantly modified. Such notable elastic effects at such low polymer concentrations have usually only been reported in the context of turbulent drag reduction [2].

Motivated by these observations, experimental findings are complemented by a series of computational fluid dynamics simulations, and here we report our results which provide additional insight into how the instability mechanism is modified by the presence of fluid elasticity. The numerical simulations performed, employ an in-house CFD code which is based on an implicit finite-volume method that is appropriate for collocated numerical grids [3].

The FENE-MCR model [4] is employed in order to express the polymeric component of the stress tensor in the momentum equation, which is a constant viscosity viscoelastic model with bounded extensional viscosity. The numerical results demonstrate a qualitative agreement with the experimentally observed behaviour, where by decreasing β in a range equivalent to ppm polymer concentrations, a significant reduction in both $\mathrm{Re_c}$ and the vorticity growth with Re for $\mathrm{Re} \geq \mathrm{Re_c}$ results.

References:

[1] SJ Haward et al, Phys Rev E, 93:031101 (2016)

[2] MD Graham, Phys Fluids, 26:101301 (2014)

[3] MA Alves et al, J Non-Newton Fluid Mech, 110:45 (2003)

[4] PJ Coates et al, J Non-Newton Fluid Mech, 42:141 (1992)

10:00-10:20 **Quantitative Rheological Model Selection with Bayesian Analysis**
J. Freund and R. Ewoldt

Any simulation of non-Newtonian flow must start with selection of a rheological model, and therein lies its own computational challenge. The more parameters in a rheological the better it will reproduce available data, though this does not mean that it is necessarily a better justified model. Good fits are only part of model selection. We employ a Bayesian inference approach that quantifies model suitability by balancing closeness to data against both the number of model parameters and their a priori uncertainty. The penalty depends upon prior-to-calibration expectation of the viable range of values that model parameters might take, which we discuss as an essential aspect of the selection criterion. Models that are physically grounded are usually accompanied by tighter physical constraints on their respective parameters. The analysis reflects a basic principle: models grounded in physics can be expected to enjoy greater generality and perform better away from where they are calibrated. In contrast, purely empirical models can provide comparable fits, but the model selection framework penalizes their a priori uncertainty. We demonstrate the approach by selecting the best-justified number of modes in a Multi-mode Maxwell description of PVA-Borax. We also quantify relative merits of the Maxwell model relative to powerlaw fits and purely empirical fits for PVA-Borax, a viscoelastic liquid, and gluten. This will be tied into ongoing flow simulation work making predictions with rheological models in modestly complex flow geometries.

Thur-B: Round Table

Chair: I. Frigaard

11:00-12:20 **Future perspectives for computational complex fluids**

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Thur-C: Free surface flows

Chair: J. Feng

2:00-2:20 **Instability and dewetting of ultra-thin nematic liquid crystal films**
L. Cummings, L. Kondic, M. Lam

A weak free surface anchoring model is presented for a thin nematic liquid crystal (NLC) film. Applying the long wave approximation to the Leslie-Ericksen equations, a fourth order nonlinear partial differential equation is derived for the free surface height. Key to the film's behavior are the dipole moments of the NLC molecules, which induce an elastic response in the bulk of the film, and the anchoring (boundary) conditions on the molecules at the free surface and substrate. In general, the anchoring conditions at the two interfaces are different (antagonistic). Strict enforcement of the antagonistic conditions for very thin films incurs an unphysically large energy penalty in the bulk of the fluid. To alleviate this issue, we present a novel weak anchoring formulation, which dynamically relaxes the free surface anchoring to that of the substrate as the thickness of the NLC film decreases. Using linear stability analysis, we are able to draw a parallel between the stability properties of our model, and the so-called "forbidden film thicknesses" seen in experiments. In addition, we present large-scale simulations, carried out using a GPU, and compare the morphology of simulated dewetted films to available experimental results.

2:20-2:40 **Magnetophoretic Interaction of a Pair of Ferrofluid Droplets in a Rotating Magnetic Field**
M. Qiu, S. Afkhami, C. Chen and J. Feng

A ferrofluid is a stable suspension of magnetic nano-particles in a carrier fluid. Thanks to the fine particle size and colloidal stability, ferrofluids mostly flow as a homogeneous Newtonian fluid, except that they can be manipulated by an external magnetic field and display a variety of novel phenomena. Recent experiments have discovered several modes of interaction between a pair of ferrofluid droplets in a rotating magnetic field, including the so-called planetary motion in which the drops spin while revolving around each other with a phase lag from the rotating field. In this study, we use direct numerical simulations to investigate pairwise drop interaction as experimentally observed. We have captured all the regimes of interaction, as well as the key features of the planetary motion. The simulations agree well with the experimental observations.

2:40-3:00 **A new mechanism for the wetting of a surface by the drops of an emulsion**
S. Borkar and A. Ramachandran

The wetting of a solid surface by the drop of an emulsion has traditionally been thought to be mediated by the formation of a liquid bridge that connects the drop and the surface. In the current work, we experimentally show that there exists a different mechanism of the spreading of a drop on a surface. Experiments were conducted for simple liquid-liquid systems, wherein drops of higher density were allowed to settle under gravity in a lighter liquid phase under conditions of small Bond numbers. The approach of the drop towards the substrate was visualized using Reflection Interference Contrast Microscopy (RICM), and the details of the film drainage dynamics and the eventual spreading mechanism of the drop on the surface were recorded. Three liquid-liquid systems were used - 1) glycerol-in-silicone oil 1000 cP (SO1000), 2) glycerol in silicone oil 500 cP (SO500), and 3) silicone oil (SO500) in paraffin oil (PO). The substrates were also varied in this study. The film shapes obtained from this were then compared with predictions from scaling analysis. The temporal variation of the minimum film heights matched theoretical expectations, except when the height reached about the order of 10 nm for silicone oil films (system 1 and 2). In this case, cessation of film drainage was observed and was attributed to the formation of an immobilized silicone oil layer due to polymer confinement. While the film appeared to be stable, after an induction period ranging from a few minutes to several hours, deformable islands of glycerol were observed to grow on the substrate. Wetting of the surface then occurs by the formation of a bridge, not between the parent drop and the surface directly, but between the parent drop and the nucleated sites. The fundamental effect discovered here will ultimately guide the tailoring of emulsion-based coatings or paints to have specific spreading times. It also has application in multiphase industrial operations such as froth floatation, where the understanding of the time scale of particle-droplet/bubble attachment is critical.

3:00-3:20 **Numerical Simulation on Impinging Droplets of Pseudo-Plastic Fluids**
H. Suzuki, R. Hidema, A. Senda, K. Ishihawa, Y. Komoda, K. Suzuki

Deformation characteristics of impinging droplets of psuedo-plastic fluids has been investigated by a numerical computation. The zero-shear and infinity viscosities of the fluids were changed in a several steps, while the surface tention and the dynamic wet angle were fixed. As an interface capture scheme, CLSVOF method was applied. The droplet size and the impinging velocity were also kept constant at 40 micron and 5 m/s, respectively. From the results, it was found that the infinity viscosity affects significantly the spread behavior of the droplets, but the zero-shear viscosity does not contribute to the spreading of the fluids on the wall.

3:20-3:40 **Numerical and nonlinear dynamic study of melt fracture**
Y. Kwon

Computationally modeling the Poiseuille flow along (and outside) contraction and straight channels with a differential viscoelastic constitutive equation, we describe various 2D elastic flow instabilities with particular emphasis on melt fracture for the extrudate exiting from the Poiseuille flow. This numerical approximation is shown to be possible, when a mathematically appropriate (evolutionary) constitutive equation is incorporated into the straightforward computation scheme (no upwinding) with the matrix-logarithmic formulation. We illustrate unstable dynamics involving a bifurcation from steady to periodic melt fracture (sharkskin instability) and its further transition to a chaotic regime. The first Hopf bifurcation results from the high stress along the streamlines and their finite curvature near the die lip. Its succeeding chaotic transition at higher level of flow elasticity that leads to gross melt fracture, seems to take a period doubling as well as quasiperiodic route. Current study suggests another possible origin for the onset of sharkskin instability and conceivably provides a robust methodology to portray various types of melt fracture if combined with an appropriate model of wall slip.

Thur-D: Numerical methods — Chair: S. Gonzalez-Andrare

4:20-4:40 **The deformation fields method revisited: stable simulation of viscoelastic fluid flow using integral models**
M. Hulsen, P. Anderson

New constitutive models for viscoelastic fluids are often formulated in terms of memory integral equations. For example, the constitutive model for complex fluids with a power-law like spectral behaviour of Jaishankar & Mckinley [1] is written in the form of a K-BKZ integral model. However, development of stable finite element methods for viscoelastic fluids has mostly been focussed on differential models. Great progress has been achieved in the field of numerical simulation of differential models. The introduction of stabilisation techniques such as SUPG, (D)EVSS-G, log-conformation, and velocity-stress decoupling schemes for zero solvent viscosity, has made it possible to solve many problems at much higher Weissenberg numbers for a large class of models of the differential type.

In this talk, new developments in the deformation fields method [2] will be presented that will give this method numerical stability properties that are comparable to state-of-the-art methods for differential models. Examples will be given on the time-dependent stability of Couette flow and the flow around a cylinder confined between two flat plates.

References:

[1] Jaishankar, A., & Mckinley, G. H. (2014). A fractional K-BKZ constitutive formulation for describing the nonlinear rheology of multiscale complex fluids. Journal of Rheology, 58(6), 1751–1788.

[2] Hulsen, M.A., Peters, E.A.J.F., & van den Brule, B.H.A.A. (2001). A new approach to the deformation fields method for solving complex flows using integral constitutive equations. Journal of Non-Newtonian Fluid Mechanics, 98, 201–221.

4:40-5:00 **A new and straightforward stabilization approach to model viscoelastic fluid flows**
C. Fernandes, M. Araújo, L. Ferrás and J. Nóbrega

The opensource finite-volume computational library OpenFOAM comprises all the major differential viscoelastic models and thus has been widely used in computational rheology studies, both in academia and industry. However, some stability issues have been reported, and, consequently, different approaches have been proposed to solve them. This work reports some recent developments made to improve the numerical stability of the viscoelastic solvers available in OpenFOAM, which are based on the modification of the traditional both-sides-diffusion stabilization approach, with a procedure that simultaneously promotes the coupling between the velocity and stress fields. The improved code capabilities are illustrated with two benchmark 2D case studies, the 4:1 contraction and the flow around a confined cylinder, of an upper-convected Maxwell fluid. For verification purposes the code predictions were compared with results from the literature. Moreover, the results obtained allowed to further improve the accuracy of the benchmark data available in the literature. These new solvers are expected to significantly enlarge the range of problems that can be solved with OpenFOAM computational library.

5:00-5:20 **Numerical Simulation of 'Extreme Fluids' - Some Examples, Challenges and Simulation Techniques for Flow Problems with Complex Rheology**
S. Turek

We present numerical simulation techniques for incompressible fluids with complex rheology due to *extreme* changes of the viscosity which may vary significantly by several orders of magnitude, for instance due to non-isothermal behavior and pressure, resp., shear dependency. Such fluids may include viscoplastic as well as viscoelastic effects which is typical for yield-stress fluids, granular material as well as polymer melts and rubber (caoutchouc). Corresponding applications are relevant for polymer processing, but include also viscoplastic lubrication, fracking and macro encapsulation. In this talk, we present special discretization and solver techniques in which case the coupling between the velocity, pressure and additional variables for the stresses, which leads to restrictions for the choice of the FEM approximation spaces, and the (often) hyperbolic nature of the problem are handled with special Finite Element techniques including stabilization methods. The resulting linearized systems inside of outer Newton-type solvers are (special) nonsymmetric saddle point problems which are solved via geometrical multigrid approaches. We illustrate and analyze numerically the presented methodology for well-known benchmark configurations as well as protoypical industrial applications for several nonlinear flow models.

5:20-5:40 **Practical aspects of implementing dual proximal gradient method for the solution of yield stress flows**
A. Roustaei, T. Treskatis, A. Wachs and I. Frigaard

The mathematically sound resolution of yield stress fluid flows requires handling of a non-smooth convex optimisation problem. Traditionally, augmented Lagrangian methods developed in 80's has been used for this purpose. The main drawback of these algorithms is the frustrating slow worst-case convergence rate of $(1/\sqrt{k})$, where k is iteration count. Recently, a new dual-based algorithm called FISTA* is introduced by Treskatis et. al [1], which achieves higher order of convergence $(1/k)$. In this talk, we will explain our experience with implementing this algorithm in two FEM packages, Rheolef (Pierre Saramito, Grenoble) and FreeFEM++ (Frèdèric Hècht, UPMC), and will mention some of the pitfalls and details to be aware of.

[1] Timm Treskatis, Miguel A. Moyers-González, Chris J. Price *An accelerated dual proximal gradient method for applications in viscoplasticity* J of Non-Newtonian Fluid Mechanics 238 (2016): 115-130.

9:00-9:20 **Mechanistic constitutive model for wormlike micelle solutions with flow-induced structure formation**
S. Dutta and M. Graham

We present a tensor constitutive model for predicting stress and flow-induced structure formation in dilute wormlike micellar solutions. The micellar solution is treated as a dilute suspension of rigid Brownian rods whose length varies dynamically. Consistent with the mechanism presented by Turner and Cates [J. Phys.: Condens. Matter 4, 3719 (1992)], flow-induced alignment of the rods is assumed to promote increase of rod length that corresponds to the formation of flow-induced structures observed in experiments. At very high deformation rate, hydrodynamic stresses cause the rod length to decrease. These mechanisms are implemented in a phenomenological equation governing the evolution of rod length, with the number density of rods appropriately modified to ensure conservation of surfactant mass. The model leads first to an increase in both shear and extensional viscosity as deformation rate increases and then to a decrease at higher rates. If the rate constant for flow-induced rod growth is sufficiently large, the model predicts a multivalued relation between stress and deformation rate in both shear and uniaxial extension. Predictions for shear and extensional flow at steady state are in reasonable agreement with experimental results. By design, the model is simple enough to serve as a tractable constitutive relation for computational fluid dynamics studies.

9:20-9:40 **The Extrudate Swell of HDPE: Experiments and Simulations**
V.K. Konaganti, M. Ansari, E. Mitsoulis and S. Hatzikiriakos

The extrudate swell of an industrial grade high molecular weight high-density polyethylene (HDPE) in capillary dies is studied experimentally and numerically using the integral K-BKZ constitutive model. The non-linear viscoelastic flow properties of the polymer resin are studied for a broad range of large step shear strains and high shear rates using the cone partitioned plate (CPP) geometry of the stress/strain controlled rotational rheometer. This allowed the determination of the rheological parameters accurately, in particular the damping function, which is proven to be the most important in simulating transient flows such as extrudate swell. A series of simulations performed using the integral K-BKZ Wagner model with different values of the Wagner exponent n, ranging from $n = 0.15$ to 0.5, demonstrates that the extrudate swell predictions are extremely sensitive to the Wagner damping function exponent. Using the correct n-value resulted in extrudate swell predictions that are in excellent agreement with experimental measurements.

9:40-10:00 **Viscoelastic Simulations with Integral Models at Extremely High Shear Rates**
E. Mitsoulis

For simulation of thin-wall injection molding, accurate viscosity data measured at shear rates up to $800,000$ s^{-1} are important. A special feature allows measuring the pressure dependency of viscosity using closed-loop counter pressure control. Experimental data are evaluated taking into account the melt temperature rise due to dissipative heating. Using capillary dies having different diameters, D, and length-to-diameter L/D ratios, a full rheological characterization has been carried out for a polypropylene-filled nanocomposite, and the experimental data have been fitted with a viscoelastic model (the Kaye - Bernstein, Kearsley, Zapas / Papanastasiou, Scriven, Macosko or K-BKZ/PSM model). Four injection molding dies have been also used to reach apparent shear rates up to $800,000$ s^{-1}. Particular emphasis has been given on the pressure-dependence of viscosity. It was found that the viscoelastic simulations were capable of reproducing the experimental data well with a pressure-dependence of viscosity, especially at the higher apparent shear rates and L/D ratios.

10:00-10:20 **Polymer effects on the development and bursting of turbulent vortices: implication on high-extent drag reduction**
L. Zhu, X. Bai, L. Xi

Two major problems in viscoelastic turbulence, the effects of polymers on the laminar-turbulent transition dynamics and the origin of the maximum drag reduction asymptote, are both better understood in the regime near the margin of turbulence. Direct numerical simulation trajectories initiated from the edge state are used to follow its unstable manifold into the turbulent basin. In Newtonian flow, the growth of turbulence starts with the intensification of velocity streaks and a sharp rise in the Reynolds shear stress. It is followed by a quick breakdown into high-intensity small-scale fluctuations before entering the core of turbulence. This breakdown process not only occurs during the transition but also shows up in steady-state turbulence as intermittent bursting events. Adding drag-reducing polymers does not affect the initial growth of turbulence but stabilizes the primary streak-vortex structure. As a result, the breakdown stage is circumvented. Throughout the process, polymers act in reaction to the growing turbulence and do not drive the instability. Before the MDR regime, there is also a transition between low-extent and high-extend drag reduction (LDR vs. HDR) where qualitative differences are observed in flow statistics. Its existence indicates that there are at least two primary mechanisms for drag reduction. Our research shows that the second one, which does not occur until the LDR-HDR transition, results from the suppression of bursting and the corresponding shift of vortex-sustaining mechanism. Understanding this transition is important for achieving high-extend drag reduction in flow control practices.

10:20-10:40 **Effects of extensional rheological properties of polymer solutions on vortex deformation in a two-dimensional turbulent flow**
R. Hidema and H. Suzuki

An experimental study has been performed in order to investigate the relationship between the extensional rheological properties of polymer solutions and the vortex deformation in turbulent flow. Polyethyleneoxide as a flexible polymer and hydroxypropyl cellulose as a rigid polymer were added to two-dimensional (2D) turbulent flow respectively. 2D flow has a benefit to examine the effect of extensional rheological properties of polymers on the flow. 2D turbulent flow and the vortex shedding on 2D flow were observed by interference patterns and particle image velocimetry (PIV). Power spectrum of the turbulent flow images, and turbulent flow statistics calculated by PIV analysis indicated that there are three flow regimes of the vortex shedding in the polymer added turbulent flow. The vortex shed in 2D flow was categorized in three types, which is affected by the relaxation time of the polymer solutions measured under extensional stresses.

11:20-11:40 **Particles in a yield-stress fluid**
E. Chaparian, A. Wachs and I. Frigaard

In Stokes flow of a particle settling within a yield-stress fluid, the resistive force of the yield stress must be overcome in order for the particle to move. This leads to a critical ratio of the buoyancy stress to the yield stress: the yield number. This translates geometrically to a critical envelope around the particle in the limit of zero flow, that contains both the particle and encapsulated unyielded fluid. Such unyielded envelopes and critical yield numbers are becoming well understood for single (2D) particles, as well as the means of calculating [1,2]. Here we study multiple particles, which introduces interesting complications. Firstly, plug regions can appear between the particles and connect them together, depending on the proximity. The combination forms larger (and heavier) particle with a different yielding behaviour. Thus, small particles (that cannot move alone) can be pulled by larger particles. Increasing the number of particles leads to more complicated dynamics.

References:

[1] E. Chaparian, I.A. Frigaard, Yield limit analysis of particle motion in a yield-stress fluid, Journal of Fluid Mechanics 819 (2017) 311–351.

[2] E. Chaparian, I.A. Frigaard, Cloaking: Particles in a yield-stress fluid, Journal of Non-Newtonian Fluid Mechanics 243 (2017) 47–55.

11:30-11:50 **A partially extending strand convection model with Newtonian solvent for modeling thixotropic yield stress fluids: stability of shear-banded flow**
Y. Renardy and M. Renardy

A viscoelastic constitutive model for thixotropic yield stress fluids is constructed with a partially extending strand convection model for an entangled microstructure and a Newtonian solvent (PECN). This approach has been used for homogeneous parallel shear flow, for an asymptotic analysis for large relaxation time. A multiple time scale analysis for the initial value problem displays key features of observed data for suspensions and gels such as delayed yielding, and hysteresis upon unyielding. The steady solution curve is non-monotone for a range of parameters that apply to suspensions, and allows for the co-existence of two shear rates, or shear banding. Linearized stability of shear-banded flow is discussed.

11:50-12:10 **Computing critical yield numbers in yield stress fluids**
I. Frigaard

In many situations involving yield stress fluids, the frontier between flowing and not flowing is defined by a critical yield number Y_c, which represents the dimensionless ratio between yield stress effects and the driving force of the flow, e.g. buoyancy driven settling of a particle. We show here the relevance of these critical limits to flow stability and give an overview of methods for computing (or at least approximating) Y_c in different flow situations. Joint work with: E. Chaparian & A. Wachs (UBC, Canada), J. Iglesias & G. Mercier (RICAM, Linz, Austria); C. Posch (U. Klagenfurt, Austria); O. Scherzer (U. Vienna, Austria), I. Karimfazli (Concordia U., Canada)

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