International Workshop on Mesoscale and Multiscale Description of Complex Fluids

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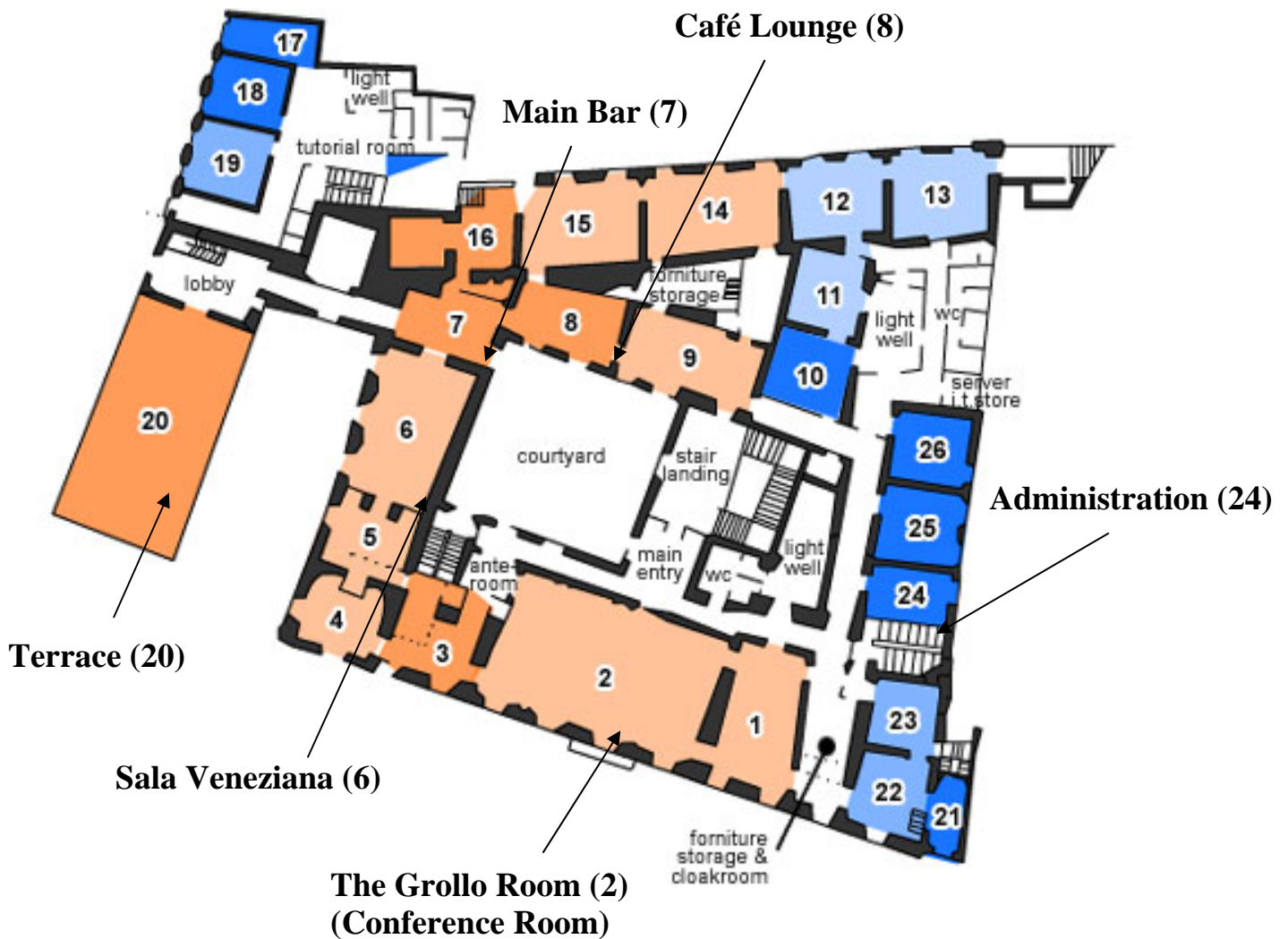
International Workshop on Mesoscale and Multiscale Description of Complex Fluids

Map of the
Monash University Centre, Prato

Café Lounge (8)

Main Bar (7)

Terrace (20)

Sala Veneziana (6)

The Grollo Room (2)
(Conference Room)

Administration (24)

International Workshop on Mesoscale and Multiscale Description of Complex Fluids

Workshop Program

Sessions	Thermodynamics & Coarse-graining Issues		Phase Behavior & Dynamics	Linear and Non-Linear Rheology	Multiscale Modelling
Time	5-Jul-06		6 - 8 July 2006		

Time	5-Jul-06
8:00	Registration
9:00	Welcome
9:20	C1: Sevick (Keynote)
9:55	C2: Olmsted
10:20	Coffee
10:40	C3: Evans (Keynote)
11:15	C4: Oettinger
11:40	C5: Prakash
12:05	C6: Prabhakar
12:30 - 13:30	Lunch
13:30	P1: Wilding (Keynote)
14:05	P2: Duenweg
14:30	P3: Pagonabarraga
14:55	Coffee
15:20	P4: Del Gado
15:55	P5: Zakin
16:20	End

Time	6 July 2006 Thursday	7 July 2006 Friday	8 July 2006 Saturday
8:30	P6: Cates (Keynote)	R7: Larson (Keynote)	R20: McKinley (Keynote)
9:05	P7: Fuller	R8: Denn	R21: Purnomo
9:30	P8: Yamaue	R9: Schieber	R22: Goddard
9:55	P9: Head	R10: Shnidman	M1: Sung-Joon Moon
10:20	Coffee	Coffee	Coffee
10:40	P10: Pasquali (Keynote)	R11: Bonn (Keynote)	M2: Kroeger (Keynote)
11:15	P11: Green	R12: Shaqfeh	M3: Boek
11:40	P12: Pereira	R13: Sridhar	M4: Dupuis
12:05	P13: Abou	R14: Fielding	M5: Kolomeisky
12:30 - 13:30	Lunch	Lunch	Lunch
13:30	R1: MacKintosh (Keynote)	R15: Sood (Keynote)	M6: Khomami (Keynote)
14:05	R2: Friedrich	R16: Lourdes de Vargas	M7: Behr
14:30	R3: Sunarso	R17: Russo	M8: Braun
14:55	Coffee	Coffee	Coffee
15:20	R4: Williams	R18: Marenduzzo	M9: Clementi
15:55	R5: Clasen	R19: Alok Paul	M10: Brenner
16:20	R6: Marrucci	End	Discussion
16:45	End		
17:05			End
18:30		Discussion	Conference Dinner
19:30			
20:00		Poster Session & Refreshments	

International Workshop on Mesoscale and Multiscale Description of Complex Fluids

PROGRAM

Wednesday Morning, 5 July 2006
Registration 8:00 AM
Welcome 9:00 AM

Thermodynamics and Coarse Graining
Chairman: Prof. Tamarapu Sridhar

9:00 AM **Introduction**

9:20 AM **E. M. Sevick (Keynote)**
Experimental demonstrations of new theorems in non-equilibrium thermodynamics

9:55 AM D. K. West, E. Paci**, P. D. Olmsted**
Mechanical unfolding of proteins: reduction to a single-reaction coordinate unfolding potential, and an application of the Jarzynski relation

Break: 10:20 – 10:40 AM

Thermodynamics and Coarse Graining Contd.

10:20 AM **R. M. L. Evans (Keynote)**
Does statistical mechanics apply to driven steady states of matter?

11:15 AM **H. C. Öttinger**
Coarse graining = understanding

11:40 PM **J. R. Prakash**
Convergence of Experiment and Theory for Dilute Polymer Solutions with Successive Fine Graining

12:05 AM **R. Prabhakar,** E. M. Sevick, D. R. M. Williams
Coarse-graining of hydrodynamic and excluded volume interactions in polymer chains

Wednesday Afternoon, 5 July 2006

Lunch: 12:30 – 1:30 PM

Phase Behaviour and Dynamics
Chairman: Prof. Peter Olmsted

1:30 PM **N. B. Wilding,** P. Sollich, M. Buzzacchi (**Keynote**)
Simulation studies of bulk and surface phase behaviour of polydisperse fluids

2:05 PM **B. Duenweg,** V. Lobaskin, S. H. Krishnan, C. Holm
Computer simulation of colloidal electrophoresis

2:30 PM **I. Pagonabarraga**
Mesoscopic modelling of biocolloidal hydrodynamics

Break: 2:55 – 3:20 PM

Phase Behaviour and Dynamics Contd.

3:20 PM **E. Del Gado**, W. Kob
Length scale dependent relaxation in colloidal gels

3:55 PM W. Ge, E Kesselman, Y Talmon, **J. L. Zakin**
Correlation of the relations of micellar microstructure of dilute CTAC/counterion systems with counterion chemical structure, counterion/CTAC ratio, drag reduction and rheological behavior

4:20 PM **End**

Phase Behaviour and Dynamics Contd.
Chairman: Prof. Hans Christian Öttinger

8:30 AM **M. E. Cates (Keynote)**
Interruption of coarsening in binary fluid mixtures

9:05 AM **G. G. Fuller**
Polymers in Two Dimensions: Spanning Solutions, Melts, and Glasses

9:30 AM **T. Yamaue,** M. Doi
The kinetics of dot formation induced by Marangoni flow in the drying process of polymer solution drop with mixed solvent

9:55 AM **D. A. Head**
Elastic deformation of non-uniform polymer crusts formed by droplet evaporation

Break: 10:20 – 10:40 AM

Phase Behaviour and Dynamics Contd.

10:40 AM **M. Pasquali (Keynote)**
Single-walled carbon nanotubes in liquids: basic science and applications to processing.

11:15 AM **M. J. Green**, R.C. Armstrong, R. A. Brown
Spinodal decomposition of a rigid-rod system

11:40 AM **G. G. Pereira**, S. K. Pattanayek
Shape instabilities of polyelectrolytes

12:05 PM **B. Abou**, F. Gallet, P. Monceau & N. Pottier
Fluctuation-dissipation relation in a colloidal glass: frequency and aging time dependence

Thursday Afternoon, 6 July 2006

Lunch: 12:30 – 1:30 PM

Linear and Non-Linear Rheology
Chairman: Prof. Gerald Fuller

1:30 PM **F. C. MacKintosh (Keynote)**
Cytoskeletal networks: polymer physics meets cell biology

2:05 PM **B. Grimminger**, Chr. Friedrich
Linear and non-linear viscoelastic properties of fiber networks

2:30 PM **A. Sunarso**, T. Yamamoto
Prediction of shear and elongational properties of polymeric fluids using reversible network with non-interacting dumbbell model

Break: 2:55 – 3:20 PM

Linear and Non-Linear Rheology Contd.

3:20 PM **M. A. K. Williams**, R. R. Vincent, D.N Pinder, Y. Hemar
Micro-rheological studies with multiple particle tracking

3:55 PM **C. Clasen**, R. Ewoldt, W. M. Kulicke, G. H. McKinley
Micro bulk rheology of complex fluids – the non-linear properties of snail mucus

4:20 PM Y. Masubuchi, G. Ianniruberto, F. Greco, **G. Marrucci**
Primitive chain network simulations for branched polymers

4:45 PM   **End**

Friday Morning, 7 July 2006

Linear and Non-Linear Rheology Contd.
Chairman: Prof. Giuseppe Marrucci

8:30 AM **R. G. Larson**, S. J. Park, S., Y. Heo, and Q. Zhou **(Keynote)**
Linear and nonlinear rheology of semi-dilute polymer solutions and melts

9:05 AM F. Xu, **M. M. Denn,** J. D. Schieber
A full-chain stochastic tube model for entangled melts and solutions of linear Polymers

9:30 AM **J. D. Schieber**, R. Khaliullin
A stochastic slip-link model with discrete numbers of Kuhn steps.

9:55 AM **Y. Shnidman**
Dynamic self-consistent field theory of polymer fluids: Beyond singlet-level mean-field, Markovian transport and Wiener walks

Break: 10:20 – 10:40 AM

Linear and Non-Linear Rheology Contd.

10:40 AM **D. Bonn (Keynote)**
Yield stress and thixotropy: on the difficulty of measuring a yield stress in practice

11:15 AM **E. S.G. Shaqfeh**
Ergodicity breaking and glassy dynamics in the stretching flows of single polymer molecules

11:40 AM **T. Sridhar**
Observation of Bulk Stress Hysteresis in the Elongational Flow of a Polymer Solution

12:05 PM **S. Fielding**, P. Olmsted
Complex dynamics in simple models of shear banding.

Lunch: 12:30 – 1:30 PM

Linear and Non-Linear Rheology Contd.
Chairman: Prof. Morton Denn

1:30 PM **A. K. Sood (Keynote)**
Route to rheochaos in nonlinear flow of surfactant gels.

2:05 PM B. M. Marín-Santibáñez, J. Pérez-González, **L. de Vargas,**
F. González, G. Huelsz
Rheo-PIV of shear-thickening wormlike micelles

2:30 PM **L. Russo**, P. Luca Maffettone, S. Crescitelli
Arnold tongues in liquid crystals under a periodic shear flow

Break: 2:55 – 3:20 PM

Linear and Non-Linear Rheology Contd.

3:20 PM **D. Marenduzzo**, A. Dupuis, E. Orlandini, J. M. Yeomans
Rheology of cholesteric blue phases

3:55 PM S. Sukumaran**, Alok K. R. Paul**, S. Ramaswamy, P. R. Nott,
V. Kumaran
Rheology of disordered lamellar phases

4:20 PM **End**

6:30 PM **Discussion**

8:00 PM **Poster Session & Reception**

Saturday Morning, 8 July 2006

Linear and Non-Linear Rheology Contd.
Chairman: Prof. Jay Schieber

8:30 AM **G. H. McKinley (Keynote)**
Extensional rheometry on a chip: flows of dilute polymer solutions in microfluidic geometries

9:05 AM **E. H. Purnomo**, D. van den Ende, F. Mugele, J. Mellema
Rheological properties of aging suspensions

9:30 AM **J. D. Goddard**
A general theory for the viscoplasticity of dry and fluid-saturated granular media

9:55 AM **S. Moon**, S. Sundaresan, I. G. Kevrekidis **(Multiscale Modelling)**
Coarse-grained dynamics of gas-fluidized beds

Break: 10:20 – 10:40 AM

Multiscale Modelling

10:40 AM **M. Kroeger (Keynote)**
Multiscale modeling of simple and polymeric liquids

11:15 AM **E. Boek**, J. Padding
Mesoscale simulation of the flow of complex oilfield fluids: wormlike micelles and asphaltene colloidal suspensions

11:40 AM **A. Dupuis**, P.G. Gonnet, P. Koumoutsakos
Coupling Lattice Boltzmann and Molecular Dynamics models for dense fluids

12:05 PM **Anatoly B. Kolomeisky**
Growth dynamics of cytoskeleton proteins: multiscale theoretical approach

Saturday Afternoon, 8 July 2006

Lunch: 12:30 – 1:30 PM

Multiscale Modelling Contd.
Chairman: Dr. Burkhard Duenweg

1:30 PM V. Venkataramani, A. Koppol, R. Sureshkumar, **B. Khomami (Keynote)**
Dynamics of dilute polymeric solutions: coarse graining strategies and multi-scale flow simulations

2:05 PM **Marek Bher**
Challenges in computational hemodynamics

2:30 PM **A. Braun,** M. Dressler, E. J. Windhab
Extrusion flow of polymer blends with droplet morphology

Break: 2:55 – 3:20 PM

Multiscale Modelling Contd.

3:20 PM **Cecilia Clementi**
Adaptive multiscale modeling of water

3:55 PM **Howard Brenner**
A simple multiscale model of the Soret effect (thermal diffusion) in liquids

4:20 PM **Discussion**

5:05 PM **End**

6:30 PM **Conference Dinner**
 (Bus departs to Artimino from Piazza Delle Carceri)

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5th-8th July, Prato, Italy

ABSTRACTS

THERMODYNAMICS AND COARSE GRAINING

C1 (Keynote)
Experimental demonstrations of new theorems in non-equilibrium thermodynamics

Edith M. Sevick

Research School of Chemistry, The Australian National University

Thermodynamics is the study of the flow of heat between states and its transformation into work. Our understanding of thermodynamics is largely confined to equilibrium states. The field of "nonequilibrium thermodynamics" represents a simple-minded extension of the 19th century concepts of equilibrium thermodynamics to systems that are close to, or near equilibrium. Moreover, these traditional concepts are limited in application to large systems, referred to as the "thermodynamic limit". However, in the last decade, two new theorems have been proposed to revolutionise the field of thermodynamics and its application to modern systems.

These new theorems firstly, lift the restriction of the thermodynamic limit, allowing thermodynamic concepts to be applied to small systems, and secondly, characterise systems that may be far-from-equilibrium. The first of these theorems, the Fluctuation Theorem (FT), generalises the Second Law of Thermodynamics so that it applies to small systems, including those that evolve far from equilibrium. The second, the Work Relation (WR), provides a method of predicting equilibrium free energy di_erences from the experimental trajectories of systems, including those that traverse far from-equilibrium states. Both of these theorems are at odds with a traditional understanding of 19th century thermodynamics where equilibrium is central and the Second Law inviolate. However these theorems are critical to the application of thermodynamic concepts to systems of interest to scientists and engineers in the 21st century. Both theorems, the FT and WR, embody concepts that are not fully explored and are not necessarily accepted amongst scientists; consequently, the practical theorems are not yet widely used. In this talk we will describe the theorems in practitoners' language, along with our optical tweezers experiments that irrefutably demonstrate the theorems.

C2
Mechanical unfolding of proteins: reduction to a single-reaction coordinate unfolding potential, and an application of the Jarzynski relation

D. K. West, E. Paci, P. D. Olmsted

University of Leeds

Single molecule force spectroscopy (AFM, optical tweezers, etc) has revolutionized the study of many biopolymers, including DNA, RNA, and proteins. In this talk I will discuss recent work in the Leeds group on modelling of mechanical unfolding of proteins, as often probed by AFM. I will address the unfolding of protein concatamers, what can be learned from prising apart proteins in different directions, and different ways for coarse-graining the entire energy landscape onto an effective one dimensional unfolding potential. Finally, I will discuss the application of the Jarzynski Relation to extract equilibrium free energies from nonequlibrium unfolding experiments.

C3 (Keynote)
Does statistical mechanics apply to driven steady states of matter?

R. M. L. Evans

University of Leeds

Complex fluids are easily and reproducibly driven into non-equilibrium steady states by the action of shear flow. Such states are as diverse and interesting as equilibrium states,

but are not governed by the same statistics of Boltzmann's law and detailed balance. Under flow, the statistically steady states of, e.g., worm-like micelles are ergodic, and are governed by microscopically reversible laws of motion, as is the case at equilibrium. We can therefore find a non-equilibrium counterpart to the canonical foundations of statistical mechanics, including a principle analogous to detailed balance, with significant consequences for activated processes.

C4

Coarse graining=understanding

Hans Christian Öettinger
ETH Zürich, Department of Materials, Institute of Polymers, HCI H 543
CH-8093 Zürich, Switzerland

Coarse graining is NOT a necessary evil required to solve problems which are computationally too large. Coarse graining rather is the art to simplify to the essentials and hence to provide understanding. Systematic coarse graining procedures are therefore needed, which are the topic of statistical equilibrium and nonequilibrium thermodynamics. This does not sound controversial but it immediately becomes massively so when illustrated for rarefied gases. We show that any coarse graining step should be accompanied by an increase in irreversibility and is potentially accompanied by the same kind of historical confusion that was created by the passage from reversible to irreversible equations.

C5

Convergence of experiment and theory for dilute polymer solutions with successive fine graining

Ravi Prakash Jagadeeshan
Department of Chemical Engineering, Monash University, Australia

The importance of incorporating fluctuating finite extensibility, hydrodynamic interactions and excluded volume effects into molecular theories for dilute polymer solutions, in order to adequately describe their complex behaviour, has become increasingly apparent over the past few years, and a number of different approaches for achieving this objective, all based on using exact Brownian dynamics simulations in the context of bead-spring chain models, have been proposed recently. In addition to making an essentially arbitrary choice of the number of beads in the chain (or the degree of coarse-graining), these approaches also adopt various schemes for determining the values of the parameters associated with the description of these mesoscale phenomena. The method of successive fine graining offers a means of overcoming some of the ambiguities associated with these approaches. In this talk, the validity of this method is demonstrated by comparing predictions with exact bead-rod simulations, and with experimental observations of static and dynamic equilibrium properties, and nonlinear rheological properties.

C6

Coarse-graining of hydrodynamic and excluded volume interactions in polymer chains

R. Prabhakar, E. M. Sevick, D. R. M. Williams
The Australian National University

Conventional bead-spring models of linear polymers incorporating hydrodynamic and/ or excluded volume interactions assume that the coarse-grained polymer segments represented

as springs are essentially isotropic i.e. the beads are always spherical. While this approach works well for static and dynamic properties of long, flexible molecules near equilibrium, in situations where molecules are likely to be stretched out, spherical beads with fixed constant friction and excluded-volume parameters cannot accurately represent interactions between elongated segments. We treat polymer segments as diffuse axissymetric ellipsoids to derive expressions for the configuration-dependent mobility matrix and excluded-volume potential which account for the effects of segmental anisotropy and orientation on inter-segmental interactions. Brownian dynamics simulations' results for static and dynamics properties obtained with coarse representations of flexible and semiflexible chains are compared with results obtained with finer representations using conventional bead-spring chains.

PHASE BEHAVIOUR AND DYNAMICS

P1 (Keynote)
Simulation studies of bulk and surface phase behaviour of polydisperse fluids

Nigel B. Wilding, Peter Sollich, Matteo Buzzacchi

Dept. of Physics, University of Bath, UK

In a polydisperse fluid, the particles exhibit continuous variation in some attribute such as size, shape, charge etc. The phase behavior of polydisperse fluids is considerably richer in both variety and form than that of their monodisperse counterparts. The source of this richness is traceable to fractionation effects: the distribution of the polydisperse attribute in general differs from one coexisting phase to another. In this talk I will first outline principal aspects of the phenomenology of phase separation in polydisperse systems, before proceeding to describe new finite-size scaling strategies for obtaining accurate estimates of coexistence properties from Monte Carlo simulation. I will then detail the results of recent simulation studies of bulk and wetting phase behaviour in prototype model systems. These reveal novel polydispersity-specific features such as a strong sensitivity of coexistence properties to the tail of the particle size distribution, and first order wetting lines which traverse the coexistence region.

P2
Computer simulation of colloidal electrophoresis

Burkhard Duenweg, Vladimir Lobaskin, Krishnan S. H., Christian Holm

Max Planck Institute for Polymer Research, Mainz, Germany

We study the motion of a charged colloidal sphere surrounded by solvent, counterions, and salt ions, under the influence of an external electric field. The ions are modeled as particles which interact dissipatively with a lattice Boltzmann background, such that hydrodynamic interactions are taken into account. Similarly, the colloid is modeled as a spherical array of such point particles. Finite concentration values are taken into account by simulating the system in a box with periodic boundary conditions. In terms of dimensionless reduced parameters, the results compare favorably with experimental data. As a complementary approach, we solve the electrokinetic equations by a finite element method.

P3
Mesoscopic modelling of biocolloidal hydrodynamics

I. Pagonabarraga

[1]Departament de Física Fonamental, Universitat de Barcelona, Carrer Martí i Franqués, 1, 08028 Barcelona (Spain), Email: ipagonabarraga@ub.edu

I will describe how to use well known methods from soft matter to study the dynamics of systems motivated biologically. In particular, I will address the effect of hydrodynamics on the motion of self-propelled particles (a simplified model for swimming microorganisms), emphasyzing their similarities and differences with colloidal suspensions. I will also analyze the role hydrodynamic plays in the dynamics of semiflexible filaments, both passive and active. An idealized model which captures inextensibility (a characteristic feature of biofilaments such as actin or microtubules) will serve to highlight the influence of hydrodynamic interactions in the motion of these systems.

Length scale dependent relaxation in colloidal gels

Emanuela Del Gado* and Walter Kob

Dipartimento di Scienze Fisiche, Universitri di Napoli "Federico II", Italia
Laboratoire de Colloi'des, Verres et Nanomateriaux, Universiti Montpellier II, France

Although gels are ubiquitous in fundamental science, technological applications and also in our daily life, their structural and dynamical properties are not well understood. In contrast to other systems that show a slow relaxation, such as glass-forming liquids, the structure of gels is given by an open network that is thought to be responsible for the unusual dynamical properties of these systems. Apart from the dramatic slowing down of the relaxation dynamics with increasing interaction strength between the particles, one finds a complex dependence of the dynamics on the length scale considered: The relaxation functions are often stretched and/or, most remarkably, compressed, i.e. the time correlators decay faster than an exponential. Due to the large variety of gel-forming systems (colloidal gels, chemical gels, ...) it has so far not been possible to obtain a clear picture on which ones of these phenomena are universal and which ones are specific to just a subclass of these systems. The same is true for their theoretical description since various mechanisms have been proposed to rationalize certain observations from experiments or computer simulations, but so far no unifying picture has emerged yet. We present the results of a recent study based on a simple model that does indeed have the characteristics of (colloidal) gelforming systems at a finite temperature. By means of molecular dynamics computer simulations, we investigate the gel formation from the equilibrium sol phase. At low volume fraction and low T particles are linked by long-living bonds and form an open percolating network. Our results on the structural and dynamical properties [1, 2] shed some light on the mechanism that is responsible for the slow dynamics in these systems. In particular we show that the strong length scale dependence of the dynamics in gel forming systems is tightly related to the formation of the gel structure and is therefore a general feature. This study allows for the first time to investigate on a microscopic level the relaxation processes in the incipient gel and to understand why they must strongly depend on the length scale investigated. In our model the mesh-size of the incipient gel network corresponds to a crossover length between dramatically different relaxation processes, from stretched to compressed exponentials. Moreover our results link the super-exponential relaxation at low temperature to the motion of pieces of the incipient gel structure.

* Corresponding author: delgado@na. infn. it
[1] E. Del Gado and W. Kob, Europhys. Lett. (2005, in press; cond-mat/0507085).
[2] E. Del Gado and W. Kob, cond-mat/0510690.

Correlation of the relations of micellar microstructure of dilute CTAC/counterion systems with counterion chemical structure, counterion/CTAC ratio, drag reduction and rheological behavior

W. Ge[1], E Kesselman[2], Y Talmon[2], and J. L. Zakin[1]

[1]Dept of Chemical & Biomolecular Engineering, Ohio State University Columbus, OH, USA
[2]Dept of Chemical Engineering, Technion-Israel Institute of Technology, Haifa, Israel

Counterion chemical structure and counterion/cationic surfactant ratio control the micelle microstructures, drag reduction effectiveness and rheological behavior of quaternary ammonium surfactant systems. Correlation of physical properties of dilute solutions of CTAC and their microstructures with the chemical structures of four para-halo-benzoate (F, Cl, Br, I) counterions and with different counterion/CTAC ratios will be shown. Microstructures are determined by cryo-TEM imaging. Drag reduction effectiveness is measured over a range of temperatures and Reynolds numbers and, along with micelle microstructures, shear viscosities, dynamic viscosities and N1, will

be related to the chemical structures of the four counterions and their molar ratios to CTAC.

Micelle microstructures of the four systems at low (0.6) and high (4.0) counterion to CTAC ratios will be shown. At 30 C the para-F-benzoate system at ratio 0.6 shows only short threadlike micelle structures, is not drag reducing and has zero N1 At ratio 4.0, the Fluoro system is also not drag reducing and has zero N1 while the Chloro, Bromo and Iodo systems are all drag reducing and have appreciable N1. The Fluoro system also

showed only small zeta potential reductions at all ratios while the other three showed moderate to large decreases in zeta-potential with increase in counterion/CTAC ratio, crossing from positive to negative values at higher ratios. The ratios at the crossing points followed the order of the Hofmeister series: I, Br and Cl. The effects of counterion chemical structure on relaxation times from dynamic viscosity measurements and estimates of counterion binding ratios obtained from NMR measurements will also be shown.

P6 (Keynote)
Interruption of coarsening in binary fluid mixtures

M. E. Cates
University of Edinburgh

I will describe two ways to prevent coarsening in a system of binary fluids en route to macroscopic phase separation: one by adding colloidal particles, and one by steady shearing. Both have been studied in our group using lattice Boltzmann simulations. Inclusion of neutrally wetting colloids in symmetric pair of demixing fluids can jam the interface and arrest the dynamics altogether [1]; I hope to report some new results for off-symmetric cases. For a two dimensional
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binary fluid system (without colloids) undergoing steady shear, we have recently established the first clear numerical evidence of non-equilibrium steady states with finite correlation lengths [2]. Preliminary results for three dimensions may be discussed.

[1] K. Stratford et al, Science, 309, 2198 (2005).
[2] P. Stansell et al, Phys Rev Lett, in press (2006)

P7
Polymers in Two Dimensions: Spanning Solutions, Melts, and Glasses

Gerald G. Fuller
Chemical Engineering, Stanford University, Stanford, CA 94305-5025

Many polymers are amphiphilic and strong attach themselves to fluid/fluid interfaces. Many configurations are possible and the one explored here has the chains adsorbed in a flat configuration, executing a two-dimensional random walk on the surface. This can result in strongly nonlinear interfaces that produce non-Newtonian surface flows and a corresponding complex interfacial rheology. Experiments are offered that demonstrate that such chains produce isotherms that are independent of

molecular weight and that contain a number of conformational and morphological transitions. The first transition has the chains passing from non-overlapping and compressed configurations over to multilayers. This is demonstrated by interfacial rheological measurements coupled with Monte Carlo simulations. The influences of temperature and chemical modification of the chains to systematically vary hydrophobicity are also investigated.

The kinetics of dot formation induced by Marangoni flow in the drying process of polymer solution drop with mixed solvent

Tatsuya Yamaue and Masao Doi
Department of Applied Physics, The University of Tokyo,
Hongo 7-3-1, Bunkyo-ku, Tokyo 113-8656, Japan.

How to control the shape of the solute deposit in the drying process of a polymer solution drop on a substrate is an important problem in the ink-jet printing. In the case of dilute solution, a commonly observed phenomena is the "coffee stain" : the evaporation of solvent induces an outward flow and creates a ring-like deposit after drying. [1] The outward flow is a result of the combined action of the increased evaporation rate at the droplet edge, and contact line pinning caused by solute deposition near the edge.(self-pinning) [2] De Gans et.al. showed that when a polymer solution is dried on a glass slide coated with hydrophobic materials, it leaves a small dot after the evaporation. [3] They observed that the dots have small dimple in the center, the size of which can be changed by solvent. They, however, did not conduct any quantitative study for the phenomena. Here, we studied the shape change, flow and contact line motion in drying process of polystyrene polymer solution drops about $100\mu m$ radius having anisole/etylacetate mixed solvents, whose evaporation rates are quite different, placed on a hydrophobic substrate. The drying process takes place in three stages. First, the droplet evaporates keeping the contact line fixed. Second the droplet shrinks with receding contact line. Finally the contact line pinned again by self-pinning, and the droplet starts to be deformed. When the solvent is pure anisole, the shape of the final polymer deposit changes from concave dot for dilute cases, to flat dot for $5wt\%$ initial density case, and then to concave dot again in dense cases with the increase of the initial polymer concentration. This shape change is caused by the gradual transition from the solute piling mechanism proposed by Deegan et.al. to the crust buckling mechanism proposed by de Gennes and Pauchard. [5] As the mixed ratio of etylacetate increases from pure anisole in the initial density $0.5wt\%$ case, the dimple of the final polymer deposit decreases, and the shape becomes flat, when anisole/etylacetate mixting ratio is about 60/40. This change is considered to be caused by the temperature Marangoni flow induced by high volatile solvent conponent and the density Marangoni flow induced by the difference of surface tensions of mixed solvents. In the other hand, the mixed ratio of etylacetate increases between 60% and 80%, the dimple of the final polymer deposit increases again. This change is considered to be caused by increasing of the outward flow induced by high volatile solvent. When the mixed ratio of etylacetate is about 90%, both a ring-like deposit and a dot-like deposit in it can be observed together. We analyze and simulate the flow of polymer solute in the evaporation process of polymer solution drops using the competetion model of the Marangoni flow and the outward flow, each model is based on Hu-Larson model [6], and the shape change in the evaporation and gelation process after selfpinning using the stress diffusion coupling model of gel dynamics based on the two fluids model of polymer and solvent. [7]

[1] R. D. Deegan, et. al. : Nature **389**, 827 (1997) : Phys. Rev. **E62**, 756 (2000) : Phys. Rev. **E61**, 475 (2000).
[2] M. D. Haw, M. Gillie and W. C. Poon, Langmuir **18**, 1620 (2002).
[3] B. J. de Gans and U. S. Schubert : Langmuir **20**, 7789 (2004).
[4] L. Pauchard, et. al. : Europhys. Lett **62**, 897 (2003) : Phys. Rev. **E68**, 052801 (2003) : Langmuir **20**, 5138 (2004).
[5] T. Kajiya, E. Nishitani,T. Yamaue,M. Doi : Phys. Rev. **E73**, 11601 (2006).
[6] H. Hu and R. G. Larson : Langmuir **21**, 3963 (2005) : Langmuir **21**, 3972 (2005).
[7] T. Yamaue and M. Doi : Phys. Rev. **E70**, 011401 (2004) : J. Chem. Phys.**122** 084703 (2005).

P9

Elastic deformation of non-uniform polymer crusts formed by droplet evaporation

D. A. Head

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Crust formation of an evaporating polymer solution is an important technical process for micron-scale manufacturing processes. For a droplet on a wetting surface, the crust takes a cap-shape that elastically deforms under the osmotic pressure arising from continuing evaporation through the porous solid. A variety of shapes have been observed in experiments, including so-called "craters" and "mexican hats" - however, it is not clear for what parameters (crust thickness, contact angle etc.) each shape arises. We have investigated this phenomenon using quasi-static simulations and have constructed a "phase diagram" of contact angle versus crust thickness to show where each shape arises. Our protocol is pressure-controlled rather than volume-controlled, both to simplify the numerical procedure and to allow us to draw on a significant literature of elastic spherical caps. We have also looked into the effects of non- uniform shell thickness, since the nature of droplet evaporation suggests the crust formed will be thicker near the contact line than the apex. In parallel with these numerical studies, we will also present some approximate theoretical calculations that incorporate non-linear strains. This is crucial, as the various shapes only emerge under non-linear deformation; linear strains always produce qualitatively similar results. Some recent results on symmetry- breaking deformations will also be given

P10 (Keynote)

Single-walled carbon nanotubes in liquids: basic science and applications to processing.

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Single Walled Nanotubes (SWNTs) have remarkable electrical, thermal, and mechanical properties. Neat, well-aligned SWNT fibers and sheets could be the ultimate building blocks of strong, ultra-light multifunctional materials for aerospace applications, and could yield electromechanical actuators and sensors with unprecedented performance. After the achievement of scalable production of SWNTs, the difficulty of processing pristine SWNTs by liquid-phase methods has been the single most important roadblock to manufacturing macroscopic materials composed solely of SWNTs.

Here we show that SWNTs dissolve at high concentration in acids; the SWNTs are stabilized because acids protonate their sidewalls, balancing wall-wall van der Waals forces. Acid strength controls the phase behaviour. At low concentration, SWNTs in acids dissolve as individual tubes which behave as Brownian rods. At higher concentration, SWNTs form a highly unusual nematic liquid phase consisting of spaghetti-like self assembled supermolecular strands of mobile, solvated tubes in equilibrium with a dilute isotropic phase. At even higher concentration, the spaghetti strands self-assemble into a polydomain nematic liquid crystal, where the domains are entangled with each other. Under anhydrous condition, the liquid crystalline phase can be processed into continuous highly aligned fibers of pure SWNTs without the aid of surfactants or polymers. The phase behavior can be controlled by changing the strength of the acid solvent, and can be exploited for separating SWNTs by length. By using a new fluorescent staining technique, we measure the rotational diffusivity and persistence length of SWNTs suspended in water with the aid of surfactants, and show that SWNTs behave as Brownian rods. We apply this understanding of stabilized SWNTs in water to making thin sheets and coatings.

P11

Spinodal decomposition of a rigid-rod system

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The spinodal decomposition of rodlike particles is simulated for a one-dimensional system with both periodic boundaries and hard wall boundaries. The nonhomogeneous Doi equation for the rod distribution function is discretized by the finite element method and integrated forward in time using a parallel, semi-implicit scheme. The simulation uses a discretized form of the full nonhomogeneous Onsager intermolecular potential which models interactions of the rods on the scale of a single rod length. This intermolecular potential makes it possible to characterize nonhomogeneous structures and interfaces in terms of the rod length with no adjustable parameters. The method is applied to isotropic-nematic spinodal decomposition and to the behavior of misaligned nematic grains. The effects of rotational and translational diffusivity ratios are computed, and the mechanisms for alignment and phase separation are analyzed. These results mark the first full computation of the distribution function's evolution for spinodal decomposition in nonhomogeneous rigid-rod systems.

P12

Shape instabilities of polyelectrolytes

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Polyelectrolytes are charged polymers where some fraction, f, of the chain's monomers are charged. This imparts to the polelectrolyte many desirable properties, which make these polymers useful in many industrial applications. In a poor solvent, an (uncharged) polymer will tend to collapse to a spherical globule, so as to minimize polymer-solvent contact. Polyelectrolytes in poor solvents also collapse, but due to charge repulsion along the chain it was originally proposed the collapse would be to a cylindrical globule. Subsequently, it was shown this cylindrical globule is unstable to capillary wave fluctuations and the pearl necklace, consisting of spherical beads joined by long strings of polymer, is the optimal shape. Although this was predicted over a decade ago, direct evidence (i.e, from imaging such as using Atomic Force Microscopy where the polyelectrolyte absorbs on the solid substrate) of the pearl-necklace structure has not been definitive. Thus we theoretically analyze how a substrate can interact with a polyelectrolyte in a poor solvent. We show that the substrate can infact inhibit the shape instability and a new shape – an elliptical globule, becomes stable. The results are validated with three independent theoretical techniques.

P13

Fluctuation-dissipation relation in a colloidal glass: frequency and aging time dependence

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Glassy systems are characterized by slow relaxation processes; they therefore remain far from equilibrium on long time scales. Recently, there have been serious attempts to approach and understand aging phenomena on a theoretical level. Many efforts have been devoted to apply statistical physics description - in particular fluctuation-dissipation relations (FDR) – to such out-of-equilibrium systems. At thermodynamic equilibrium, FDR relate the

response function of the system to its autocorrelation function, involving a single thermodynamic parameter, the equilibrium temperature. However, FDR apply only to ergodic systems at equilibrium, and is not expected to hold in out-of-equilibrium systems. The idea that a timescale dependent nonequilibrium temperature or *effective* temperature could describe the slow relaxation modes has received a lot of attention.

We present an experimental investigation of the Generalized Einstein Relation (GER), a particular form of a fluctuation-dissipation relation, in an out-of-equilibrium complex fluid. Micrometer beads used as thermometers are immersed in an aging colloidal glass to provide both fluctuation and dissipation measurements. At a given aging time of the system, we measure the fluctuating motion of a micrometric tracer bead immersed in the glass, leading to the direct measurement of the mean square displacement of the bead. At the same aging time, we apply an oscillatory or step force on the tracer bead with an optical tweezer, and measure its mobility. From these measurements, the fluctuation-dissipation ratio – also expressed in terms of an *effective* temperature – is derived as a function of frequency and aging time. The deviations from the GER, observed during the glass formation process, suggest that the effective temperature can be directly related to the relaxation times of the glass.

B. Abou & F. Gallet, Phys. Rev. Lett. **93** *160603 (2004)*
N. Pottier, Physica A **317***, 371 (2003)*

LINEAR AND NONLINEAR RHEOLOGY

R1 (Keynote)
Cytoskeletal networks: polymer physics meets cell biology

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Networks of filamentous proteins play a crucial role in cell mechanics. These *cytoskeletal* networks, together with various crosslinking and other associated proteins largely determine the (visco)elastic response of cells. Cytoskeletal biopolymers have also provided new insights into basic aspects of polymer physics. In contrast to common flexible polymer materials, the response of these networks is highly non-linear, and their rheological properties can be tuned with small changes in density or local network connectivity. In the cell, these systems are also out of equilibrium in a way unique to biology: their rheological properties can reflect internal active force generation by molecular motors. We discuss recent theoretical and experimental efforts to understand these essential materials of the cell.

R2
Linear and non-linear viscoelastic properties of fiber networks

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The molecular dispersion of carbon nanotubes (CNTs) in matrices is of crucial importance for the beneficial combination of CNTs superior properties with that of matrix fluids. Therefore, we dealt with methods enabling the molecular dispersion of CNTs in low molecular weight fluids and the characterization of dispersions properties.

We found that CNTs are very well dispersed in ionic liquids such as 1-butyl 3-methyl imidazolium tetrafuoroborate (BMIBF$_4$) together with cosolvents and surfactants. Already for concentrations higher than 0.01 wt.%, the rheological response of these compounds resembles that of isotropic fiber networks. These networks were characterized morphologically by TEM and rheologically by mechanical spectroscopy in the linear and non-linear deformation ranges.

Using models developed for semi flexible biopolymer networks we can understand the obtained results quantitatively. In contrast to actin-networks, the CNT-networks display rather energetic elasticity than entropic. We discuss the reasons for this peculiarity.

R3
Prediction of shear and elongational properties of polymeric fluids using reversible network with non-interacting dumbbell model

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Recently, reversible network with non-interacting dumbbell model has been proposed by Cifre et al. (J. Non-Newtonian Fluid Mech. 113 (2003) 73-96) to model the shear viscosity of associative polymer. It has been shown that this model is capable to predict the main features of associative polymer, such as the presence of Newtonian plateau at low shear rates followed by shear thickening at moderate shear rates and shear thinning at high shear rates. Although this model was initially derived for associative polymer, the basic

concept of association and disassociation of network junctions can also be applied to model non-associative polymers such polymer solutions and melts in general. To use the model in the simulation of flow of polymeric fluids in complex channel, the prediction capability of the model should be further investigated. In the present work, we perform a Brownian dynamics simulation based on the work of Cifre et al. to investigate the capability of the reversible network with non-interacting dumbbell model in predicting the shear and elogation properties of polymer solutions and melts. In order to obtain more realistic prediction of elongational properties, we use a FENE connector force instead of a Hookean connector force. By adjusting the parameters controlling the association process of the dumbbells to the networks, we obtain the correct trend in prediction of rheological properties. If the association rate is proportional to the dumbbell length, the model predicts the presence of shear thickening which is typical for associative polymer, otherwise, with a constant association rate, the model predicts only shear thinning behavior (without shear thickening), which is typical for polymer solutions and melts. In the elongational flow, the increasing association rate results in elongational viscosity which is characterized by strain thickening at moderate strain rates followed strain thinning and the second strain thickening at high strain rates. For the constant association rate, there is no second strain thickening region, and the maximum extension parameter governs whether the strain thinning region at high strain rates exists or not exist. The trend in elongational viscosity in the case of constant shear rate is in agreement with the available experimental data of elongation viscosity of polymer solutions and melts.

R4
Micro-rheological studies with multiple particle tracking

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It is well known that a plethora of biologically relevant soft materials exhibit heterogeneous hierarchical architectures, that arise naturally from the propensity of constituent biopolymers to self-assemble and aggregate[1]. Thus, understanding how to probe the viscoelastic properties of such systems is expected to have wide relevance, both from the fundamental and the industrial view-points.

We describe micro-rheological measurements[2] carried out with multiple particle tracking (MPT) on a series of model biological systems of increasing structural and temporal complexity. We start with purely viscous media, progress to entangled polymeric solutions, gels, and ultimately systems with designed heterogeneous microstructures that exhibit a spatial distribution of mechanical properties. At each stage of the study we compare our MPT results with those obtained by additional passive micro-rheological experiments carried out using diffusing wave spectroscopy and those obtained using a conventional rheometer. Carefully consideration is given to the comparison of the results obtained by the different techniques.

References
[1] Hemar, Y. and Pinder D.N. DWS microrheology of a linear polysaccharide. (in Press) Biomacromolecules.

[2] Waigh, T.A., Microrheology of complex fluids, Reports on progress in physics, 68 (3), 685, (2005).

Micro bulk rheology of complex fluids – the non-linear Properties of snail mucus

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Investigating the material properties of biological liquids often hinges on the ability of measuring the viscoelastic properties of very small quantities of the fluid on length scales relevant to their actual application in nature. A number of techniques have been developed for measuring the microrheological response of l samples of complex fluids by probing the local *linear* response of the system via particulate probes or AFM techniques. In contrast, in this paper we present bulk rheological investigations of minute amounts of fluid under both linear and nonlinear deformation conditions.

Utilizing a flexure-based microgap rheometer (FMR) we measure the rheological properties of slug and snail pedal mucus for film thicknesses of 20-40 micrometer that are representative of the natural slime carpet employed by the snails for locomotion. The complex physically-crosslinked structure of the aqueous mucin gel that is secreted during locomotion results in an effective yield stress, which allows part of the snail foot to glide forward over a viscous fluid region while the remaining portions remain elastically-attached to the substrate in a yielded state. The time and strain-dependent structural changes of these complex mucus gels are presented in the form of Pipkin diagrams which constitute a readily-accessible 'fingerprint' of the viscoelastic properties of the slime carpet for a specified deformation history.

Primitive chain network simulations for branched polymers

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We present simulations of branched polymer dynamics based on a sliplink network model, which also accounts for topological change around branch points. It is well known that, with the exception of stars, branched polymers may show a peculiar rheological behavior due to the exceptionally slow relaxation of the backbone chains bridging branch points. Though Brownian simulations based on sliplinks are a powerful tool to study motion of polymers and to predict rheological properties, relaxation of the bridge chains in multibranched structures remains an open problem, due to lack of a definite rule for network topology rearrangement around branch points. We here introduce a branch point mobility rule into our primitive chain network model. For both star and H-shaped polymers, diffusion was simulated both with and without the new rule, and the linear relaxation modulus was determined.

Linear and nonlinear rheology of semi-dilute polymer solutions and melts

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Molecular rheological theories based on the tube model have, for the most part, only been able to predict successfully the nonlinear rheological properties of *well entangled*

polymers. For semi-dilute solutions that may not be well enough entangled for the tube model to apply, the concept of a renormalized monomer called a "blob" provides a basis for universal rheological scaling behavior, with the concentration parameter c/c_e replacing the normalized molecular weight M/M_e as the index of the degree of entanglement. Raspaud et al. (1995) have confirmed the prediction of the "blob" theory that there is scaling law $\eta_p/\eta_{Rouse} \approx (c/c_e)^{2.4/(3v-1)}$ for polymer solutions at concentrations ranging from well entangled to below the onset for entanglement, with v the excluded volume exponent (whose value for good solvents is 0.589), $\eta_{p,0} = \eta_0 - \eta_s$ is the polymer contribution to the zero shear viscosity with η_0 the zero-shear viscosity of the solution and η_s the solvent viscosity; η_{Rouse} is the hypothetical Rouse polymer viscosity. We here describe vastly extended scaling laws based on a "Rouse relaxation time" $\tau_{Rouse} = (\eta_s/k_B T)R_g^3(c/c^*)^{(2-3v)/(3v-1)}$ that predicts that all frequency dependent moduli for semi-dilute solutions should fall onto master curves at each value of c/c_e when plotted against frequency times the Rouse time. Similarly, nonlinear rheological data should also collapse onto master curves. We tested these predictions using carefully chosen polystyrene, polybutadiene, and other solutions in the linear viscoelastic regime, and to a limited extent in the nonlinear regime, and find that general agreement with the predictions of the scaling laws of the "blob" theory. In principle, the scaling laws should also encompass the melt state, once a proper definition of the Rouse time is settled. Our findings also carry implications for the value of the "dilution exponent" α relating entanglement density to concentration. Finally, we present recent results from the pearl necklace model for weakly and modestly entangled polymer melts that bear on the formation of the entanglement "tube," the dilution exponent, and mechanisms of relaxation in entangled polymers.

Raspaud, E., D. Lairez, and M. Adam, Macromolecules 28, 927-933 (1995).

R8

A full-chain stochastic tube model for entangled melts and solutions of linear Polymers

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We describe a full-chain stochastic tube model for entangled melts and solutions of linear polymers. The model incorporates two forces that result from chain confinement: a tensile force along the chain that prevents chain collapse and a transverse force that keeps the chain within the virtual tube. The model tracks conjugate constraint pairs and utilizes a consistent approach to constraint renewal. Chain loops within the tube are permitted. There is good agreement with published transient and steady-state data on two entangled polystyrene solutions with a single time-scaling adjustable parameter.

R9

A stochastic slip-link model with discrete numbers of Kuhn steps.

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Doi and Edwards originally used a slip-link picture to justify a certain stress tensor expression in their tube model. We have instead been using the slip-link picture to

derive all dynamics and stresses in a thermodynamically consistent way. Key to this novel development is the use of monomer density between entanglements as a stochastic variable. The resulting model contains only a single phenomenological parameter (a time constant), which is determined by linear viscoelastic experiments (or possibly by molecular dynamics). All nonlinear flow dynamics are then explained without adjusting parameters. This approach offers a way to model systems that have been modeled by separate equations, to date. So far, theoretical predictions for linear chains in a melt have shown an ability to make accurate, quantitative predictions of transient and steady shear flows, and of steady elongational flows. However, a description of transient elongational melt, and steady elongational solution predictions are off. Here we examine assumptions in our stochastic model by considering a more fundamental description of dynamics, which avoids arbitrary assumptions about the dynamics at the ends of the chains. We can then use this more-fundamental model to re̎examine elongational flows, and to study star-branched relaxation dynamics. We argue that slip-links offer a way to unify the description of linear and branched liquids, and lightly cross-linked elastomers.

R10

Dynamic self-consistent field theory of polymer fluids: Beyond singlet-level mean-field, Markovian transport and Wiener walks

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The author's group has recently developed a dynamic self-consistent field (DSCF) theory on a lattice [M. Mihajlovic, T. S. Lo and Y. Shnidman, Phys. Rev. E **72**, 041801 (2005)] for modeling the time evolution of composition, mass and momentum densities, and of chain conformation statistics in inhomogeneous polymer fluids under shear. It assumed a singlet-level dynamic mean-field approximation, a Markovian model for diffusive and viscous transport, and an anisotropic Wiener random walk for generating chain conformation in a self-consistent potential relating anisotropic stepping probabilities to the gradient of the velocity by means of an elastic dumbbell model. The theory above was applied to unentangled polymer blends that are sheared in a planar channel, and compared with a molecular dynamics study of the same systems [T. S. Lo *et al.*, Phys. Rev. E **72**, 040801(R) (2005).]. We will discuss a reformulation of the DSCF theory to make it applicable to entangled polymer fluids under shear, incorporating (a) non-Markovian mean field time evolution of occupancy probabilities for oriented pairs of adjacent sites coupled to the gradient of the velocity, and (b) a stochastic process generating chain conformation statistics that transcends the anisotropic Wiener random walk in a singlet-level self-consistent potential.

R11 (Keynote)

Yield stress and thixotropy: on the difficulty of measuring a yield stress in practice

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The yield stress of many yield stress fluids has turned out to be difficult to determine experimentally. This has led to various discussions in the literature about those experimental difficulties, and the usefulness and pertinence of the concept of yield stress fluids. I will argue that most of the difficulties disappear when taking the thixotropy of yield stress fluids into account, and will demonstrate an experimental protocol that allows to obtain reproducible results on the critical stress necessary for flow of these fluids. As a bonus, I will show that the interplay of yield stress and thixotropy allows one to account for the ubiquitous localization of shear in these materials. The price to pay, however, is high:

due to the thixotropy the yield stress is no longer a material property, since it depends on the (shear) history of the sample.

R12

Ergodicity breaking and glassy dynamics in the stretching flows of single polymer molecules

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DeGennes 1974 described in his seminal paper the possibility that near the well-known coil-stretch transition of polymers in extensional flows, there could exist two kinetically separated or "glassy" dynamic states simultaneously at the same applied extension rate. The simultaneously existing coiled and stretched states were postulated as a product of intramolecular hydrodynamic interactions along the chain backbone. Since this original work, many researchers have weighed in on DeGennes' theory with no clear consensus and much debate. Thirty years after DeGennes' original publication, Schroeder et al. 2003 presented the first clear, unambiguous experimental evidence that conformational hysteresis existed by examining the dynamics of single molecule, genomic length E Coli DNA. Moreover, theoretically, it was demonstrated by Schroeder et al. 2004 that these kinetically separated states were separated by an effective activation energy that could be hundreds of kT.

In this talk, the findings of Schroeder, Babcock, Shaqfeh and Chu 2003, 2004 will be reviewed from the point-of-view of a conformational Kramers' rate theory. Moreover, we will demonstrate that the presence of "glassy" or "kinetically separated" conformational states is far more general than

originally thought, if one considers nonlocal or nonlinear flows i.e. flows which vary along a molecule's length. These flows have application in microfluidics. We will take two examples in detail and demonstrate that an effective Arrhenius expression for the rate of hopping from coiled to stretched polymer states describe the results of large scale computer simulation quantitatively. Furthermore, we demonstrate that the activation energy in these Arrhenius expressions becomes infinite in the thermodynamic limit of $N_k \rightarrow \infty$ where N_k is the Kuhn step number and therefore ergodicity is broken. Thus the idea of glassy dynamic states must be included in any description of the rheology of this class of flows even for isolated chains. Finally, we will extend these ideas to consider "mixed" flows where there is significant vorticity in the flow. We will demonstrate that the addition of vorticity modifies these theories primarily in changing the size of the fluctuations in the polymer length, thus providing a source of convective fluctuations. Thus vorticity, in an otherwise extension dominant flow, can increase the "hopping" rate between the conformational states in a manner that can be understood using advective (Taylor) dispersion theory.

R13

Observation of Bulk Stress Hysteresis in the Elongational Flow of a Polymer Solution

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Nearly all currently popular models in polymer rheology assume that the steady state stress in a polymer solution is uniquely determined by the rate of deformation to which the solution is subjected. Yet in a seminal paper in 1974, de

Gennes proposed arguments to suggest that in fact, under certain circumstances, the time history of deformation experienced by the solution might have a crucial bearing on the steady state value of stress attained for a given

deformation rate. The importance of de Gennes contention has paradigm changing implications for the modelling of polymer rheology, as was recognized at about the same time by Tanner. The accurate estimation of the relationship between stress and strain in a solution lies at the heart of being able to develop a realistic description of the flow of polymer solutions. The microfluidics of biopolymer solutions is just one example of a number of current contexts in which such a description is crucial for efficient design. Serious early doubts, however, about the theoretical validity of de Gennes arguments, and the absence until recently of any supporting experimental evidence, has implied that the need for a fundamental change in the modeling of polymer solution rheology has not been widely recognized so far.

In ground breaking experiments on ultra-dilute solutions of DNA molecules subjected to planar elongational flow, Shaqfeh and coworkers have shown recently that even though solutions experience identical rates of deformation, individual DNA molecules can have widely disparate conformational states—either coiled or highly stretched—depending on the time history of the solutions's deformation. Since the stress in a polymer solution has its origin predominantly in the entropic resistance of individual polymer molecules to deformation from their equilibrium coiled state, the Stanford groups results clearly validate De Gennes hypothesis (albeit indirectly) of different deformation histories leading to disparate states of stress.

The design of the flow cell used in the Stanford experiments, while being ideal for the observation of single molecules for extended periods of time, does not currently enable the simultaneous measurement of fluid stresses. Additionally, the existence of disparate conformational states has only been demonstrated unambiguously so far for the particular case of E-Coli DNA in a sucrose-water solution.

In this paper, we report the measurement of bulk stresses in a synthetic polymer solution undergoing uni-axial elongational flow, with appreciably different magnitudes at identical values of strain rate, depending on the time history of the solution's deformation. This demonstration has been achieved by exploiting the simple fact that though under certain circumstances the steady state stress in a solution can be a multi-valued function of the strain rate, and consequently exhibit hysteretic behaviour, the strain rate is a single valued function of stress—under all circumstances. The experimental challenge of generating a uniform elongational flow field in which a desired value of stress can be achieved and maintained constant, while carrying out measurements of the resultant strain rate, has been met by successfully extending the domain of operation of the filament stretching rheometer from its usual constant strain rate mode to a constant stress mode. Computer simulations carried out to mirror the constant stress experiments are shown to reproduce the experimental observations, and indicate as conjectured originally by de Gennes that the origin of the
deformation history dependence of stress lies in the conformation dependence of hydrodynamic forces.

R14

Complex dynamics in simple models of shear banding.

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Complex fluids commonly undergo flow instabilities and flow-induced transitions that result in spatially heterogeneous "shear banded" states. Often, these banded states display oscillatory or chaotic dynamics, measured in the bulk rheological signals and in the motion of the interface between the bands. Until recently, however, theory considered a steady state comprising stationary bands separated by a flat interface. We therefore discuss recent theoretical progress in capturing complex dynamics of the banded state: first in a model in which the interface remains flat but moves in a chaotic way; second in a model that explicitly allows for undulations along the interface.

R15 (Keynote)
Route to rheochaos in nonlinear flow of furfactant gels.

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The nonlinear flow behaviour of a viscoelastic gel formed due to entangled cylindrical worm-like micelles of the surfactant CTAT shows rheochaos [1, 2]: for a suitable range of concentrations and temperatures, the stress vs shear-rate curve shows a plateau signaling a rheological phase coexistence and, in the plateau region, the time series of the shear and normal stresses at constant shear rate show deterministic chaos. Recently [3] we have shown experimentally that the route to chaos is via intermittency in the CTAT gels where the strength of flow-concentration coupling is tuned by the additional of salt. A Poincare first return map of the time series and the probability distribution of laminar lengths between burst events shows that our data is consistent with type-II intermittency. The coupling of flow to concentration fluctuations is evidenced by the "Butterfly" intensity pattern in Small Angle Light Scattering (SALS) measurements performed simultaneously with the rheological measurements.

The scattered depolarised intensity in SALS, sensitive to orientational order fluctuations, shows the same time-dependence (like intermittency) as that of shear stress. We will also present our recent experiments when shear stress is kept constant. Attempts to understand rheochaos in our theoretical model will also be presented [4,5].

[1] R. Bandyopadhyay, G. Basappa, and A. K. Sood, Phys. Rev. Lett. 84, 2022 (2000).
[2] R. Bandyopadhyay and A. K. Sood, Europhys. Lett. 56, 447 (2001).
[3] R. Ganapathy and A. K. Sood, Intermittency route to rheochaos in wormlike micelles with flow-concentration coupling, To appear in Phys. Rev. Lett. (2006).
[4] B. Chakrabarti, M. Das, C. Dasgupta, S. Ramaswamy and A. K. Sood, Spatiotemporal rheochaos in nematic hydrodynamics, Phys. Rev. Lett. 92, 55501-1 (2004).
[5] M. Das, B. Chakrabarti, S. Ramaswamy and A. K. Sood, Routes to spatio-temporal chaos in the rheology of nematogenic fluids, Phys.Rev.E 71, 021707(2005).

R16
Rheo-PIV of shear-thickening wormlike micelles

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The shear thickening behavior of an equimolar semidilute aqueous solution of 40 mMol/l cetylpyridinium chloride and sodium salicylate was studied in this work by using a combined method of rheometry and particle image velocimetry (PIV). Experiments were conducted at 27.5 °C with Couette, vane-bob, and capillary rheometers in order to explore a wide shear stress range, as well as the effect of boundary conditions and time of flow on the creation and destruction of shear induced structures (SIS). The use of the combined method of capillary rheometry with PIV allowed the detection of fast spatial and temporal variations in the flow kinematics,

which are related to the shear thickening behavior and the dynamics of the SIS, but are not distinguished by pure rheometry. A rich in details flow curve was found for this solution, which includes five different regimes. Namely, at very low shear rates a Newtonian behavior was found, followed by a shear thinning one in the second regime. In the third, shear banding was observed, which served as a precursor of the SIS and shear thickening. The fourth and fifth regimes in the flow curve were separated by a spurt-like behavior, and they clearly evidenced the existence of shear thickening accompanied by stick-slip oscillations at the wall of the rheometer, which subsequently

produced variations in the shear rate under shear stress controlled flow. Such a stick-slip phenomenon prevailed up to the highest shear stresses used in this work, and was reflected in asymmetric velocity profiles with spatial and temporal variations linked to the dynamics of creation and breakage of the SIS. Increasing the residence time of the fluid in the flow system enhanced the shear thickening behavior.

R17

Arnold tongues in liquid crystals under a periodic shear flow

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It is well known that polymers in liquid crystalline nematic phase exhibit a complex rheological behavior. Under steady shear flow and in homogeneous conditions, theoretically and experimental studies have proved the existence of a variety of periodic regimes as well as aperiodic behaviour. In particular, periodic regimes have been predicted both with mesoscopic models for the second moments of the orientation distribution and with continuous kinetic models based on a Smoluchowski equation.

In this work we study the influence of a parallel sinusoidal field superimposed on top of steady shear. The mesoscopic model adopted to describe the liquid crystalline nematic phase of finite aspect-ratio rodlike molecules is based on a quadratic closure capable of reproducing the complex dynamics predicted by the kinetic theory. The analysis is performed through bifurcation analysis applying a parameter continuation technique to the Poincarè map of the system. When the unforced system is in a periodic regime, the interaction of the forcing frequency with the natural one gives rise the frequency locking phenomena. We delimited parameter regions (Arnol'd tongues) in the plane of forcing parameters (amplitude and frequency) where periodic frequency locked regimes can been found. Finally we discuss how periodic shear flow experiments can be performed to give more insights on the dynamics of the liquid crystals under steady state shear flow.

R18

Rheology of cholesteric blue phases

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Blue phases of cholesteric liquid crystals offer a spectacular example of aturally occurring disclination line network. Here we use a lattice Boltzmann algorithm to investigate the response of three types of blue phases to an imposed Poiseuille flow. Our algorithm solves the Beris- Edwards equations of motion, which comprise an equation for the order parameter evolution and the Navier-Stokes equation. Our simulations show that the disclination network and director field configuration couple together to yield a very rich phenomenology as far as the rheological properties of the system are concerned. We show that shear forces bend and twist and can unzip the disclination lines. Under gentle forcing the network opposes the flow and the apparent viscosity is significantly higher than that of an isotropic liquid. In this regime we also observe a mild shear thickening regime, whose magnitude depends on the topology of the blue phase under consideration. With increased forcing we find strong shear thinning corresponding to the disruption of the defect network. As the viscosity starts to drop, the imposed flow sets the network into motion. Disclinations breakup

and re-form with their neighbours in the flow direction. This gives rise to oscillations in the time-dependent measurement of the average stress. We compare our results with experimental observations on the rheological properties of blue phases and of disclination line networks in colloidal intrusions in cholesteric liquid crystals.

R19

Rheology of disordered lamellar phases

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We explain the rheological properties of disordered smectics using a theory of polydomain smectics and with lattice Boltzmann (LB) simulations of oscillatory rheological experiments. A proper averaging of the smectic stress field has two contributions: the first from assuming a constant stress field and the second, from a constant strain field. This computation of the complex dynamical modulus yields a zero frequency elastic shear modulus G0 and also !1/2 behavior at intermediate frequencies. The LB simulations indicate the plateau regime with a constant elastic modulus. Interestingly, a fourth regime due to smectic permeation is shown to exist at frequencies less than a critical frequency.

R20 (Keynote)

Extensional rheometry on a chip: flows of dilute polymer solutions in microfluidic geometries

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Applications as diverse as DNA separation and ink-jet printing involve microfluidic geometries which generate strong elongational flows of dilute polymer solutions. In this work, we investigate the non-Newtonian flow of dilute aqueous polyethylene oxide (PEO) solutions through microfabricated planar abrupt contraction-expansions. The contraction geometries are fabricated from a high-resolution chrome mask and cross-linked PDMS gels using the tools of soft-lithography. The small length scales and high deformation rates near the contraction plane lead to significant extensional flow effects even with dilute polymer solutions having time constants on the order of milliseconds. Conventional rheological characterization of such fluids even in simple homogeneous flows is challenging because of the need to generate large deformation rates; under such conditions the low levels of viscoelasticity can easily be swamped by inertial effects. To determine the relaxation time we therefore use capillary break-up rheometry and high-speed video imaging. The measured viscometric properties can then be used to quantify the dynamics of the extensional flows arising in microfluidic devices such as planar contractions. Our ultimate goal is to construct a microfluidic-based extensional rheometer on-a-chip. Measurements show that the dimensionless extra pressure drop associated with non-Newtonian flow across the contraction plane increases by more than 200% and is accompanied by significant upstream vortex growth. Streak photography and video-microscopy using epifluorescent particles shows that the flow ultimately becomes unstable and three-dimensional. The moderate Reynolds numbers ($0.03 \leq Re \leq 44$) associated with these high Deborah number ($0 \leq De \leq 600$) microfluidic flows results in the exploration of new regions of the Re-De parameter space in which the effects of both elasticity and inertia can be observed. Understanding such interactions will be increasingly important in microfluidic applications involving complex fluids and can best be interpreted in terms of the Elasticity number, $El = De/Re$.

Rheological properties of aging suspensions

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The slow dynamics of soft glassy materials have attracted quite some attention in the last decades and have been found in amorphous polymers, spin glasses, foams, densely packed suspensions, and living cells. Aging of the materials is one of the consequences of the slow dynamics: the relaxation processes slow down with the age of the material but it never achieves an equilibrium state.

We have examined the linear viscoelastic behavior of poly-N-isopropylacrylamide (PNIPAM) microgel suspensions in order to obtain insight in the aging processes in these densily packed suspensions. The viscoelastic moduli are compared to the prediction of the soft glassy rheology model of Sollich *et al.* [1]. The model predicts *quantitavely* the loss modulus $G''(\omega,t)$, the elastic modulus $G'(\omega,t)$, and their ratio $G''(\omega,t)/G'(\omega,t)$. The relative noise-temperature (x/x_g) of the PNIPAM suspension obtained from the analysis is smaller at lower temperature, when the microgel particles are more swollen, indicating a lower mobility of the microgel particles in a denser suspension.

[1] P. Sollich: *Rheological constitutive equation for a model of soft glassy materials. Phys. Rev. E 58, 738-759 (1998).*

A general theory for the viscoplasticity of dry and fluid-saturated granular media

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This paper revisits the "purely dissipative" model proposed several years ago [1] as a general continuum model for the history-dependent viscoplasticity of non-colloidal particle dispersions. Essential to the model is a positive-definite fourth-rank viscosity tensor _ depending on the history of deformation. In the reduced form considered here, _ is an isotropic function of a history-dependent 2nd-rank "texture" or "fabric" tensor A, which gives stress as a tensor-valued function of fabric and strain-rate tensors. This paper considers several special cases appropriate to systems ranging from Stokesian suspensions to dry granular media. For Stokesian suspensions, a formula for _(A) given by the analogous theory of linear elasticity, together with a corotational memory integral for A, provides a compelling model of transient viscosity and normal stresss evolution in simple shear [5, 3]. However, one extremely rapid mode of relaxation is required to mimic the incomplete reversal of stress on abrupt reversal of shearing. This suggests that nonhydrodynamic effects are implicated, and it establishes a kinship to liquid-saturated granular media with sustained particle contact. In the case of granular media, the isotropic version of the above model reduces to the Reiner-Rivlin form proposed previously [2], which encompasses a quasi-linear model proposed recently for dense rapid granular flow [4]. Since isotropic models cannot represent the effect of flow-induced anisotropy on yield surfaces and viscometric normal stresses, attention is given here to a more general forms, involving nonlinear dependence on both fabric and strain rate. Two important time scales are highlighted, a grain-inertia time scale for dry granular media [2, 4], and a viscous-frictional time scale that appears to be implicated in recent experiments on completely saturated granular media.

References
[1] J. D. Goddard. *Dissipative materials as models of thixotropy and plasticity. Journal of Non-Newtonian*

Fluid Mechanics, 14:141–60, 1984.

[2] J. D. Goddard. Dissipative materials as constitutive models for granular materials. Acta Mechanica, 63:3–13, 1996.

[3] J.D. Goddard. A dissipative anisotropic fluid model for non-colloidal particle dispersions. submitted for publication, 2005.

[4] P. Jop, Y. Forterre, and O. Pouliquen. Crucial role of sidewalls in granular surface flows: consequences for the rheology. Journal of Fluid Mechanics, 541:167–92, 2005.

[5] V. G. Kolli, E. J. Pollauf, and F. Gadala-Maria. Transient normal stress response in a concentrated suspension of spherical particles. Journal of Rheology, 46:321–34, 2002.

MULTISCALE MODELLING

M1

Coarse-grained dynamics of gas-fluidized beds

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Particulate flows involving granular materials, powders, and gas-particle mixtures are widespread in nature and industry. Although kinetic theory-based continuum models for rapid granular flows (of large particles) have been developed in the literature, these models have not been tested against flows where the particle assemblies undergo rapid compaction or dilation; most gas-particle flows occurring in industrial practice do manifest such inhomogeneities.

There are also a number of particulate systems, involving fine particles, where cohesive forces become important, and for which continuum models are simply unavailable; either validated continuum models or "equation-free" multiscale computational schemes, which do not require explicit closures are needed to analyze large scale flows involving such particles.

We describe in this paper a computational study of model problems addressing both of these issues. We model gas-fluidized beds of grains and powders using a hybrid approach by combining dissipative particle dynamics with volume-averaged gas hydrodynamics.

First, we simulate planar traveling waves in gas-fluidized beds and by ensemble averaging the data in a co-traveling frame we determine variables that typically appear in continuum models for gas-particle mixtures. These results are then used to interrogate the adequacy of constitutive models for the stresses in the granular phase which are commonly used in the literature. We find that the particle phase stresses exhibit pronounced compaction/dilation rate dependence, which is not captured by the commonly used constitutive models.

Second, we study the mixing/de-mixing phenomena in fluidized beds of binary mixtures, using descriptions at different levels of coarse-graining. The coarse-grained dynamics of this "model" problem are explored without explicit derivation of the corresponding governing equations, following an "equation-free" multiscale computational approach. Through this example, we demonstrate how such a multiscale approach can be applied to gas-particle flow problems for which reasonable continuum models are unavailable.

M2 (Keynote)

Multiscale modeling of simple and polymeric liquids

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A) I will offer an introduction to the so-called beyond-equilibrium molecular dynamics method which requires and recognizes a separation of time scales. The method is of particular use for the study of nonequilibrium molecular dynamics subject to weak external fields, a regime usually difficult to access using brute-force simulation approaches.

B) A method similar in spirit, the so called quasi equilibrium approximation, will be used to obtain 'macroscopic' equations for the theoretical description of ferrofluids and liquid crystals starting from a 'mesoscopic' description. For these systems,

we also discuss on how closure relationships with correct tensorial symmetry lead to closed nonlinear equations for the orientation tensor, and offer a nonequilibrium phase diagram.

C) As long as there will be no overlap with the presentations by Vlasis Mavrantzas or Ronald G. Larson, I will report on recent developments in the identification and analysis of 'tubes' from atomistic and mesoscopic simulations of polymer melts.

D) Eventually, I may present some recent modifications of the smooth particle dynamics method to incorporate viscoelasticity by treating the stress tensor as a dynamical variable.

Mesoscale simulation of the flow of complex oilfield fluids: wormlike micelles and asphaltene colloidal suspensions

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We have developed mesoscopic simulation models to calculate the flow of complex oilfield fluids. These include 1) the rheology of wormlike micellar fluids and 2) the aggregation and deposition of asphaltene colloidal suspensions in capillary flow. First, we develop a multi-scale simulation model for the rheology of wormlike micelles, This model can be used to predict the shear rheology and normal stress differences, particularly at high shear rates [1]. Such a model gives valuable insight, particularly because the available rheological equations of state [2] are incomplete with respect to extensional rheology [3] and predict the wrong behaviour for normal stress differences. The aim of the model is to understand the link between mechanical properties of the wormlike micelle on the one hand, and the dynamics and rheology of a solution of entangled wormlike micelles on the other hand. A mesoscopic approach is necessary because it is impossible to reach large enough length and time scales using atomistic simulation methods. The simulation method is based on Brownian Dynamics (BD) of coarse-grained pieces of wormlike micelle. To guarantee the predictive power of the BD simulations, the mesoscopic interaction parameters are derived as much as possible from the results of Molecular Dynamics (MD) simulations. We calculate the mechanical properties of a small segment of a wormlike micelle, including the persistence length and elastic modulus, from MD simulations. Then we use these properties in the mesoscopic BD simulation, where the smallest unit is the persistence length. In the BD simulation, the ends of wormlike micelles can approach each other and, if a certain activation barrier is overcome, fuse together. The specific kinetics with which this happens can be investigated for different scission energies, activation barriers and environment parameters such as temperature, concentration and deformation rates. Entanglements are very important for the rheology of a solution of concentrated wormlike micelles. Entanglements emerge naturally whenever a wormlike micelle tries to cross another. By means of the TWENTANGLEMENT algorithm, originally developed for polymer melt simulations, these crossings are monitored and entanglement points are inserted whenever a crossing is imminent. Preliminary results are very encouraging. For example, the predicted shear thinning of EHAC surfactants is in good agreement with experimental results. Second, we study the aggregation and deposition of asphaltene colloids in capillary flow. The deposition of asphaltene solids in oil pipe lines and reservoir rock is poorly understood and hard to study experimentally. Therefore we have developed a mesoscopic simulation model, using the Stochastic Rotation Dynamics techniques. We study the aggregation and deposition of asphaltene colloids in capillary flow, as a function of flow rate and interaction potential between colloid and the walls. We find that the colloidal aggregates and deposits break up with increasing flow rate. Also we observe an decrease of the permeability with increasing depth of the interaction potential well.

[1] J.T. Padding, E.S. Boek and W.J. Briels, ``Rheology of wormlike micellar fluids from Brownian and Molecular Dynamics simulations'', J. Phys.: Condens. Matter 17, S3347S3353 (2005).
[2] O.Manero, F.Bautista, J.F.A.Soltero and J.E.Puig, J. Non Newton. Fluid Mech. 106, 1-15 (2002).
[3] E.S. Boek, J.T. Padding, V. Anderson, P. Tardy, J. Crawshaw and J.R.A. Pearson, ``Constitutive Equations for Extensional flow of wormlike micelles: Stability analysis of the Bautista-Manero model'', J. Non-Newtonian Fluid Mech. 126, 39-46 (2005).

Coupling Lattice Boltzmann and Molecular Dynamics models for dense fluids

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The advent of nanofabrication provides us today with enhanced capabilities for sensors and actuators. A particular challenge involves the embedding of these de- vices in liquid environments when considering biological applications. The difficulty of carrying out controlled experiments on nanoscale systems makes computational studies potent alternatives for characterizing their properties. Molecular Dynamics (MD) simulations are a useful approach that allow the in- vestigation of such flows by modeling the interactions between atoms. State of the art MD have been used to simulate systems that can be described with up to a few millions atoms and a few nanoseconds. However, as nanoscale devices are often embedded in micro and macroscale systems, the computation of such flows requires a proper integration of atomistic simulations with computational methods suitable for larger scales.

Lattice Boltzmann (LB) models are a class of numerical techniques well suited to probing the behavior of fluids at a mesoscopic scale [1]. In this work we use a LB model which solves the Navier-Stokes equations for an incompressible fluid by following the evolution of distribution functions on a lattice at discrete time steps. LB models for meso/macro scale flow modeling enjoy several advantages. They are highly efficient as there is no need to compute a Poisson equation, pressure being locally available. The computational implementation of LB is straightforward and its local character makes it well suited to parallel computing architectures.

Finally, the method can handle easily complex boundaries. In this work we propose a domain decomposition algorithm that allows the coupling between an MD description, of a dense fluid, with an LB model solving the Navier-Stokes equations of an incompressible fluid. The flow domain is decomposed into two overlapping regions: an atomistic and a mesoscopic region. The two scales are matched at an overlapping region via an alternating Schwarz method matching the solutions in the two domains [2]. The present novel MD-LB method is tested on nanoscale Couette and Poiseuille flows. The molecular regime is composed of liquid argon, coupled with an LB solver for the Navier-Stokes regime. We compare the results of the present hybrid method with analytical solutions. We report on the convergence of the hybrid method and demonstrate good quantitative agreement in both test cases. The convergence of the method is analyzed in terms of the overlapping region size and the number of iterations performed within the molecular dynamics model.

References

[1] S. Succi. The Lattice Boltzmann Equation, For Fluid Dynamics and Beyond. Oxford University Press, 2001.

[2] T. Werder, J.H. Walther, and P. Koumoutsakos. Hybrid atomistic-continuum method for the simulation of dense fluid flows. J. Comp. Phys., 205:373, 2005.

Growth dynamics of cytoskeleton proteins: multiscale theoretical approach

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Cytoskeleton proteins, such as actin filaments, microtubules, intermediate filaments, play an important role in the functioning of biological systems. The cellular functions of these rigid filament proteins are defined by their growth processes. A theoretical analysis of the growth dynamics of cytoskeleton proteins is presented from the point of view of different length scales. It is argued that simple phenomenological models cannot reasonably

describe the polymerization processes, while the atomic scale analysis is still technically not feasible. We present a mesoscopic theoretical approach that takes into account the structure and geometry of the growing proteins, chemical processes and chemical interactions between the subunits. The method is successfully applied to explain and to analyze the experimental observations. It is shown that chemical processes on the microscopic level might lead to large macroscopic fluctuations in cytoskeleton proteins.

M6 (Keynote)
Dynamics of dilute polymeric solutions: coarse graining strategies and multi-scale flow simulations

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Traditionally, coarse-grained kinetic theory based models of dilute polymeric solutions have relied on reduction of the internal degrees of freedom in the micro-mechanical description of the macromolecule. However, in recent years fluorescence microscopy of model macromolecules, namely DNA, in a variety of flow fields has shown that multi-segment bead-rod and bead spring descriptions are required to describe both single molecule dynamics such as molecular individuality, unraveling/tumbling dynamics as well as the rheological properties of the solution, namely, viscosity and the mean molecular extension. These findings clearly underscore the fact that a multi-segment description of the macromolecule or reduced order coarse grained models that contain information regarding the internal degrees of freedom of the chain are required for accurate modeling of polymer dynamics under flow. Motivated by this fact, we have been involved in developing novel coarse graining strategies as well as highly efficient multiscale simulation techniques for dynamics of polymeric solutions under flow. In this presentation our progress in both areas will be discussed. Specifically, I will address the following issues,

1. Development of a reduced-order configuration-based model for dilute macromolecular solutions that relies on partitioning the phase space accessible to macromolecules into a few configuration classes, namely, folds, half dumbbells, kinks, dumbbells, coils and extended states. In turn, the evolution of the probability distribution of these classes is determined via a population balance model and the configurational details of molecules within each class are coarse-grained into a single micro-mechanical variable. Macroscopic properties such as the stress are calculated as a sum over the contributions from the configuration classes weighted by their respective probability of occurrence by using a unique force law that is consistently derived from Brownian dynamics simulations. The accuracy and efficiency of the configuration-based model is demonstrated by studying the startup of steady uniaxial extensional flow followed by relaxation and the startup of steady shear. Furthermore, the applicability of the configuration-based model to multi-scale flow calculations is demonstrated.

2. Development of a highly efficient algorithm for multiscale large-scale flow simulation of dilute polymeric solutions described by multi-segment bead-spring micro-mechanical models. The accuracy and efficiency of the algorithm is demonstrated via flow simulations in simple and complex kinematics flows (i.e., plane-Couette, Poiseuille, and 4-1-4 contraction/expansion).

M7

Challenges in computational hemodynamics

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Modeling and computational analysis play an increasingly-important role in bioengineering, particularly in the design of ventricular assist devices. Numerical simulation of flow in blood pumps has the potential to shorten the design cycle and give the designers important insights into causes of blood damage and suboptimal performance. A set of modeling techniques will be presented which are based on stabilized space-time finite element formulation of the Navier-Stokes equations, with a shear-slip mesh update used to accommodate the movement of the impeller with respect to a non-axisymmetric housing. The computed global flow characteristics (performance curves) are compared with experimentally measured data. This application presents a ripe target for shape optimization and optimal control. In order to assess the influence of the fluid constitutive model on the outcome of shape optimization tasks, a comparison of model problem computations based on the Navier-Stokes equations on one hand, and on a more accurate shear-thinning modified Cross model on the other, will be presented. More complex description of blood behavior takes into account viscoelastic phenomena, in particular via an Oldroyd-B constitutive model. Recent developments in stabilized methods of GLS-type for simulation of Oldroyd-B flows using low-order extra-stress interpolations will be outlined. Finally, in order to obtain quantitative hemolysis prediction, cumulative tensor-based measures of strain experienced by individual blood cells are being developed and correlated with available blood damage data. In the first approximation, red blood cells under shear are modeled as deforming droplets, and their deformation is tracked along pathlines of the computed flow field.

M8

Extrusion flow of polymer blends with droplet morphology

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The thermodynamically consistent blend model of Dressler and Edwards [1] has been solved computationally to understand the flow of polymer blends with droplet morphology in the metering section of a single screw extruder. Extending the method proposed in Dressler and Edwards [2] to non-symmetric flow fields, the dynamic model has been solved for a mixed Couette/Poiseuille flow as encountered in the metering section of a single screw extruder. In our code we consider both the mixing flow perpendicular to the flights of the extruder and the conveying flow parallel to the flights. We have performed calculations for different model (e. g. blend component viscosity ratio) and flow geometry parameters (e. g. helix angle of the extruder screw) to nderstand qualitatively microstructure-rheology relationships for polymer blends in extrusion flows. Macroscopic flow characteristics such as the volumetric throughput, the residence time distribution function, and the non-Newtonian flow stresses are discussed along with microscopic characteristics of the blend such as oblate/prolate configurations of the droplets, break-up/coalescence rates, and matrix microstructural characteristics.

[1] Dressler, M. and Edwards, B. J. (2004). Rheology of polymer blends with matrix- hase viscoelasticity and a narrow droplet size distribution. J. Non-Newtonian Fluid Mech., 120:189–205. [2] Dressler, M. and Edwards, B. J. (2005). A method for calculating rheological and morphological properties of constant-volume polymer blend models in inhomogeneous shear fields. J. Non-Newtoian Fluid Mech., 130:77–95.

Adaptive multiscale modeling of water

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We propose a multiscale model to simulate water molecules, their interaction with other water molecules and with solutes. The resolution of the model changes on-the-fly from coarse-grained to all-atom depending on the local environment. We present the method and results in the context of simulation of water absorption by an hydrophilic surface. The adaptive model allows to simulate water molecules in full atomic details in proximity of the absorbing surface (where a few layers of molecules organize into a thin ice-like structure) while maintaining an overall coarse-grained description for water molecules in lower density region. We show that this model correctly reproduces the structural and thermodynamic properties of the system, and significantly simplifies the calculations.

A simple multiscale model of the Soret effect (thermal diffusion) in liquids

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The Soret effect [1] refers to the resulting inhomogeneity in composition created in an otherwise homogeneous binary liquid solution confined between parallel walls by the imposition of a steadystate temperature gradient across the walls. The Soret effect is a special case of the general phenomenon of thermal diffusion. While the mechanism by which the separation occurs in *gases* has been well understood for almost a century as a result of the work of Chapman and Enskog based on solving the Boltzmann equation [2], no comparable explanation has existed in the case of *liquids* owing to the greater complexity of the molecular forces existing in liquids. Our presentation outlines a simple multiscale model [1,3] of the phenomenon in liquids whereby the separation is explained in terms of "thermo-osmotic" forces [3] acting on a dilute suspension of Brownian particles (the solute, species 1) dispersed in a liquid (the solvent, species 2). The analysis uses these temperature gradient-induced forces acting on individual colloidal particles (i.e., solute "molecules") to model the overall macroscale Soret effect. The analysis parallels Einstein's (1905) classical analysis of Brownian diffusion in *isothermal* binary liquids. Despite the model's simplicity, the results of the Soret model are shown to compare well with experimental data [4] over a wide range of solutes and solvents.

References

*[1] J. R. Bielenberg and H, Brenner, "A hydrodynamic/Brownian motion model of thermal diffusion in liquids," Physica A **356**, 279-293 (2005).*

[2] S. Chapman and T. G. Cowling, The Mathematical Theory of Non-Uniform Gases, rd. ed. (Cambridge University Press, Cambridge, 1970).

*[3] H. Brenner, "Nonisothermal Brownian motion: Thermophoresis as the macroscopic manifestation of thermally biased molecular motion," Phys. Rev. E **72**, 061201-1 to 16 2005).*

*[4] S. Iacaponi, R. Rusconi and R. Pizza, "The "macromolecular tourist": Universal temperature dependence of thermal diffusion in aqueous colloidal suspensions," Eur. hys. J. E **19**. 59-67 (2006).*

POSTERS

PT1

Viscoelastic surfactant fluids in the application of hydraulic fracturing

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Hydraulic fracturing is a reservoir stimulation technique in which fractures are created by the injection of viscous fluids and/or slurry into the rock mass. Conductive passages are developed for the flow of hydrocarbons by either placing solid particles to prop the fracture open or by etching the rock surfaces with acid. Self-assembling viscoelastic surfactant based (VES) fluids have been widely used in the application of hydraulic fracturing for their advantages over crosslinked polymer fluids in frictional pressure reduction and the ability to transport solid particles. The rheology of these VES fluids has shown distinct characteristics of either a nearly constant shear stress plateau or shear rate softening in the flow curves. Experimental results obtained from rheometers as well as pipe and slot tests suggest strong links between flow behavior and shear-induced structures. A better understanding of how the rheological properties and macroscale shear-induced structures are affected by the microscale properties as well as how the macroscale structures can be predicted based on rheology would be extremely valuable for practical purposes. In this presentation, a phenomenological model is formulated to describe the flow in the fracture. A conceptual hypothesis is also proposed to account for the transport of particles.

PT2

Numerical simulation of deformation of newtonian and viscoelastic droplets in shear flows

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The deformation of Newtonian and viscoelastic droplets in shear flows was numerically simulated. The droplet deformation deeply relates the flow of emulsions. Emulsions are dispersions of immiscible liquids and are found in foodstuffs, pharmaceutical products, cosmetics, and coating materials. It is important to investigate the droplet deformation in lows because it relates both the function and properties of emulsion products. In addition, it is also interesting to analyze the relation between rheology of emulsions and the deformation behavior of droplets in flows. In the present simulation, the interface between two liquids is implicitly expressed using a color function F, which takes a value of 1 in one liquid and 0 in the other liquid. The interface is expressed by a contour of $F = 0.5$. The movement of the interface is described by an advection equation of F. The advection equation was solved with the CIP (Cubic-Interpolated Propagation) method. The flow of surrounding liquid was computed with the MAC method. The Phan-Thien Tanner model was employed as a constitutive equation for viscoelastic liquids. The effect of interfacial tension was introduced with the CSF model. The deformation of droplets under shear flows between parallel plates was numerically simulated. Both the upper and the lower plates move in the counter direction to each other. Periodic boundary conditions were applied to the boundaries except for the upper and lower plates. Moreover, the droplet deformation after the cessation of shear was also simulated. The

numerical simulation predicted that viscoelastic droplets deform more easily than Newtonian droplets because the viscoelastic fluid has shear-thinning viscosity. The stress in a viscoelastic droplet rapidly increased at an early stage of deformation and relaxed with time. This phenomenon is typical for viscoelastic droplets and appeared more remarkably for a fluid with stronger stretch-thickening property in elongation viscosity. Furthermore, the present computation can simulate the emergence of satellite droplets at the breakup of droplet, which has been experimentally observed. The predictions of the present numerical simulation qualitatively agree with experimental results and hence the present approach will be applicable for the simulation of flows of emulsion.

PT3

Investigation of the structuration of micellar solutions by using rheometry and electric current measurements

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Surfactants in solution are able to form molecular aggregates known as micelles, which can take different shapes depending on the concentration and ionic strength of the solution. In the semidilute regime cylindrical wormlike micelles are able to entangle and exhibit a highly viscoelastic behavior that sometimes resembles that observed in high molecular weight polymers. However, in contrast to polymers in which the contour length of the molecule is fixed, micelles in solutions can break and recombine, thus permitting modes of stress relaxation that are absent in polymeric systems. This characteristic along with variations in surfactant concentration and ionic strength of the solutions give rise to a wealth of rheological behaviors, including flow instabilities such as shear banding and spurt, flow induced phase transitions, and shear thickening resulting from shear induced structures. In this work, the structuration of shear banding and shear thickening aqueous micellar solutions formed by cetylpyridinium chloride and sodium salicylate is studied by a combined method of rheometry and electric current measurements. It is shown that the flow field induces changes in the electric resistance of the solutions, which are related to the dynamics of shear induced structures. In fact, the electric current as a function of the shear stress faithfully mimics the flow curves for the studied solutions, thus providing further evidence of changes in the fluid structure.

PT4

Modelling of drop deformation: A combination of the VOF method and the finite element method.

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The Volume of Fluid (VOF) method has been applied extensively for tracking interfaces when modelling the merging and breakup of droplets in dispersed systems. Most commonly the VOF method is coupled to a finite difference scheme or a finite volume scheme which limits the possibility to handle complex geometries. In our work we are interested in simulating the deformation and breakup of drops in complex flow fields which requires the solution of the flow variables in complex domains. We have therefore implemented the VOF method together with a finite element formulation of the Stokes equation. Interfacial tension is included using the continuous surface stress (CSS) formulation of Lafaurie et al. [1]. The CSS formulation is well suited for the finite element formulation because the interfacial stress tensor enters as a natural boundary condition. The interface between the continuous phase and the disperse phase is reconnected using piecewise linear interface calculation (PLIC). In order to make the VOF implementation compatible with the finite element formulation the interface normal is calculated using finite element shape

functions. The finite element solver is based on hexahedral Q2P0 elements. By introducing 8 VOF cells per finite element (in 3D) the vertices of each VOF cell coincide with the finite element velocity nodes. Advection of the two phases is carried out by solving the transport equation dF/dt + r · (Fv) = 0 where F is the colour field associated with the VOF method and v is the velocity.

References
[1] Bruno Lafaurie, Carlo Nardone, Ruben Scardovelli, Stéphane Zaleski, and Gianluigi Zanetti. Modelling Merging and Fragmentation in Multiphase Flows with SURFER. Journal of Computational Physics, 113:134–147, 1993.

PT5

A mesoscopicmodel for (De)wetting

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We present a mesoscopic model for simulating the dynamics of a non-volatile liquid on a solid substrate. The wetting properties of the liquid can be tuned from complete wetting to total non wetting. The velocity boundary condition at the solid interface can be controlled so that either perfect stick or slip can be induced. This model opens thus the way to study the dynamics of drops and liquid thin films at mesoscopic lengths scales. As applications, we study the role of thermal fluctuations on the spreading of nanodroplets and the effect of slip on the morphology of dewetting thin films.

PT6

Macroscopic dynamics of magnetic gels – surface waves and Rosensweig instability

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Introduction: Ferrogels are chemically cross-linked polymer networks that are generated using a ferrofluid as a solvent. While isotropic ferrogels experimentally show a superparamagnetic behavior like usual ferrofluids [1], anisotropic ones are characterized by a nonvanishing magnetization even without any external magnetic field. To produce these uniaxial gels, the cross-linking process is performed in an external magnetic field [2, 3]. In this situation the nanosized particles very likely form columns and fibers due to the necessarily lowered pH-value to get the cross-linking process started. These chains are then fixed in the network, leading to a frozen-in magnetization.

Macroscopic dynamics: Here we generalize the set of hydrodynamic equations for isotropic ferrogels [4] to uniaxial ferrogels. Ferromagnetic gels are uniaxial, if the frozen-in magnetization denotes the only preferred direction. On the one hand they show similarities to other anisotropic gels like, for example, nematic elastomers as well as to isotropic ferrofluids and ferrogels, but on the other hand the combination of preferred direction, magnetic degree of freedom and elasticity makes them unique and very special. Prominent features [5] are the relative rotations between the magnetization and the elastic network, which couple dynamically flow, shear, and magnetic reorientation. As a result, hear flow in a plane that contains the frozen-in magnetization induces a rotation of the magnetization, not only within the shear plane, but also out of the shear plane. Another outstanding aspect of the hydrodynamics of this material is the difference between the mass current density (mass density times velocity) and the momentum density due to a nonvanishing magnetization vorticity. This difference also appears in uniaxial quantum fluids but this is the first time a macroscopic, classical system shows up that coupling. Finally an oscillating external magnetic field induces not only an oscillation of the magnetization in the direction of the external field, but also oscillating shear strains. The latter are found in planes that contain the

frozen-in magnetization and either the external field or the third, perpendicular direction. In addition, the external magnetic field also induces a magnetization component perpendicular to both, the field and the frozen-in magnetization.

Rosensweig instability: It is known from usual ferrofluids, that if a magnetic field is applied normal to a free surface of that ferrofluid, an instability of the surface occurs above a certain threshold resulting in a periodic, stationary structure of spikes [6]. The threshold field depends on the surface tension and gravity, but is independent of the viscosity of the ferrofluid. Within the framework of a linear stability analysis we could show however [7], that for a uniaxial ferrogel the elasticity does influence the threshold, whereas the characteristic wavelength at onset does not change with respect to ferrofluids. We discuss also the possible influence of the viscosity of the ferrogel on the instability. In addition we derive the dispersion relation for surface waves on a uniaxial ferrogel and show how the Rosensweig instability emerges from surface waves, if the field reaches the threshold value.

References
[1] M. Zrinyi, Trends Polym. Sci. 5, 280 (1997)
[2] Z. Varga, J. Feher, G. Filipcsei and M. Zrinyi, Macromol. Symp. 200, 93 (2003).
[3] D. Collin, G. K. Auernhammer, O. Gavat, P. Martinoty and H. R. Brand, Macromol. Rapid Commun. 24, 737 (2003).
[4] E. Jarkova, H. Pleiner, H.-W. M¨uller and H. R. Brand, Phys. Rev E 68, 041706 (2003).
[5] S. Bohlius, H. R. Brand and H. Pleiner, Phys. Rev. E 70, 061411 (2004).
[6] R. E. Rosensweig, Ferrohydrodynamics, Cambridge University Press, Cambridge, U.K., 1985.
[7] S. Bohlius, H. R. Brand and H. Pleiner, Z. Phys. Chem. (2005), to be published [8] S. Bohlius, Diploma Thesis, University of Bayreuth (2005), unpublished.

PT7

Structural interpretation of waxy crude oil gels

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The phase separation of paraffinic crystals from crude oil constitutes a major operating issue for the petroleum industry because their aggregation generates an extended network structure which leads to severe flow assurance problems. The starting point to understand these phenomena is the observation that crude oil gels display features common to those of gels formed from dispersions of weakly attractive colloidal particles.

In this work we have develop a quantitative interpretation of their internal structure by means of fractal geometry and the comparison between three waxy oil gels (by two crude and one model oil) and other colloidal particle gels. It has been possible to estimate the fractal dimension in the gelation regime and a parameter (α) which defines the balance between the magnitude of intra and inter-floc links. This approach has allowed us to formulate a mechanism of waxy crude oil gel formation which is fully consistent with experimental observations.

An important result is the finding that the fractal formed flocs are more rigid than the interfloc links: it is the strength of the interfloc links that determines the elasticity of the gel. Crude oil gels, in fact, behave like an elastic solid until the interfloc links can bear the stress application: after a critical value of deformation these links are damaged and the mechanical properties will degrade smoothly, due to the minor degree of connectivity of the dispersion of (unlocked) aggregates.

PT8
Rheological characterisation of complex fluids in electro-magnetic field

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The paper is dedicated to the rheological investigation and modeling of complex fluids behavior in the presence of electro-magnetic fields (the samples are crude oilswater emulsions enriched with ferrofluids and normal blood). The study is focused on the determination of the electro-magneto-rheological properties of the samples, respectively: (i) measurement of magnetic permeability, electric permittivity and conductivity, (ii) modeling the magnetic field influence on samples viscosity (the start-up of simple shear motion in presence of magnetic field, applied normal to the direction of velocity). Our results include the tested samples in the category of thixotropic, viscoelastic, paramagnetic and semi-conductor fluids. The experiments, corroborated with numerical simulation of the process, put in evidence the capability of electromagneto-rheology to produce value information, both on the micro-scale formulation of complex fluid and on the flow dynamics at the macro-scale. In particular: (i) viscosity sensitivity on magnetic field intensity and variation of electric permittivity might be correlated with changes in the local flow kinematics, (ii) differences between samples chemical formulation and rheology (asphalt and paraffin based crude oils, respectively) correspond to differences of their electro-magnetic properties. The present results have the potential applicability in building a special device to investigate non-invasively the flow structure of complex fluids in micro-geometries.

PT9
Dispersion mechanisms of carbon black in an elastomer under shear

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Silica and carbon black are traditionally used as reinforcing filler in rubber applications (tires and technical rubber parts). These types of filler present a multiscale organisation. The filler is introduced as pellets (100 μm to the millimetre size) in the matrix. These pellets are agglomerates constituted by smaller entities which are aggregates, themselves resulting from the aggregation of elementary particles. During the mixing operation of the filler, the elastomer and other constituents (vulcanising agent, oil, antioxidant…), the filler is dispersed in the matrix, that is its size is reduced down to the smallest attainable size (aggregate size), and spatially distributed in the matrix. A good dispersion and a good distribution of the filler in the matrix are a necessary condition for a reinforced material. Although mixing filler particles in a matrix is a common operation, the elementary mechanisms responsible for the size reduction of the filler are not fully understood. One way to optimise this state would be to be able to observe inside the mixer what happens, which is not possible. Rheo-optical techniques were recently shown as a good tool to investigate in-situ dispersion but in a simpler flow (shear).

In this work, we studied the elementary mechanisms of dispersion (rupture and erosion) of commercial carbon blacks in a SBR matrix using a transparent counter-rotating shear cell coupled to an optical microscope in order to observe in-situ during the shear the behaviour of a carbon black pellet suspended in a SBR matrix. The effect of hydrodynamic parameters (quantity of strain units, applied shear stress, pellet size) and intrinsic parameters of the carbon black (structure, specific area) was investigated. This study led to the determination of a critical condition for rupture and a mastercurve for erosion kinetics. The mechanisms of dispersion will be discussed.

PT10

Tunable micro- and nano-periodic structures in a free-standing flexible urethane: experiments and modelling

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The control and manipulation of tuneable structures that develop at rest in a free-standing urethane/urea elastomer film have been studied by means of atomic force microscopy AFM), small-angle light scattering (SALS) and polarizing optical microscopy (POM). The urethane/urea film was produced by means of a shear-casting technique, by extending a poly(propylenoxide)-based triisocyanate-terminated prepolymer PU) with poly(butadienediol) (PBDO) with a weight ratio of 60% PU/40% PBDO. UV irradiation results in latent micro- and nano-periodic patterns which can be `developed' by applying a uniaxial strain, or by immersing the elastomer in an appropriate olvent and then drying it. For this elastomer we describe six pattern states, how they are related and how they can be manipulated. The morphological features of the UV-exposed ilm surface can be tuned, in a reproducible and reversible manner, by switching the direction of the applied mechanical field. Elastomers extracted in toluene exhibit different surface patterns depending upon the state in which they were developed. Sress-strain data collected for the films before and after UV irradiation, allowed the detection of orientational order induced by the shear casting direction and enhanced by the mechanical field.

We have attempted to model the strain-induced textures by a ssuming the film to consist of a thin, stiff surface layer (`skin') atop a thicker, softer substrate (`bulk'). The skin's higher stiffness is hypothesised to be due to the crosslinking of chains near the surface by UV radiation. Patterns thus arise as a competition between the effects of bending the skin and stretching the bulk. This model has been simulated using the finite-element package ABAQUS; some preliminary results are presented which show promising agreement with experiment.

PT11

Structures formation in shear flow of mixtures of rough particles and Newtonian fluids

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The interaction in a fluid of two rough particles is analysed in the lubrication limit. Because particles have asperities they may collide and exert a rebound force on one another. The insight obtained from the analysis is deployed in a numerical simulation of many particles in a fluid. This is done by shearing two rough walls in a discrete element method. The resulting flow patterns are reported and analysed. One feature that comes to the fore is the formation of ephemeral structures, consisting of alignments of particles in the direction of the compressive quadrant of the shear.

These structures are quantified by means of a spatial-temporal spectral analysis of the particle concentrations. These are reported for various microscopic and macroscopic parameters: surface asperity size, channel width and particle concentration. The work will contribute to the phrasing of overall constitutive laws for this type of slurry.

PT12

Micro-Macro Simulation of Viscoelastic Flows at High Weissenberg Number

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We present here a micro-macro approach based on combining the Brownian configuration fields (BCF) method (van den Brule et al, JNNFM 1997) with the Galerkin finite element method, to compute both a viscoelastic flow around a cylinder and a slot coating flow (free surface flow). A distinct advantage of the BCF method is its ability to treat models for which no exact closed-form constitutive equations exist, such as FENE dumbbells or models with hydrodynamic and excluded volume interactions.

Most of the studies in literature on viscoelastic flow around a cylinder are limited to the use of an Oldroyd-B constitutive equation, which is a poor constitutive model compared to other more sophisticated constitutive models such as FENE-P, FENE etc. Here, we show numerical results for different constitutive models with both linear and non-linear dumbbells using BCF. We are able to obtain solutions beyond the limiting Weissenberg numbers (Wi) typically encountered in macroscopic schemes. In particular, we show that the FENE and FENE-P models produce mesh converged results with relatively coarse meshes at high Wi number compared to the meshes used to solve an Oldroyd-B constitutive model.

Computations were also found to be stable at much higher Wi number using the BCF method for a slot coating flow. We observe that the slot coating flow behaviour of dilute polymer solutions is dramatically different from that of ultra-dilute solutions (studied previously by Pasquali and Scriven, JNNFM, 2002) in terms of the failure of flow computations at high Wi.

PT13

Simulation of macromolecules dynamics: an implicit solvent method

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When studying the dynamics of macromolecules, solvent molecules are responsible of the long range hydrodynamic interactions. Unfortunately, simulations of such systems which explicitily include solvent particles, even if coarse grained, are often computationally unaffordable. We use an implicit solvent method, in which an hydrodynamics solver replaces the solvent particles and is coupled to the macromolecular dynamics. In our model, fluctuating hydrodynamic equations are solved by a recently developed finite-volume method[1], which ensures thermodynamic consistency and readily allows variations of temperature and viscosity of the fluid. Following Alhrics and D¨unweg[2], a Stokesian term is responsible for the coupling of the macromolecule to the fluid. In this paper, we present results of Zimm-like dynamics for a polymer in good solvent and for the collapse of a polymer in poor solvent.

References
[1] G. De Fabritiis, R. Delgado-Buscaglioni, P.V. Coveney, Submitted
(2006).
[2] P. Ahlrichs, B. D¨unweg, J. Chem. Phys. 111 8225 (1999).

PT14

Non-fickian interdiffusion of dynamically asymmetric species: A molecular dynamics study

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We use Molecular Dynamics combined with Dissipative Particle Dynamics to construct a model of a binary mixture where the two species differ only in their dynamic properties (friction coefficients). For an asymmetric mixture of slow and fast particles we study the interdiffusion process. The relaxation of the composition profile is investigated in terms of its Fourier coefficients. While for weak asymmetry we observe Fickian behavior, a strongly asymmetric system exhibits clear indications of anomalous diffusion, which occurs in a crossover region between the Cases I (Fickian) and II (sharp front moving with constant velocity), and is close to the Case II limit.

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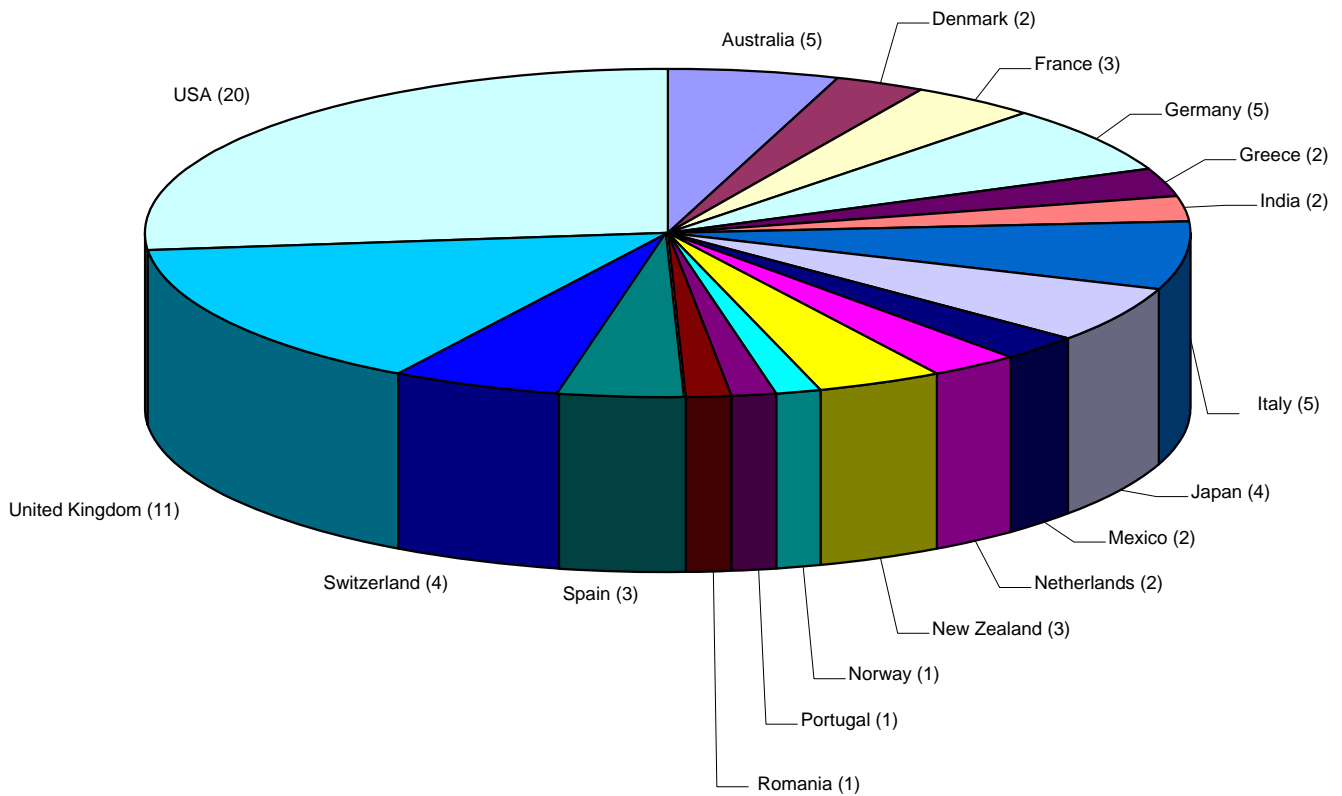
[§] This list was compiled on 9 June 2006, at the time of going to press. A list of participants registering after this date will be circulated at the workshop.

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