

Hydrodynamic Fluctuations in Soft-Matter Simulations

*February 09, 2016 - February 12, 2016
Monash University Prato Centre, Italy
<http://www.ita.monash.edu/>*

Burkhard Duenweg

*Max Planck Institute for Polymer Research, Mainz, Germany
Institute for Solid State Physics, Technical University Darmstadt, Germany
Monash University, Melbourne, Australia*

Ravi Prakash Jagadeeshan

Monash University, Melbourne, Australia

Friederike Schmid

Institute of Physics, Johannes Gutenberg University, Mainz, Germany



1 Description

For details concerning venue, accommodation, etc. please see the Prato meeting web site <http://users.monash.edu.au/~rprakash/cecarn2016/home.html>.

Langevin noise [1] is the standard description for thermal fluctuations in equilibrium. In 1957, Landau and Lifshitz (LL) [2] solved the problem of applying the formalism to a Navier-Stokes continuum fluid. The subject has found renewed interest in the computer simulation community with the advent and refinement of "mesoscopic" techniques like Dissipative Particle Dynamics (DPD) and Smoothed Dissipative Particle Dynamics (SDPD) [3], Multi-Particle Collision Dynamics (MPCD) [4], the Lattice Boltzmann (LB) method [5], and (more recently) direct numerical solution of the discretized LL equations [6].

As documented in the literature, there has been significant progress in the field, but some issues need further improvement. These include: (i) issues of thermodynamic consistency (for example, there are still deep fundamental problems when attempting to apply LL noise to multiphase LB methods [7]); (ii) convergence to the continuum limit; and (iii) the role of non-hydrodynamic degrees of freedom. A synoptic view on all the existing complementary methods will be very helpful.

The meeting aims at bringing together researchers with different and complementary backgrounds, ranging from physicists to chemical engineers and applied mathematicians, who are experts in their respective fields. The goal is to promote the efficient application of advanced numerical methods through a deep understanding of the physical and mathematical background. It is anticipated that a discussion of the relevant questions will lead to a comparison of observations, a sharing of procedures, and foster new collaborations among a multidisciplinary group of scientists and engineers working on an important contemporary problem.

The format of the meeting is planned as a two-day tutorial, followed by a two-day workshop.

Key references

- [1] H. C. Oettinger, *Stochastic Processes in Polymeric Fluids*, Springer Berlin Heidelberg 1995.
- [2] L.D. Landau and E. M. Lifshitz, *Soviet Physics JETP* 5, 512 (1957); *Fluid Mechanics: Course of Theoretical Physics vol. 6*, Elsevier 2013.
- [3] P. Espanol and P. Warren, *Europhys. Lett.* 30, 191 (1995); P. Espanol and M. Revenga, *Phys. Rev. E* 67, 026705 (2003); A. Vazquez-Quesada, M. Ellero, P. Espanol, *The Journal of Chemical Physics* (2009), 130, 3, 034901; Xin Bian, Sergey Litvinov, Rui Qian, Marco Ellero, Nikolaus A Adams, *Physics of Fluids* (2012) 24, 1, 012002.
- [4] G. Gompper, T. Ihle, D. M. Kroll, and R. G. Winkler, *Adv. Polym. Sci.* 221, 1 (2009).
- [5] S. Succi, *The Lattice-Boltzmann Equation*, Oxford University Press 2001; B. Duenweg and A. J. C. Ladd, *Adv. Polym. Sci.* 221, 89 (2009); A. J. C. Ladd, *J. Fluid Mech.* 271, 285 (1994); 271, 311 (1994); R. Adhikari, K. Stratford, M. E. Cates, and A. J. Wagner, *Europhys. Lett.* 71, 473 (2005); B. Duenweg, U. D. Schiller, and A. J. C. Ladd, *Phys. Rev. E* 76, 036704 (2007); G. Kaehler and A. J. Wagner, *Phys. Rev. E* 87, 063310 (2013).
- [6] N. Sharma and N. A. Patankar, *J. Comp. Phys.* 201, 466 (2004); G. De Fabritiis, M. Serrano, R. Delgado-Buscalioni, and P. V. Coveney, *Phys. Rev. E* 75, 026307 (2007); J. B. Bell, A. L. Garcia, and S. A. Williams, *Phys. Rev. E* 76, 016708 (2007); S. Williams, J. Bell, and A. Garcia, *Multisc. Model. Simul.* 6, 1256 (2008); A. Donev, E. Vanden-Eijnden, A. Garcia, and J. Bell, *Commun. Appl. Math. Comp. Sci.* 5, 149 (2010); P. J. Atzberger, *J. Comp. Phys.* 230, 2821 (2011); F. Balboa Usabiaga, J. Bell, R. Delgado-Buscalioni, A. Donev, T. Fai, B. Griffith, and C. Peskin, *Multisc. Model. Simul.* 10, 1369 (2012); F. Balboa Usabiaga, I. Pagonabarraga, R. Delgado-Buscalioni, *J. Comp. Phys.* 235, 701 (2013).
- [7] M. Gross, R. Adhikari, M. E. Cates, and F. Varnik, *Phys. Rev. E* 82, 056714 (2010).

2 Program

Day 1 - Tuesday February 9, 2016

8:00 - 8:45	Registration
8:45 - 9:00	Welcome and Introduction
9:00 - 10:30	Burkhard Duenweg: Introduction to hydrodynamics and Langevin theory
10:30 - 11:00	Coffee Break
11:00 - 12:30	Piotr Szymczak: Brownian Dynamics for systems with hydrodynamic interactions
12:30 - 13:30	Lunch
13:30 - 14:15	Burkhard Duenweg: Introduction to fluctuating hydrodynamics
14:15 - 15:00	Ravi Prakash Jagadeeshan: Treating fluctuating hydrodynamic interactions in polymer solutions far from equilibrium: Closure approximations beyond Zimm theory (part 1)
15:00 - 15:30	Coffee Break
15:30 - 17:00	Tony Ladd: An introduction to Lattice Boltzmann methods
17:00 - 18:30	Alexander Wagner: Thermal fluctuations in Lattice Boltzmann

Day 2 - Wednesday February 10, 2016

9:00 - 10:30	Mike Graham: Stokes flow, Green's functions and advanced Brownian Dynamics
10:30 - 11:00	Coffee Break
11:00 - 12:30	Marco Ellero: Dissipative Particle Dynamics and Smoothed Dissipative Particle Dynamics
12:30 - 13:30	Lunch
13:30 - 15:00	Alejandro Garcia: Direct simulation Monte Carlo
15:00 - 15:30	Coffee Break
15:30 - 17:00	Thomas Ihle: Multi-Particle Collision Dynamics: Kinetic theory
17:00 - 17:45	Ravi Prakash Jagadeeshan: Treating fluctuating hydrodynamic interactions in polymer solutions far from equilibrium: Closure approximations beyond zimm theory (part 2)
17:45 - 18:30	Rafael Delgado-Buscalioni: Fluctuating hydrodynamics and minimal models for Immersed Boundaries

Day 3 - Thursday February 11, 2016

8:30 - 9:00	Registration
9:00 - 9:45	Pep Español: Brownian motion of sub-grid nanoparticles from the theory of coarse-graining
9:45 - 10:30	Giovanni Ciccotti: Hydrodynamics from Dynamical Non-Equilibrium Molecular Dynamics
10:30 - 11:00	Coffee Break
11:00 - 11:45	Aleks Donev: Fluctuating hydrodynamics of suspensions of passive and active rigid bodies
11:45 - 12:30	Rafael Delgado-Buscalioni: Tumbling stars under stress in melt and solution
12:30 - 13:30	Lunch
13:30 - 14:15	Mike Graham: Margination regimes and drainage transition in confined multicomponent suspensions
14:15 - 17:00	Poster session with integrated coffee
17:00 - 17:45	Marco Ellero: Smoothed Particle Hydrodynamics simulations of shear-thinning behavior in a non-colloidal suspension under flow
17:45 - 18:30	Holger Stark: How fluctuations govern the dynamics of active and passive colloids

Day 4 - Friday February 12, 2016

9:00 - 9:45	Tony Ladd: Self-organization and pattern formation in geological systems
9:45 - 10:30	Piotr Szymczak: Polymorphism and chirality in the formation of fibrous aggregates
10:30 - 11:00	Coffee Break
11:00 - 11:45	Suzanne Fielding: Hydrodynamics and phase behaviour of biologically active suspensions
11:45 - 12:30	Robin Ball: Stochastic wavelet hydrodynamics
12:30 - 13:30	Lunch
13:30 - 14:15	Alexander Wagner: Lattice Boltzmann studies of nucleation phenomena
14:15 - 15:00	Thomas Ihle: Kinetic theory of self-propelled particles: Invasion waves and correlation effects
15:00 - 15:45	Alejandro Garcia: Fluctuating hydrodynamics for electrolytes
15:45 - 16:00	Summary & Conclusions
16:00 - 17:00	Coffee Break

3 Abstracts. Invited Talks

Introduction to hydrodynamics and Langevin theory

Burkhard Duenweg [1][2][3]

[1] Max Planck Institute for Polymer Research, Mainz, Germany;

[2] Institute for Solid State Physics, Technical University Darmstadt, Germany;

[3] Monash University, Melbourne, Australia

The lecture is split into two parts, both of which serve the purpose of introducing basic concepts central to the rest of the school. Part 1 provides a phenomenological derivation of the deterministic Navier-Stokes equations for a simple Newtonian fluid, based upon the principles of local conservation laws, local equilibrium, symmetries, and linear Onsager-type non-equilibrium thermodynamics. Part 2 introduces the concept of a Fokker-Planck type Markov process and the Fokker-Planck equation, plus its equivalent stochastic differential equation, the Langevin equation. Furthermore, the lecture discusses basic simulation algorithms to numerically solve such stochastic differential equations. An important concept in that context is the fluctuation-dissipation relation, which establishes that, in case of thermal equilibrium, the temperature can always be written as a ratio between the noise strength and a dissipative transport coefficient.

Brownian Dynamics for systems with hydrodynamic interactions

Piotr Szymczak [1]

[1] University of Warsaw, Poland

The lecture will give an introduction to the Brownian Dynamics (BD) simulation technique, a mesoscale method which takes advantage of the time-scale separation between the rapid momentum relaxation and the much slower evolution of the positional degrees of freedom of Brownian particles. In BD, the collisions between the Brownian particles and the fluid particles are accounted for by inclusion of the stochastic displacements of the Brownian particles. Moreover, for the proper description of the system one needs to take into account hydrodynamic interactions mediated by the solvent: the motion of one particle induces a flow which affects all the other particles. The lecture will start with a discussion of the hydrodynamics at low Reynolds number - introducing Stokes equations and their fundamental solution (Oseen tensor). Next, we will define the mobility tensor, which couples the forces and torques on particles to their velocities and provides a complete characterization of the hydrodynamic interactions. In particular, we will discuss the construction of the mobility tensor by means of the multipole expansion, examine the short- and long-range behaviour of hydrodynamic interactions, and present various approximations to the full hydrodynamic tensor. Next, a classical Brownian dynamics algorithm will be discussed, with a special attention paid to the bottlenecks limiting its computational efficiency, such as the Cholesky decomposition of the mobility matrix needed for the calculation of the hydrodynamically correlated random displacements. Various methods of accelerating BD will then be presented.

Introduction to fluctuating hydrodynamics

Burkhard Duenweg [1][2][3]

[1] Max Planck Institute for Polymer Research, Mainz, Germany;

[2] Institute for Solid State Physics, Technical University Darmstadt, Germany;

[3] Monash University, Melbourne, Australia

The lecture combines the general concepts of hydrodynamics, Langevin theory, and fluctuation-dissipation relations, in order to derive the equations of fluctuating hydrodynamics, as first pioneered by Landau and Lifshitz. Some remarks about the interpretation in terms of numerical discretization are given.

Treating fluctuating hydrodynamic interactions in polymer solutions far from equilibrium: Closure approximations beyond Zimm theory

Ravi Prakash Jagadeeshan [1]

[1] Monash University, Melbourne, Australia

The Rouse model is the simplest description of dilute polymer solutions that captures some aspects of their flow behaviour. Polymer molecules are represented in the model by linear chains of identical spherical beads connected by 'Hookean' springs, and the solvent is modelled as a Newtonian fluid, characterised by its viscosity. The motion of each bead on a polymer chain is affected by the presence of solvent molecules through a hydrodynamic drag force, and a Brownian force. The Rouse model, however, has several shortcomings. For instance, in steady shear flow, it predicts shear rate independent material functions, and a vanishing second normal stress difference coefficient. Additionally, it predicts that the polymer contribution to viscosity scales as molecular weight squared, in disagreement with experimental data. The drawbacks of the Rouse model can be traced to its neglect of the nonlinear phenomena of hydrodynamic interactions, which is the perturbation of the solvent velocity field caused by the motion of polymer chains. Essentially, the hydrodynamic drag force on each bead is affected by the motion of all the other beads on the chain. Zimm improved the Rouse model by taking hydrodynamic interactions into account in a pre-averaged form, i.e., by averaging the hydrodynamic interaction tensor with the probability distribution function that describes the equilibrium configurations of a polymer chain. Predictions by the Zimm model of small amplitude oscillatory shear flow material functions are in excellent agreement with experiment, as is the prediction of the molecular weight scaling of the polymer contribution to viscosity. However, the Zimm model, like the Rouse model, predicts shear rate independent material functions, and a vanishing second normal stress difference coefficient. Significant improvement in the prediction of far from equilibrium material functions have been made more recently in models proposed by Oettinger, by carrying out the average of the hydrodynamic interaction tensor with the non-equilibrium distribution function (the consistent- averaging approximation), and by accounting for fluctuations in hydrodynamic interactions (the Gaussian approximation).

In this talk, I will motivate the development of the basic equations of conventional polymer kinetic theory, which are, (i) the evolution equation for the configurational distribution function (the diffusion equation), and, (ii) the Kramers expression for the stress tensor, which involves complicated moments of the distribution function. I will show that all treatments of hydrodynamic interactions proposed so far in the literature are essentially closure approximations, necessary for obtaining an independent set of evolution equations for the second moments of the distribution function. The importance of accounting for fluctuations in hydrodynamic interactions will be established by comparing the predictions of the various approximations with the exact results of Brownian dynamics simulations. Finally, I will discuss the universal character observed for many polymer properties, independent of the detailed chemical structure of the polymers, and how such properties can be predicted when hydrodynamic interactions are investigated in a systematic manner.

An introduction to Lattice Boltzmann methods

Tony Ladd [1]

[1] University of Florida, Gainesville, USA

In this lecture I will present an overview of the application of lattice-Boltzmann methods to simulations of soft matter. I will briefly describe the LB method and then focus on different methods for coupling fluid and particle systems. I will discuss some of the complications that arise in colloids and other particulate matter, including the effects of lubrication and contact forces. I will illustrate the talk with examples from simulations of colloids and polymers.

Thermal fluctuations in Lattice Boltzmann

Alexander Wagner [1]

[1] North Dakota State University, Fargo, USA

In this talk I will discuss how lattice Boltzmann methods can be adapted to simulate fluctuating hydrodynamics, and the inevitable disconnects from trying to generate a fluctuating theory from a continuous model. In doing so I will focus on fundamentals and demonstrate the issues involved in simple toy models.

Stokes flow, Green's functions and advanced Brownian Dynamics

Mike Graham [1]

[1] Dept. of Chemical and Biological Engineering, University of Wisconsin, Madison, USA

This lecture covers the foundations of low Reynolds number hydrodynamics that are necessary to understand the dynamics of small objects suspended in a flow. The following issues will be addressed: * General properties of the Stokes equations: Linearity, reversibility, reciprocal theorems. * Point force solution (Green's function) in an unbounded domain: the Stokeslet. * Point force solution in a triply periodic domain; Ewald sums. * Point force solutions in bounded domains: reciprocity property of Green's functions; solutions in a half-space and slit; images. * Force dipoles and freely suspended particles; stress in a suspension; hydrodynamic migration of deformable particles near walls. * Mobility and resistance tensors for a multiparticle system. * Boundary integral equations. * Brownian dynamics for a system of hydrodynamically interacting particles in an arbitrary confined geometry. * Fluctuating hydrodynamics; Derivation of the random force on a Brownian particle from a reciprocal theorem. * Application: polymer solutions in confined geometries.

Dissipative Particle Dynamics and Smoothed Dissipative Particle Dynamics

Marco Ellero [1]

[1] University of Swansea, United Kingdom

Dissipative Particle Dynamics (DPD) [1,2] is a mesoscopic mesh-free particle-based method which can be understood as a coarse-graining version of Molecular Dynamics [3]. The method is able to reproduce fluctuating hydrodynamics behavior bypassing some grid-artifacts present in original versions of other mesoscopic grid-based techniques, such as lattice gas automata. Although having been very successful in modelling complex mesoscopic systems, as a model of fluid particles DPD suffers from the conceptual problem that it has no thermodynamic scale associated with the particles. Therefore, a DPD simulation requires an ambiguous fine-tuning of the model parameters with the physical parameters, i.e. to specify the fluid transport coefficients one needs to rely on approximate kinetic theory [4,5] or to map and calibrate the parameters in ways that are not always systematic [6,7]. A corrected version of DPD that does not suffer from this problem is Smoothed Dissipative Particle Dynamics (SDPD) [8,9]. SDPD is, in fact, a version of the well-known Smoothed Particle Hydrodynamics method (SPH) - a mesh-free Lagrangian Navier-Stokes solver - albeit with the proper inclusion of thermal fluctuations. The SDPD model is entirely embedded in the GENERIC framework, therefore it maintains the thermodynamic consistency of the original DPD method, but in addition allows for a direct specification of the transport coefficients as input parameters. Another remarkable advantage of the method is that the application of GENERIC lead directly to a size-dependent thermal noise which satisfies the Fluctuation-Dissipation Theorem [9]. In other words, whenever the fluid particle size is large enough, no thermal noise is present in the hydrodynamic variables, whereas it shows up only when the fluid description needs to be miniaturized, e.g. under microflow conditions. This property allows to formally unify the Lagrangian description of fluid flow based on a stochastic mesoscopic approach (SDPD) with a fluctuations-free deterministic macro-continuum methods (SPH) [10]. In the first part of this talk I will review the SDPD method, discussing the link with the standard DPD and the macroscopic SPH methods for the modelling of a simple Newtonian solvent. In the second part I will present some applications of SDPD for the modelling of complex fluids, i.e. in the context

of viscoelastic polymeric solutions [11,12,13] and particle suspensions [14,15,16] based on a hierarchical description of the fluid microstructure.

- [1] P. J. Hoogerbrugge and J. M. V. A. Koelman, *Europhys. Lett.* 19, 155, 1992.
- [2] P. Español and P. B. Warren, *Europhys. Lett.* 30, 191, 1995.
- [3] G. De Fabritiis, P.V. Coveney, E.G. Flekkøy, *Phil. Trans. R. Soc. Lond. A* 360 317–331, 2002
- [4] C. Marsh, G. Backx, and M. Ernst, *Phys. Rev. E* 56, 1676, 1997.
- [5] R. D. Groot and P. B. Warren, *J. Chem. Phys.* 107, 4423, 1997.
- [6] R. Qiao and P. He, *J. Chem. Phys.* 128, 126101, 2008.
- [7] A. Moshfegh, A. Jabbarzadeh, *Soft Materials* 13 106, 2015.
- [8] P. Espanol, M. Revenga, *Phys. Rev. E* 67, 026705, 2003
- [9] A. Vazquez-Quesada, M. Ellero, P. Espanol, *J. Chem. Phys.* 130, 034901, 2009.
- [10] J. J. Monaghan, *Annu. Rev. Astron. Astrophys.* 30, 543, 1992.
- [11] A. Vazquez-Quesada, M. Ellero, *J. Non-Newt. Fluid Mech.* 167, 1-8, 2012.
- [12] A. Vazquez-Quesada, M. Ellero, P. Espanol, *Phys. Rev. E* 79, 056707, 2009.
- [13] S. Litvinov, M. Ellero, X.Y. Hu, N.A. Adams, *Phys. Rev. E*, 77, 066703, 2008.
- [14] X. Bian, S. Litvinov, R. Qian, M. Ellero, N. A. Adams, *Phys. Fluids* 24 012002, 2012.
- [15] X. Bian, M. Ellero. *Comp. Phys. Comm.* 185, 53-62, 2014.
- [16] A. Vazquez-Quesada, M. Ellero, , *J. Non-Newt. Fluid Mech* , to appear, 2016.

Direct simulation Monte Carlo

Alejandro Garcia [1]

[1] San Jose State University, San Jose, California, USA

For over 50 years Direct Simulation Monte Carlo (DSMC) has been the dominant molecular algorithm for modeling rarefied gas flow. Originally developed for aerospace engineering, its applications now range from nanofluidics to planetary weather. The capabilities of the method include the simulation of realistic chemistry, dense gases, and granular flows. DSMC has a very successful track-record due to its strong foundation in kinetic theory and stochastic processes; its popularity is due to its elegant simplicity. The presentation will provide a general introduction to DSMC, including guidance for implementing the algorithm. The use of DSMC for the study of hydrodynamic fluctuations will be highlighted.

Multi-Particle Collision Dynamics: Kinetic theory

Thomas Ihle [1]

[1] Ernst-Moritz-Arndt University Greifswald, Greifswald, Germany

In this tutorial, I will introduce Multi-Particle Collision Dynamics (MPC), also called Stochastic Rotation Dynamics, a mesoscale particle-based simulation method for fluid flow [1]. The method consists of two steps: streaming, where all particles are advanced according to their velocities, and collision, where particles exchange momentum according to simple collision rules. MPC requires a discrete time step and is off-lattice; however, a lattice is still needed to identify collision partners. Advantages of MPC include easy implementation and the fact that both hydrodynamic interactions and Brownian fluctuations are intrinsically contained in a thermodynamically consistent way. The original algorithm [1] was not Galilean invariant due to the underlying lattice structure, and I will review how this invariance can be exactly restored by introducing random shifts of the lattice [2]. After explaining the algorithm and discussing its implementation, I will outline several applications such as suspensions of colloids and polymers. More recent developments of the algorithm such as ways to conserve angular momentum will also be discussed. Since the collision rules conserve momentum and energy, the MPC-fluid is described by the Navier-Stokes equations in the limit of large length and time scales. In the second part of the tutorial I will introduce and contrast several analytical methods to calculate the transport coefficients of this fluid. These approaches include Green-Kubo relations obtained from a Projector-Operator approach, a nonequilibrium approach [3], and a kinetic theory that leads to an Enskog-like equation which is then treated by a Chapman-Enskog expansion [4].

- [1] A. Malevanets, R. Kapral, *J. Chem. Phys.* 110, 8605 (1999).
- [2] T. Ihle, D. Kroll, *Phys. Rev. E* 63, 020201 (2001).
- [3] K. Kikuchi et al., *J. Chem. Phys.* 119, 6388 (2003).
- [4] T. Ihle, *Phys. Chem. Chem. Phys.* 11, 9667 (2009).

Fluctuating hydrodynamics and minimal models for Immersed Boundaries

Rafael Delgado-Buscalioni [1]

[1] Depto. Fisica Teorica Materia Condensada and IFIMAC, Universidad Autonoma de Madrid, Spain

This lecture explains in some details the implementation of fluctuating hydrodynamics based on finite volumes and the basis of immersed boundary methods to include particles in the fluctuating hydrodynamic solvent. From the computational standpoint it will focus on how to include scalars, vector, and tensor fields in staggered grids and the basis of some famous integration schemes, such as Cranck-Nicholson. I will focus on periodic systems, where the use of fast-fourier transform allows maximal efficiency, at the cost of explicit boundary (walls) treatment. The lecture will also explain the particularities of the immersed boundary method applied to the minimal "blob" particle model, with an excellent ratio of accuracy over computational cost. Physical properties of the blob and ways to generalize the model (adding compressibility or more complex shapes) will be addressed (see also Donev lecture for rigid constraints). Practical computational problems and tricks appearing in applications (colloidal gelation, viscosity calculations, ultrasound forces) will be briefly discussed.

F Balboa Usabiaga. Minimal models for finite particles in fluctuating hydrodynamics. Tesis Univ. Autonoma Madrid (2014)

Staggered schemes for fluctuating hydrodynamics. F Balboa Usabiaga, JB Bell, R Delgado-Buscalioni, A Donev, TG Fai, Multiscale Modeling & Simulation 10 (4), 1369-1408

Inertial Coupling Method for particles in an incompressible fluctuating fluid. F Balboa Usabiaga, R Delgado-Buscalioni, BE Griffith, A Donev, Computer Methods in Applied Mechanics and Engineering 269, 139-172

Brownian dynamics without Green's functions. S Delong, FB Usabiaga, R Delgado-Buscalioni, BE Griffith, A Donev. The Journal of chemical physics 140 (13), 134110

Minimal model for acoustic forces on Brownian particles. F Balboa Usabiaga, R Delgado-Buscalioni. Physical Review E 88 (6), 063304

A multiblob approach to colloidal hydrodynamics with inherent lubrication. A Vázquez-Quesada, F Balboa Usabiaga, R Delgado-Buscalioni. The Journal of chemical physics 141 (20), 204102

Brownian motion of sub-grid nanoparticles from the theory of coarse-graining

Pep Español [1]

[1] Universidad Nacional de Educacion a Distancia, Madrid, Spain

We formulate the dynamics of a nanoparticle floating in a fluid starting from the microscopic dynamics of the system. The distinctive feature of the present approach is that the nanoparticle is assumed to be smaller than the discrete grid in which the fluctuating hydrodynamics is formulated (i.e. we have a sub-grid nanoparticle). This avoids the need to resolve the particle and describe the coupling with the fluid through costly (and uncertain) boundary conditions. We obtain a coupled set of equations for the stochastic evolution of the position of the particle and the stochastic evolution of the discrete hydrodynamics. These equations obtained microscopically are very similar to recent popular continuum equations used in the simulation of colloidal particles in fluctuating fluids, once they are discretized with the Petrov-Galerkin method. This gives light and theoretical support to these continuum phenomenological blob models.

Pep Español, Aleksandar Donev, "Coupling a nano-particle with isothermal fluctuating hydrodynamics: Coarse-graining from microscopic to mesoscopic dynamics", <http://arxiv.org/abs/1509.01540>, to appear in J. Chem. Phys.

Hydrodynamics from Dynamical Non-Equilibrium Molecular Dynamics

Giovanni Ciccotti [1]

[1] Universita di Roma "La Sapienza", Italy

We present a way to extend stationary state (equilibrium and nonequilibrium) Molecular Dynamics to time dependent nonequilibrium situations, including the dynamical processes of response and relaxation. The procedure, which we have called Dynamical Non-Equilibrium Molecular Dynamics (D-NEMD), to distinguish it from standard NEMD, only used to simulate stationary nonequilibrium states, is based on a generalization of linear response theory. The idea has been formulated by Onsager in the thirties in metaphysical language; given a solid foundation in the fifties by Green and Kubo (in the linear and nonlinear regime); and adapted to MD simulations by the present author (in collaboration with G.Jacucci and I.R.Mac Donald) in the seventies. It has been called the nonlinear Kubo-Onsager relation, connecting dynamical nonequilibrium averages or dynamical relaxations to stationary probability distribution functions (initial distribution) suitably sampled. To show the power of the method we apply it to study the onset of nonlinear behavior in transport processes of simple fluids and by looking at the convective circulation in liquids, which establishes, as stationary asymptotic state, convective rolls. Moreover we will also apply the method to get the hydrodynamic relaxation of an interface between two immiscible liquids.

Fluctuating hydrodynamics of suspensions of passive and active rigid bodies

Aleksandar Donev [1]

[1] Courant Institute of Mathematical Sciences, New York University, New York, NY

I will discuss computational methods for problems involving Brownian rigid and semi-rigid structures immersed in a fluid. Examples include colloidal particles, polymer chains, and macromolecules in a solvent. There are a number of methods developed for suspensions of spheres at small Reynolds numbers, such as the well-known method of Stokesian Dynamics, or boundary-integral formulations. More complex rigid bodies suspended in fluid can be represented with different degrees of fidelity by enforcing a rigidity constraint on a collection of blobs resolving the body to some degree of fidelity. Implementing all of this in practice efficiently for suspensions of tens of thousands of particles is possible but requires some sophisticated numerical linear algebra which I will discuss in some detail. Thermal fluctuations and thus Brownian motion can be consistently modeled by including a fluctuating (random) stress in the momentum equation, as dictated by fluctuating hydrodynamics. I will discuss methods that couple an immersed-boundary Lagrangian representation of rigid bodies to a fluctuating finite-volume fluid solver. Unlike the commonly-used methods of Brownian and Stokesian dynamics, which are based on Green's functions, our techniques are based on an explicit-fluid fluctuating hydrodynamics formulation in which we add a stochastic stress tensor to the usual viscous stress tensor. Once special care is taken to construct temporal integrators that correctly capture stochastic drift terms without increasing the computational cost, our methods give the correct translational and rotational Brownian motion.

"Brownian Dynamics of Confined Rigid Bodies", S. Delong, F. Balboa Usabiaga and A. Donev, *J. Chem. Phys.*, 143, 144107, 2015 [Arxiv:1506.08868]

"An immersed boundary method for rigid bodies", B. Kalleinov and A. Pal Singh Bhalla and B. E. Griffith and A. Donev, submitted to CAMCoS, 2015 [Arxiv:1505.07865]

"Brownian Dynamics without Green's Functions", S. Delong, F. Balboa Usabiaga, R. Delgado-Buscalioni, B. E. Griffith and A. Donev, *J. Chem. Phys.*, 140, 134110, 2014 [Arxiv:1401.4198]

Tumbling stars under stress in melt and solution

Rafael Delgado-Buscalioni [1], J. Sablić [2] and M. Praprotnik [2]

[1] Depto. Fisica Teorica Materia Condensada and IFIMAC, Universidad Autonoma de Madrid, Spain

[2] Laboratory for Molecular Modeling, National Institute of Chemistry, Slovenia

I will first present a numerical study [1] on the rheology of star polymer melts performed under two different external constraints: fixed volume and shear rate (closed) and fixed normal pressure and shear stress (open). This second ensemble (fixed pressure tensor) is modelled in a grand-canonical fashion, using Open Boundary Molecular Dynamics (OBMD). OBMD uses Adaptive Resolution Scheme (AdResS) to coarse-grain the system's buffers where new polymer molecules are inserted or removed according to the external pressure balance. OBMD conserves the overall momentum balance across the system's interfaces, and it uses a DPD thermostat to preserve the local momentum upon each monomer collision. Interestingly, we find that the system's rheology depends on the external constrain (open vs. closed). As a second contribution we show that the models rheology greatly depends on the friction kernel used to thermalize the chains "blobs" (or "monomers"). This fact indicates that the choice of the DPD-thermostat's kernel should be taken as part of the coarse-graining protocol, something however seldom considered. In the second part of the talk I will present preliminary results on a study on the tumbling dynamics of star polymers under shear flow. This study compares the motion of polymer molecules in melt and in dilute solution (single chain dynamics) was solved using a Brownian dynamics code which allows to compare the free draining case (no-hydrodynamics) with the effect of hydrodynamic couplings between monomers, solved via the Rotne-Prager mobility tensor. Our study shows discrepancies with previous published studies which shall be highlighted.

[1] J. Sablić, M. Praprotnik and R. Delgado-Buscalioni, *Open boundary molecular dynamics of sheared star-polymer melts*, *Soft Matter*, 2016, DOI: 10.1039/C5SM02604K

Margination regimes and drainage transition in confined multicomponent suspensions

Mike Graham [1]

[1] Dept. of Chemical and Biological Engineering, University of Wisconsin, Madison, Wisconsin, USA

Blood is a suspension of objects of various shapes, sizes and mechanical properties, whose distribution during flow is important in many contexts. Red blood cells tend to migrate toward the center of a blood vessel, leaving a cell-free layer at the vessel wall, while white blood cells and platelets are preferentially found near the walls, a phenomenon called margination that is critical for the physiological responses of inflammation and hemostasis. Additionally, drug delivery particles in the bloodstream will also undergo segregation and the influence of these phenomena on the efficacy of such particles is unknown. This talk describes efforts to gain a systematic understanding of flow-induced segregation phenomena in blood and other complex mixtures, using a combination of theory and direct simulations. Contrasts in size, deformability and shape can all lead to segregation. A kinetic theory model based on pair collisions and wall-induced hydrodynamic migration can capture the key effects observed in direct simulations, including a drainage transition in which one component is completely depleted from the bulk of the flow. Experiments performed in the laboratory of Wilbur Lam indicate the physiological and clinical importance of these observations.

Smoothed particle hydrodynamics simulations of shear-thinning behavior in a non-colloidal suspension under flow

Marco Ellero [1], Adolfo Vazquez-Quesada [1]

[1] University of Swansea, United Kingdom

Shear-thinning, i.e. the reduced suspension viscosity at increasing shear rates, although being relatively well understood in Brownian colloidal systems as a result of the decreasing relative contribution of entropic forces [1], it has been often reported also in experiments with Brownian-less non-colloidal systems at high volume fractions [2-5]. Despite this phenomenon has been known for a long time the origin of non-colloidal shear-thinning is still theoretically puzzling and difficult to reproduce by numerical simulations where typically opposed shear-thickening is observed instead [6-9]. By proposing a non-Newtonian model of interparticle lubrication forces, we show that hidden shear-thinning effects of the suspending medium, i.e. occurring at shear rates orders of magnitude larger than the range investigated experimentally, can eventually produce significant shear-thinning of the overall suspension at the much smaller shear rates explored experimentally. This is due to the fact that at high volume fractions, 'local' shear rates occurring in the domain, especially in the narrow gaps between approaching particles, can be significantly larger than the 'averaged' one imposed by the viscometric flow, therefore allowing the suspending medium to probe possibly its high-shear non-Newtonian regime. In this talk a Smoothed Particle Hydrodynamics (SPH) simulation model of a noncolloidal suspension of spherical particles presented in [9-11] is modified by incorporating high-shear non-Newtonian interparticle lubrication effects and the resulting rheology studied showing good agreement against experimental data [5].

[1] J. Mewis and N. J. Wagner, "Colloidal Suspension Rheology" (Cambridge University Press, 2011)

[2] F. Ferrini, D. Ercolani, B. de Cindio, L. Nicodemo, L. Nicolais, and S. Ranaudo, *Rheologica Acta* 18, 289 (1979).

[3] F. Gadala-Maria and A. Acrivos, *Journal of Rheology* 24, 700 (1980).

[4] Zarraga, I. E., D. A. Hill, and D. T. Leighton, Jr., "The characterization of the total stress of concentrated suspensions of noncolloidal spheres in Newtonian fluids," *J. Rheol.* 44, 185–220 (2000).

[5] SC Dai, E. Bertevás, FZ Qi, RI Tanner, "Viscometric functions for noncolloidal sphere suspensions with Newtonian," *Journal of Rheology* 57 (2), 493-510 (2013).

[6] Sierou A, Brady J, "Rheology and microstructure in concentrated noncolloidal suspensions". *J Rheol* 46(5):1031–1056 (2002).

[7] Bertevás E, Fan X, Tanner RI "Simulation of the rheological properties of suspensions of oblate spheroidal particles in a Newtonian fluid." *Rheologica Acta* 49(1):53–73 (2010).

[8] X Bian, S Litvinov, M Ellero, NJ Wagner, "Hydrodynamic shear thickening of particulate suspension under confinement", *Journal of Non-Newtonian Fluid Mechanics* 213, 39-49 (2014).

[9] A. Vazquez-Quesada, M. Ellero, "Rheology and microstructure of noncolloidal suspensions under shear studied with Smoothed Particle Hydrodynamics", *J. Non-Newt. Fluid Mech.*, to appear (2016)

[10] X. Bian, M Ellero, "A splitting integration scheme for the SPH simulation of concentrated particle suspensions" *Computer Physics Communications* 185 (1), 53-62 (2014).

[11] A. Vazquez-Quesada, X. Bian, M. Ellero, "Three-dimensional simulations of dilute and concentrated suspensions using Smoothed Particle Hydrodynamics", *Comp. Part. Mech.*, online (2015).

How fluctuations govern the dynamics of active and passive colloids

Holger Stark [1]

[1] Institute of Theoretical Physics, Technische Universität Berlin, Germany

In this contribution I review some of our work on active and passive colloids in non-equilibrium stressing the role of fluctuations or stochastic events. A squirmer is a generic active particle or microswimmer driven by surface flow. We discuss here the realization of a squirmer, where a mixture of surfactants can spontaneously demix and thereby initiates Marangoni flow at the droplet interface [1]. Thermal noise in the diffusion-reaction-advection equation, governing the dynamics of the surfactant mixture, is crucial for the coarsening of the mixture and also for the persistent random walk of the droplet. Second, we use multi-particle collision dynamics (MPCD) to simulate the collective behavior of active colloids or squirmers [2]. In a quasi-two-dimensional geometry phase separation occurs depending on the swimmer type. With large-scale simulations we map out the phase diagram for mean area fraction versus swimming velocity. Third, using MPCD we investigate passive colloids under Poiseuille flow in a microchannel [3]. At sufficiently large densities and driving they develop regular velocity pulses, which we explore by implementing

elastic interactions and Coulomb friction between the colloids. Force chains create jammed regions, which are unjammed by rarefaction pulses traveling upstream.

[1] M. Schmitt and H. Stark, *Europhys. Lett.* 101, 44008 (2013).

[2] A. Zöttl and H. Stark, *Phys. Rev. Lett.* 112, 118101 (2014).

[3] P. Kanehl and H. Stark, *J.Chem. Phys.* 142, 214901 (2015).

Self-organization and pattern formation in geological systems

Tony Ladd [1]

[1] University of Florida, Gainesville, USA

When water percolates through a carbonate bed containing faults or fractures, the solutional attack of dissolved CO₂ starts to widen them. Dissolution of fractured carbonate rocks is often accompanied by the formation of highly localized flow paths, with patterns that are somewhat reminiscent of viscous fingering. Numerical simulations of fracture dissolution show a systematic reduction in the number of flow paths as dissolution progresses, which has interesting scientific and engineering consequences. In this talk I will present results from numerical and theoretical investigations of dissolution, and compare them with some field observations.

Polymorphism and chirality in the formation of fibrous aggregates

Piotr Szymczak [1]

[1] University of Warsaw, Poland

Things are twisted, particularly if one looks at biological matter: from DNA entwined in the double helix, and coiled coils of alpha-helical proteins such as tropomyosin, to microtubules or fibrillar aggregates of proteins. The morphology of these macromolecules or their aggregates is typically determined by an interplay between cohesive and elastic forces. Using a simple coarse-grained numerical model we study structural polymorphism of aggregates of chiral elastic filaments. Three generic morphologies of the aggregates are observed: ribbons, in which the filaments are joined side-by-side, twisted, helicoidal fibrils, in which filaments entwine along each other, and tubular forms, with filaments wound together around a hollow core of the tube. A relative simplicity of the model allows us to supplement numerical simulations with an analytic description of the elastic properties of the aggregates. The model is capable of predicting geometric and structural characteristics of the composite structures, as well as their relative stabilities. We also investigate in detail the transitions between different morphologies of the aggregates.

Hydrodynamics and phase behaviour of biologically active suspensions

Suzanne Fielding [1]

[1] Department of Physics, Durham University, UK

Following a brief pedagogical introduction to the field of biologically active suspensions, we discuss recent research results for the phase behaviour and rheology of these fluids. In the first part of the talk we report simulations of a continuum model for active fluids in two dimensions (2D). We focus on extensile materials and find that steady shear bands, previously shown to arise ubiquitously in 1D for the active nematic phase at small (or indeed zero) shear rate, are generally replaced in 2D by more complex flow patterns that can be stationary, oscillatory, or apparently chaotic. The consequences of these flow patterns for time-averaged steady-state rheology are examined. In the second part we discuss particle based simulations with hydrodynamics of a suspension of active disks squirming through a Newtonian fluid. We explore numerically the full range of squirmer area fractions from dilute to close packed and show that "motility induced phase separation" (MIPS), which was recently proposed to arise generically in active matter, and which has been seen in simulations of active Brownian disks, is strongly suppressed by hydrodynamic interactions. We give an argument for why this should be the case and support it with counterpart simulations of active Brownian disks in a parameter regime that provides a closer counterpart to hydrodynamic suspensions than in previous studies.

Stochastic wavelet hydrodynamics

Robin Ball [1], Ollie Dyer [1], J Ravi Prakash [2]

[1] University of Warwick, United Kingdom

[2] Monash University, Australia

Stochastic Wavelet Hydrodynamics provides an efficient real space approach to simulating the Brownian dynamics of dilute and semi-dilute soft matter such as polymers and colloids. Hydrodynamic correlations are propagated by the use of extended wavelet moves, without any explicit treatment of the solvent. Potential interactions are incorporated exactly via Monte Carlo move acceptances. I will show that the computational cost can be Order N per physical unit of time, where N is only the number of monomers and/or colloidal particles and the unit of time is such that a particle moves of order its own size, or the range of its interaction with others - whichever is the lesser. The method is best suited to systems with truly soft interactions. Any totally forbidden hard core regions must be protected with a soft repulsion outside them, and this includes the case of any hard walls confining the simulation. For best order of algorithm there are also constraints on the continuity of interaction potentials and their derivatives. The method is straightforward to code for serial computation and should be amenable to parallel computation on a shared memory multiprocessor architecture. However the variable geometry of the wavelet moves it uses makes efficient parallelization on a distributed memory machine more of a challenge.

Lattice Boltzmann studies of nucleation phenomena

Alexander Wagner [1]

[1] North Dakota State University, Fargo, USA

I will talk about using fluctuating lattice Boltzmann simulations to look at nucleation phenomena, in particular comparing simple diffusive LB methods with experiments on multilayer di-block copolymer experiments, where as a function of temperature holes will form in the uppermost layer.

Kinetic theory of self-propelled particles: invasion waves and correlation effects

Thomas Ihle [1]

[1] Ernst-Moritz-Arndt University Greifswald, Greifswald, Germany

Models of self-driven agents similar to the Vicsek model are studied by means of kinetic theory [1,2]. In these models, particles try to align their travel directions with the average direction of their neighbours. At strong alignment a globally ordered state of collective motion forms. An Enskog-like kinetic theory is derived from the exact equation for a Markov chain in phase space using Boltzmann's mean-field approximation of molecular chaos. The kinetic equation is solved numerically by a nonlocal Lattice Boltzmann-like algorithm. Steep soliton-like waves are observed that lead to an abrupt jump of the global order parameter if the noise level is changed. The shape of the wave is shown to quantitatively agree within 3% with agent-based simulations at large particle speeds [3]. This provides a mean-field mechanism to change the second-order character of the flocking transition to first order. At small densities and realistic particle speeds, the mean-field assumption of Molecular Chaos is invalid near the onset of collective motion, and correlation effects become relevant. I will show how to self-consistently include correlation effects at the level of ring-kinetic theory [4]. Instead of just one kinetic equation, an additional equation for the time evolution of two-particle correlations will be derived. This equation is solved numerically for a homogeneous system and shown to be in excellent agreement with agent-based simulations in certain parameter ranges.

[1] T. Ihle, *Phys. Rev. E* 83, 030901 (2011).

[2] Y. L. Chou et al., *Phys. Rev. E* 86, 021120 (2012).

[3] T. Ihle, *Phys. Rev. E* 88, 040303 (2013).

[4] Y. L. Chou et al., *Phys. Rev. E* 91, 022103 (2015).

Fluctuating hydrodynamics for electrolytes

Alejandro Garcia [1]

[1] San Jose State University, USA

A series of recent papers describe efficient, accurate numerical methods for the multicomponent fluctuating hydrodynamic equations [1-5]. This talk will present the extension of this work to electrochemical systems. Electrochemistry has a broad range of applications including energy conversion in batteries and fuel cells, sensors and chemical processing. A typical electrochemical system consists of electrodes separated by an electrolyte, which is a multicomponent fluid containing mobile ions in a neutral solvent but in which the movement of free electrons is suppressed. Since we are interested in liquid systems, we focus on the development of a low Mach number model. The formulation of fluctuating hydrodynamics for electrolytes, as well as the numerical methodology and preliminary results, will be presented.

[1] K. Balakrishnan and A. L. Garcia and A. Donev and J. B. Bell, *Phys. Rev. E* 89:013017, 2014

[2] A. Donev and A. J. Nonaka and Y. Sun and T. G. Fai and A. L. Garcia and J. B. Bell, *Communications in Applied Mathematics and Computational Science (CAMCOS)*, 9-1:47-105, 2014

[3] A. J. Nonaka and Y. Sun and J. B. Bell and A. Donev, *Communications in Applied Mathematics and Computational Science (CAMCoS)* 10-2, 163-204, 2015

[4] A. Donev and A. J. Nonaka and A. K. Bhattacharjee and A. L. Garcia and J. B. Bell, *Physics of Fluids*, 27(3):037103, 2015

[5] A. K. Bhattacharjee, K. Balakrishnan, A. L. Garcia, J. B. Bell and A. Donev, *J. Chem. Phys.*, 142, 224107, 2015

4 Abstracts. Posters

Optimal propulsion of helical particles

Maria Michiko Alcanzare [1]
[1] Aalto University, Finland

Controlled nanoscale motion in a fluid environment is one of the most ambitious challenges in nanoscience. Nanomachines that are able to transform energy to mechanical work have been fabricated to perform a series of tasks such as transporting drug or genetic material in cells, fluid mixing that accelerates chemical reactions and cargo transport in microfluidic chips [1]. Helical particles have coupled translational and rotational motion therefore propulsive motion can be performed by applying an external torque [2]. The difficulty in achieving directed and controlled motion in the nanoscale lies mainly in overcoming the thermal effects which may dominate the locomotive behaviour of the helical swimmer. In this work, we study the effects of shapes, the pitch angles and helical turns, and the viscosity of the fluid on propulsive motion by using a hybrid lattice Boltzmann - molecular dynamics (LBMD) multiscale method that incorporates full hydrodynamic interactions and thermal fluctuations [3]. The increase in the length by increasing the helical turns of the chiral particle adds to the stability in its directed motion but this also increases the hydrodynamic drag. Directed motion is possible when the Peclet number is significantly larger than unity in which case the propulsive motion dominates over the thermal fluctuations. A balance between attaining stability and minimizing the hydrodynamic drag is necessary in achieving optimal propulsion and efficiency. We show results for optimizing the relevant physical parameters for maximum efficiency of passive nanoswimmers.

[1] Cohen, Richard N., et al. "Molecular motors as drug delivery vehicles." *Drug Discovery Today: Technologies* 2.1 (2005): 111-118; Tottori, Soichiro, et al. "Magnetic helical micromachines: fabrication, controlled swimming, and cargo transport." *Advanced materials* 24.6 (2012): 811-816.

[2] Walker, D., et al. "Optimal length of low Reynolds number nanopropellers." *Nano letters* 15.7 (2015): 4412-4416; Morozov, Konstantin I., and Alexander M. Leshansky. "The chiral magnetic nanomotors." *Nanoscale* 6.3 (2014): 1580-1588.

[3] Ollila, Santtu TT, et al. "Fluctuating lattice-Boltzmann model for complex fluids." *The Journal of chemical physics* 134.6 (2011): 064902; Mackay, F. E., S. T. T. Ollila, and Colin Denniston. "Hydrodynamic forces implemented into LAMMPS through a lattice-Boltzmann fluid." *Computer Physics Communications* 184.8 (2013): 2021-2031.

The in-silico lab-on-a-chip: high-throughput simulations of microfluidics at cell resolution

Dmitry Alexeev [1], D. Rossinelli [1], C. Conti [1], P. Hadjidoukas [1], S. Litvinov [1], K. Lykov [2], I. Pivkin [2], P. Koumoutsakos [1]
[1] Swiss Federal Institute of Technology, Zurich, Switzerland
[2] University of Italian Switzerland, Lugano, Switzerland

We focus on microfluidic systems for the mechanical detection and characterization of individual Circulating Tumor Cells (CTC) and CTC clusters as prognostic markers of metastatic cancer. Our goal is to help improve the rational design of such systems through simulations that capture the behaviour of fluids and cells in microscale confinement. Our simulations are based on an extension of Dissipative Particle Dynamics (DPD). DPD is a mesoscale simulation technique that has been shown to accurately resolve solid-fluid-cell interactions with sub-micron resolution. We have developed uDeviceX, a high-throughput software with kernels thoroughly optimized for GPUs, for microfluidics simulations using DPD models. The software has performed unprecedented simulations of blood flow and CTCs with sub-micron resolution in realistic microfluidic geometries. In this work as a proof of the capabilities of our software we simulate flows of RBCs and CTCs in the CTC-iChip [1]. The CTC-iChip is a microfluidics system that has shown great potential for blood separation and capture of CTCs. The one-to-one geometric correspondence between the CTC-iChip and the geometries studied herein, allow us to confirm these features.

[1] N. Karabacak, P. Spuhler, F. Fachin, E. Lim, V. Pai, E. Ozkumur, J. Martel, N. Kojic, K. Smith, P. Chen, J. Yang, H. Hwang, B. Morgan, J. Trautwein, T. Barber, S. Stott, S. Maheswaran, R. Kapur, D. Haber, and M. Toner. *Microfluidic, marker-free isolation of circulating tumor cells from blood samples. Nat. Protoc.*, 9(3):694–710, 2014.

Unravelling the salvinia effect: a route to robust submerged superhydrophobicity

Matteo Amabili [1], Alberto Giacomello [1], Simone Meloni [1], Carlo Massimo Casciola [1]
[1] University of Rome " La Sapienza"

A surface wetted by a liquid can show a number of remarkable macroscopic behaviors including self-cleaning, anti-fouling, and drag reduction to list only a few examples. Operationally, surfaces exhibiting those properties are usually referred to as superhydrophobic, and are obtained experimentally by combining materials of suitable chemical composition with a micro/nano-structuring of the surface. These surfaces exhibit two (meta)stable states: the Cassie state, responsible for the superhydrophobic properties, in which gas/vapor bubbles are entrapped in the roughness, and the Wenzel state, in which the liquid completely wets the surface corrugations. Obviously, under suitable conditions, the liquid can also be completely transformed into vapor. The simple paradigm of combination of hydrophobic chemistry with surface corrugation to enhance the water-repellent properties of the surfaces has been challenged by recent findings which show that in nature the surface of some water floating plants contains hydrophilic patches. This is the case, for example, for the *Salvinia molesta* water fern. The *Salvinia* has leaves with a unique re-entrant structure and which are characterized by heterogeneous chemistry. This combination is capable of stabilizing an air layer underwater (*Salvinia* effect). The question we try to address in this work is the combination of chemical heterogeneities and surface texturation help improving the hydrophobicity of these surfaces. To achieve this objective we have performed atomistic rare event simulations of a model system mimicking the structural and chemical features of the *Salvinia* leaves. Our results shows that the re-entrant geometry together with the heterogeneous chemistry control the free-energy barriers for the Cassie-Wenzel and Cassie-vapor states. These findings can be translated into simple design criteria which make it possible to engineer robust superhydrophobicity for submerged applications [1][2].

[1] Amabili M., Giacomello A., Meloni S., Casciola C. M. (2015). *Unraveling the Salvinia Paradox: Design Principles for Submerged Superhydrophobicity*. *Adv. Mater. Interfaces*, 2: . doi: 10.1002/admi.201500248

[2] Amabili M., Lisi E., Giacomello A., Casciola C. M. (2015). *Wetting and cavitation pathways on nanodecorated surfaces*. *In review*

Fluctuating hydrodynamics of contact lines

Daniele Belardinelli [1], Mauro Sbragaglia [1], Markus Gross [2], Bruno Andreotti [3]

[1] University of Rome "Tor Vergata", Rome, Italy;

[2] Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany;

[3] Physique et Mécanique des Milieux Hétérogènes, Paris, France

We consider the influence of thermal fluctuations on the dynamics of thin fluid films close to solid boundaries. Working within the stochastic lubrication approximation, we explore the modifications induced by thermal fluctuations to the classical (i.e. zero temperature limit) profiles describing the behaviour of a liquid wedge close to solid boundaries. The problem studied is a pre-requisite to go deeper into the non-hydrodynamical origin of the slip length, the effect which must cure the singular behaviour of the Navier-Stokes equations close to the contact line.

Brownian motion near cell membranes: theory and simulations

Abdallah Daddi Moussa Ider [1], Achim Guckenberg [1], Stephan Gekle [1]

[1] Biofluid Simulation and Modeling, Fachbereich Physik, Universität Bayreuth, Germany

We study the translational Brownian motion of a small particle nearby a realistically modeled red blood cell. At leading order (when the particle is far away from the elastic membrane) we compute the correction to the frequency dependent mobility tensor. We find that hydrodynamic interactions create a memory effect in the particle dynamics. Therefore, a generalized Langevin equation is applied in order to evaluate the particle mean-squared displacement, in the overdamped regime. At the intermediate time scales of motion, we find that the particle undergoes a subdiffusion, with a local scaling exponent as low as 0.9 in the parallel direction, and as low as 0.8 in the perpendicular direction. A good agreement is found between the theoretical predictions and the numerical simulations that we perform using a completed double layer boundary integral equation method.

Effects of hydrodynamic interactions on the apparent 1d mobility of a non-specifically bound protein following a helical path around DNA

Maciej Długosz [1]

[1] Centre of New Technologies, University of Warsaw

We investigated effects of hydrodynamic interactions on diffusivities of proteins that undergo rotation-coupled sliding along DNA [1]. For that, we applied numerical calculations of mobility and friction tensors to systems consisting of detailed bead-shell models of DNA and proteins of different size. Using tensors that result from these calculations along with an expression for the instantaneous energy dissipation rate due to motions of a non-specifically bound protein that follows a helical track around DNA, we evaluated apparent one-dimensional friction and mobility coefficients for model proteins [2]. The results that we obtained indicate that hydrodynamic interactions between DNA and proteins may substantially (even several-fold) reduce the apparent one-dimensional diffusivity of proteins, when compared with results of other theoretical analyses of the rotation-coupled sliding of proteins along DNA that neglect hydrodynamic effects [3,4]. Moreover, accounting for hydrodynamic effects decreases the gap between values of diffusion coefficients of proteins on DNA measured experimentally and those estimated based on theoretical calculations and analyses applied to model systems [1,3,4]. Altogether, our study gives insights into the significance of hydrodynamic interactions in determination of the rate of finding target sites by DNA-binding proteins.

[1] P.C Blainey, G.Luo, S.C.Kou, W.F.Mangel, G.L.Verdine, B.Bagchi, X.S.Xie, *Nat.Struct.Mol.Biol.* 16 1224 (2009)

[2] M. Długosz, *J. Phys. Chem. B* 119 14433 (2015)

[3] J.M. Schurr, *Biophys. Chem.* 9 413 (1979) 8232;

[4] B. Bagchi, P.C. Blainey, X.S. Xie, *J. Phys. Chem. B* 112 6282 (2008)

Simulating the fluctuating Lattice Boltzmann equation via Metropolis Monte Carlo: some tentative ideas, and some sobering results

Burkhard Duenweg [1][2][3], Thomas Balles [2]

[1] Max Planck Institute for Polymer Research, Mainz, Germany;

[2] Institute for Solid State Physics, Technical University Darmstadt, Germany;

[3] Monash University, Melbourne, Australia

Lattice Boltzmann simulations are based upon a fully discretized version of the linearized Boltzmann equation, and can be used as an efficient solver for hydrodynamics. At micro- and nanoscales, the inclusion of thermal fluctuations becomes a necessity. The conventional existing approach to do this is the solution of a discretized Langevin equation [1-3]. The stochastic collisions can also be viewed as a Monte Carlo procedure that satisfies the underlying principle of detailed balance [2]. The main steps of reasoning to derive the procedure are briefly outlined. So far the algorithm has been limited to a harmonic approximation to the governing Boltzmann entropy. We therefore test the idea to instead do stochastic collisions via a simple Metropolis procedure, where the full Boltzmann entropy directly enters the acceptance criterion. While it is obvious that this satisfies the detailed balance condition, it is also expected to be intrinsically stable, due to the nonlinear feedback built into the trial-accept procedure, combined with the rigorous and theory-based exclusion of negative populations. The trial populations are generated in such a way that mass and momentum are conserved; a heuristic procedure for doing this is derived from the existing algorithm of Refs. [1,2]. The dynamics of the new algorithm can be rigorously analyzed in the limit of weak collisions and weak deviation from local equilibrium, where it turns out to be equivalent to the known stochastic BGK implementation of Refs. [1,2]. The underlying reason is that in the limit of very high acceptance rates the Metropolis algorithm may be viewed as a Langevin solver [4,5]. However, it turns out that in this limit the necessary separation of time scales between local stress relaxation and large-scale hydrodynamics breaks down, such that the procedure becomes unsuitable for its original purpose. In the opposite limit of strong collisions the new procedure works, provided that complete relaxation into local equilibrium is enforced by doing not only one, but many Metropolis collision steps, which is again inefficient. Future work is needed to find a better way to do this.

[1] R. Adhikari, K. Stratford, M. E. Cates, and A. J. Wagner, *Europhysics Letters*, 71(3):473, 2005.

[2] B. Duenweg, U. D. Schiller, and A. J. C. Ladd, *Physical Review E*, 76(3):036704, 2007.

[3] G. Kaehler and A. J. Wagner, *Physical Review E*, 87(6):063310, 2013.

[4] K. Kikuchi, M. Yoshida, T. Maekawa, and H. Watanabe, *Chemical Physics Letters*, 185(3–4):335-338, 1991.

[5] K. Kikuchi, M. Yoshida, T. Maekawa, and H. Watanabe, *Chemical Physics Letters*, 196(1–2):57-61, 1992.

Simulating soft-matter with stochastic wavelet hydrodynamics

Oliver Dyer [1], Robin Ball [1]

[1] University of Warwick, Coventry, United Kingdom

A new approach is developed for simulating dilute and semi-dilute soft-matter systems, using stochastically generated wavelets to evolve the system. In this method hydrodynamics appears automatically with a large number of wavelet moves, making both the solvent molecules and diffusion tensor implicit. As a result, the use of wavelets gains both simplicity and computational efficiency over established methods, such as Lattice Boltzmann and Brownian Dynamics. The algorithm is used on polymer solutions to show its validity and to confirm the theoretical scaling of its computational costs.

Multiscale simulation with Smoothed Dissipative Particle Dynamics

Gérôme Faure [1], Julien Roussel [2], Jean-Bernard Maillet [1], Gabriel Stoltz [2]

[1] CEA, Paris, France

[2] CERMICS, Marne-la-Vallée, France

Smoothed Dissipative Particle Dynamics [1] is a mesoscopic top-down method which is based on a particle discretization of the Navier-Stokes equations. The mesoscopic size of the fluid particles are taken into account by adding thermal fluctuations. We focus on establishing a link between the SDPD model and an underlying microscopic system so as to ensure thermodynamical consistency, which constitutes the first step if one wants to couple the two methods in a multiscale hybrid simulation. We formulate the SDPD equations using energy variables rather than entropies, thus enabling natural coupling with the DPDE equations. Equilibrium NVT simulations at several thermodynamical conditions are performed in order to tabulate an equation of state for subsequent SDPD simulations, thus ensuring thermodynamic consistency between the two models. We quantify the agreement between the reference microscopic system and the SDPD systems at various resolutions, and propose finite size corrections in order to enhance the consistency for moderately large SDPD particles. With this result in mind, we propose a coupling between different SDPD scales in a concurrent multiscale simulation and test it at equilibrium. The simulation domain is divided into two main regions: one discretized with small SDPD particles and the other one with larger SDPD particles. The transition between the two sizes is done by splitting or merging particles in a buffer region at the interface between the two domains.

[1] P. Español and M. Revenga, *Phys. Rev. E* 67 026705 (2003)

The collapse of a cavitation nano-bubble near a solid boundary

Mirko Gallo [1], Francesco Magaletti [1], Luca Marino [1], Carlo Massimo Casciola [1]

[1] University of Rome "La Sapienza"

The implosion of a cavitation bubble close to a solid boundary is a widely investigated problem in fluid mechanics, due to its many scientific interactions with several fields of applied and theoretical science, such as material science, biochemistry and nanotechnology. In the present work a diffuse interface model is used to address the dynamics of a vapor nano bubble collapsing near a solid wall [1]. Bubble collapse is triggered by a normal shockwave in the liquid. This formulation enables an unprecedented description of physical phenomena occurring in cavitation collapse, namely: interfacial flow, phase transition to and from the supercritical state, shockwave emission and liquid jet formation [2]. Numerical simulations show that the bubble dynamics is characterized by a

sequence of rebounds: when the bubble reaches its minimum volume, huge temperature and pressure values are detected. These peaks are considered the precursors of the shockwaves observed in cavitation experiments. After the collapse, the bubble starts to expand back up to a maximum volume. During this stage the temperature decreases and vapor formation is observed. The process ends with the full condensation of the bubble. By increasing the strength of the triggering shockwave one observes a microjet focused toward the wall that pierces the bubble which then assumes a toroidal shape. The aforementioned effects shed light on the mechanism of cavitation damage.

[1] Magaletti, F., Gallo, M., L. Marino, and C. M. Casciola. "Shock-induced collapse of a vapor nanobubble near solid boundaries.", *In review*.

[2] Magaletti, F., L. Marino, and C. M. Casciola. "Shock Wave Formation in the Collapse of a Vapor Nanobubble." *Physical Review Letters* 114.6 (2015): 064501.

Ideal polymers: equilibrium properties from non-equilibrium processes

Raz Halifa Levi [1], Yacov Kantor [1]

[1] Tel Aviv University, Israel

We consider several cases of an ideal polymer being dragged by an external force. The work W in such a process depends on the initial state of the polymer, and its distribution can be related to the difference in the free energy ΔF between the initial and the (equilibrated) final states by the means of Jarzynski equality [1]. We consider both Newtonian and over-damped Langevin dynamics, for a polymer moving in a free space or initially located near a repulsive wall. We reconstruct (either analytically or numerically) the distribution of W , and demonstrate that there is a critical velocity v_c such that for $v > v_c$ such reconstruction is, practically, impossible. The velocity v_c depends on the number of monomers and other parameters of the problem.

[1] C. Jarzynski, *Phys. Rev. Lett.* 78.2690 (1997).

Dissipative Particle Dynamics simulation of DNA linearization by a squeezing flow in a nanoscale tube

Minsub Han [1]

[1] Incheon National University, South Korea

Deoxyribose nucleic acid (DNA) is the macromolecule for genetic information storage of all living organisms. Squeezing the solution in flexible nanoscale channel proved to be a highly effective method for fully linearizing DNA [1], which could be an initial step in one of the important methods to probe the vital information in biological and clinical settings. The detailed physical basis of the process is studied by using Dissipative Particle Dynamics simulation, whose results corresponds to the lambda DNA in the nanoscale PDMS tube in the experiment. The squeezing process typically consists of a large degree of elongational flow, which is followed by relaxing back and adjusting to the narrower confinement. Strong elongation by flow and nanoscale confinement are the major thrust for linearization in the process. The degree of the linearization primarily positively correlates with the initial degree of extension at the start of the strain release as well as the contour length.

[1] T. Matsuoka, B.C. Kim, J. Huang, N.J. Douville, M.D. Thouless, S. Takayama, *Nanoscale squeezing in elastomeric nanochannels for single chromatin linearization*, *Nano Lett.* 12 (2012) 6480-6484.

Modelling of polymer membrane formation

Manuel Hirschler [1], Christian Zander [1], Ulrich Niekén [1]

[1] Institute for Chemical Process Engineering, University of Stuttgart, Germany

Direct modelling of different preparation processes of polymer membranes is highly challenging. The basic mechanism to prepare polymer membranes is based on precipitation of a polymer solution which then separates into two stable phases forming pores and matrix of the membrane

[1]. Since the underlying physical processes (e.g. phase decomposition, coarsening, gelation, etc.) are observed on different time and length scales, the computational effort is immense for molecular simulations. In addition, the detailed mechanisms are not totally understood in theory and most of the explanations came from experimental observations. Therefore, it is recommended to find a fundamental theory to explain all observed effects on morphology of polymer membranes. Since the dynamic of pore formation like phase decomposition is driven by mesoscale effects fluctuating hydrodynamics have to be considered. One mesoscale method including fluctuations is Smoothed Dissipative Particle Dynamics (SDPD) [2]. We present a SDPD model for polymer membrane formation and discuss the effect of fluctuations on the dynamic of pore formation.

[1] S. Loeb and S. Sourirajan: *Sea Water Demineralization by Means of an Osmotic Membrane. Advan. Chem. Ser., 38, 117 (1962).*

[2] P. Espanol and M. Revenga: *Smoothed dissipative particle dynamics. Phys. Rev. E 67, 026705 (2003).*

Coil-stretch hysteresis in planar mixed flows of polymer solutions at finite concentrations

Ravi Prakash Jagadeeshan [1], Chandi Sasmal [1]

[1] Department of Chemical Engineering, Monash University, Melbourne, Australia

In 1974, de Gennes conjectured that in extension-dominated flows, depending on the deformation history, it is possible for a dilute polymer solution to manifest multiple values of stress at a single strain rate, and consequently exhibit hysteretic behaviour. The importance of de Gennes contention has paradigm changing implications for the modelling of polymer solution rheology. Experimental proof for de Gennes hypothesis was established 30 years later by showing individual DNA molecules in ultra-dilute solutions subjected to planar elongational flow can be either coiled or highly stretched depending on the history of deformation [1]. While de Gennes arguments and the experimental validation were restricted to dilute solutions, recent scaling arguments [2] and experiments [3] carried out at Monash University suggest that the concentration of polymers has a significant non-monotonic influence on the extent of coil-stretch hysteresis. Additionally, it has been known since de Gennes early theory, that increasing the fraction of shear in a mixed flow of planar shear and extension dramatically decreases the magnitude of coil-stretch hysteresis. We discuss the development of a mesoscopic Brownian dynamics simulation algorithm that is capable of accurately describing polymer solutions undergoing planar mixed flows at finite polymer concentrations [4]. The simulations permit the examination of the competing roles of polymer concentration and flow mixedness on the extent of coil-stretch hysteresis, and provide a fascinating insight into the influence of non-linear phenomena on the molecular scale on macroscopic solution properties.

[1] Schroeder, C.M., Babcock, H.P., Shaqfeh, E.S.G., Chu, S., *Observation of Polymer Conformation Hysteresis in Extensional Flow, Science, 301, 1515-1519 (2003).*

[2] Prabhakar, R., *Influence of stretching induced self-concentration and self-dilution on coil-stretch hysteresis of unentangled polymer solutions, J. Rheol., In press (2016).*

[3] Prabhakar, R., Sasmal, C., Nguyen, D. A., Sridhar, T., Prakash, J. R., *Rheological observation of coil-stretch transition in elongational flows of unentangled polymer solutions, under preparation, Phys. Rev. Lett. (2016).*

[4] Jain, A., Sasmal, C., Hartkamp, R., Todd, B.D., Ravi Prakash, J., *Brownian Dynamics Simulations of Planar Mixed Flows of Polymer Solutions at Finite Concentrations, Chem. Eng. Sci., 121, 245-257 (2015).*

Shear and bulk viscosity of a DPD-fluid

Gerhard Jung [1]

[1] Johannes Gutenberg-Universität, Mainz, Germany

Exact values for shear and bulk viscosity are important to characterize a solvent and a necessary input for a continuum description. There exist various well-known methods to study the rheology of fluids that are interacting via conservative forces only. However, the correct treatment of random and dissipative forces is still under debate. In this poster we present fully consistent results for both viscosities using Green-Kubo relations and non-equilibrium molecular dynamics (NEMD).

Green-Kubo relations are calculated using the formulas derived by Ernst and Brito [1], while NEMD results were obtained using a novel technique based on an idea of Müller-Plathe [2].

[1] M.H. Ernst, R. Brito, *Europhys. Lett.* 73 183 (2006)

[2] Florian Müller-Plathe, *Phys. Rev. E* 59 4894 (1998)

A nonlinear Langevin coarse-grained model for electrospinning simulations

Marco Lauricella [1], G. Pontrelli [1], D. Pisignano [2] [3], S. Succi [1]

[1] Istituto per le Applicazioni del Calcolo-CNR, Rome, Italy.

[2] Dipartimento di Matematica e Fisica "Ennio De Giorgi", Università del Salento, Lecce, Italy

[3] Istituto Nanoscienze-CNR, Euromediterranean Center for Nanomaterial Modelling and Technology (ECMT), Lecce, Italy.

The production of nanofibres has increasingly gained attention in recent years due to the broad number of promising applications including filtration, textile, medical, protective, structural, electrical, and optical. Nowadays, the electrospinning process is exploited on industrial scale for the production of nanofibres. In this process, the nanofiber is obtained by the stretching of a polymeric liquid droplet driven by an intense electric field which pushes the liquid jet away from a nozzle towards a conductive collector. During the jet dynamical evolution, hydrodynamic perturbations, as well as mechanical vibrations at the nozzle, usually misalign the jet from its stretching axis providing a region of chaotic bending instability, which characterizes the fluid dynamics. These instabilities increase the path traveled by the jet between the nozzle and the collector, and consequently the stream cross-section is further decreased along the way. As a consequence, bending instabilities play an important role for nanofibre quality. Following the approach of Reneker et al. [1], we present a Lagrangian coarse-grained model, where the liquid jet is modelled as a series of charged beads, connected by viscoelastic springs. By this model, we probe the effects of the dissipative air drag force combined with the other main forces (Coulombic, electrical viscoelastic, etc.) on the jet dynamics. In particular, based on experimental observations, we have included a Brownian noise to account for dissipative air drag effects, obtaining a nonlinear Langevin-like stochastic differential equation, which is solved by a modified Runge-Kutta stochastic scheme. We found that this perturbation force changes significantly the dynamics of the jet, by reducing its uni axial elongation at the early stage, and opens new perspectives to control the efficiency of the process and the quality of the spun fibres [2]. Furthermore, encompassing these efforts, we delivered, along with the overall model, a detailed algorithm and the corresponding FORTRAN code, JETSPIN, specifically designed to simulate the electrospinning process under a variety of different conditions and experimental settings [3].

[1] Reneker, D. H., Yarin, A. L., Fong, H., Koombhongse, S. (2000), *Bending instability of electrically charged liquid jets of polymer solutions in electrospinning*, *Journal of Applied physics*, 87(9), 4531-4547.

[2] Lauricella, M., Pontrelli, G., Pisignano, D., Succi, S. (2015), *Nonlinear Langevin model for the early-stage dynamics of electrospinning jets*, *Molecular Physics*, 113, 2435-2441.

[3] Lauricella, M., Pontrelli, G., Coluzza, I., Pisignano, D., Succi, S. (2015), *JETSPIN: a specific-purpose open-source software for simulations of nanofiber electrospinning*, *Computer Physics Communications*, 197, 227-238.

A finite volume method for fluctuating hydrodynamics of simple fluids

Kiran Narayanan [1], Ravi Samtaney [1], Brian Moran [1]

[1] King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Fluctuating hydrodynamics (FHD) accounts for stochastic effects that arise at mesoscopic and macroscopic scales. We present a finite volume method for numerical solutions of the fluctuating compressible Navier Stokes equations. Case studies for simple fluids are demonstrated via the use of a perfect gas equation of state. We extend the fourth order conservative finite volume scheme originally developed by McCorquodale and Colella [1], to evaluate the deterministic and stochastic fluxes. The expressions for the cell-centered discretizations of the stochastic shear stress and stochastic heat flux are adopted from the results by Espanol [2], where the discretizations were

shown to satisfy the fluctuation-dissipation theorem. A third order Runge-Kutta scheme with weights proposed by Delong et. al. [3] is used for the numerical time integration. Comparisons of the numerical solution against theoretical solutions will be presented. Accuracy of the proposed scheme will be demonstrated.

[1] P. McCorquodale & P. Colella, *A high-order finite-volume method for conservation laws on locally refined grids*, CAMCOS,6(1),2010

[2] P. Espanol, *Stochastic differential equations for non-linear hydrodynamics*, Physica A, 248,1998

[3] S. Delong, B. E. Griffith, E. Vanden-Eijnden, and A. Donev, *Temporal integrators for fluctuating hydrodynamics*, Phy. Rev. E, 87 (2013)

A study of water on metal surfaces using a simple water model

Chanwoo Noh [1], YounJoon Jung [1]

[1] Seoul National University, Seoul, Korea

We introduce a simple two dimensional water model to describe water molecules on metal surfaces. In this model, water molecules are modeled as two-dimensional Lennard-Jones disks, with three orientation-dependent hydrogen bonding arms. The phase transition between an ice and a liquid water phase is reproduced in our model. In this work, the thermodynamic and dynamic properties of water on metal surfaces are studied. The structure of water on metal surfaces is highly affected by metal surfaces. By regulating the adsorption energy of water molecules, the ice structure, which was reported in experiments, is reproduced. In addition to the thermodynamic behavior, the anomalous diffusion behavior of water is observed. The diffusion anomaly is caused by the hydrogen bonds and the empty space of water. At last, the dynamic heterogeneity of water is analyzed by the method frequently used in supercooled liquid system.

[1] J. Carrasco et al., *Nature Mater.* 11 667 (2012)

[2] K. A. T. Silverstein et al., *J. Am Chem. Soc.* 120 3166 (1998)

[3] A. Scutkins et al., *Comput. Phys. Commun.* 190 129 (2015)

Charge screening mechanism in graphene oxide supercapacitors: Molecular Dynamics simulation study

Sang-Won Park [1], Andrew D. DeYoung [2], Nilesh R. Dhumal [2], Youngseon Shim [1], Hyung J. Kim [2,3], YounJoon Jung [1]

[1] Seoul National University, Seoul, Korea;

[2] Carnegie Mellon University, Pittsburgh, USA;

[3] Korea Institute for Advanced Study, Seoul, Korea

Electric double layer capacitors (EDLCs), or supercapacitors, are promising devices for energy storage applications due to their reasonable energy density and high power density [1]. In this study [2,3], Molecular Dynamics (MD) simulations are performed to study graphene oxide supercapacitors in the parallel plate configuration. The oxidation range of the electrode is varied from 0% (pure graphene) to 100% (fully oxidized GO) by decorating the graphene surface with hydroxyl groups. Ionic liquids (IL) and organic electrolytes (OE) are employed as electrolytes, where the IL is 1-ethyl-3-methylimidazolium tetrafluoroborate (EMI+BF4-) and the OE is its solution with acetonitrile. It is found that BF4- screens the electrode charges more effectively than EMI+, and the effective shielding by BF4- arises from its small size. The area-specific capacitance tends to decrease with increasing electrode oxidation, but its detailed screening mechanism shows an interesting difference between the anode and the cathode. The details are revealed by varying the electrode oxidations and by comparing the IL and the OE. The interesting difference is explained in terms of hydrogen bonding and screening ability.

[1] Wang, G.; Zhang, L.; Zhang, J., *Chem. Soc. Rev.* 41, 797 (2012).

[2] A. D. DeYoung, S.-W. Park, N. R. Dhumal, Y. Shim, Y. Jung and H. J. Kim, *J. Phys. Chem. C* 118, 18472 (2014).

[3] S.-W. Park, A. D. DeYoung, N. R. Dhumal, Y. Shim, H. J. Kim and Y. Jung, *in preparation*.

Dynamics and growth of clusters in freely cooling granular fluid

Subhajit Paul [1], Subir K. Das [1]

[1] Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India

In this work [1], we have studied the structure and dynamics in a model granular fluid of hard particles in space dimensions $d = 1, 2$ and 3 , via event driven molecular dynamics simulations. Inelastic collisions, described by the coefficient of restitution e , among the particles lead to energy decay and clustering. We investigate both $e = 0$ and $e > 0$ cases, to be referred to as the sticky gas (SG) and granular gas (GG), respectively. Occurrence of the clustering, referred to as the inhomogeneous cooling state (ICS), is delayed for GG. In this time regime, the density inhomogeneity in the GG resembles pattern formation in a vapor-liquid phase transition. On the other hand, interesting fractal-like structures form in the case of SG, having similarity with the pattern formation in diffusion limited aggregation. Exponents related to the growth of these clusters, for various values of e and overall particle density $\hat{\rho}$, are quantified via the finite-size scaling technique. Validity of a scaling theory [2], relating the growth of average cluster mass with that of energy decay, predicted for the SG, is tested and discussed in the general context. It appears, the decay of kinetic energy in ICS, irrespective of the value of e follows power-law in time (t), $E(t) \sim t^{-\hat{\nu}}$, with unique exponent $\hat{\nu} = 2d/(d + 2)$, predicted by the above mentioned scaling theory. However, the growth of mass in GG is in disagreement with that of SG.

[1] S. Paul and S. K. Das, *Europhys. Lett.*, 108, 66001 (2014).

[2] G. F. Carnevale, Y. Pomeau, and W. R. Young, *Phys. Rev. Lett.*, 64, 2913 (1990).

Open Boundary Molecular Dynamics of sheared star-polymer melts

Jurij Sablić [1], Matej Praprotnik [1], Rafael Delgado Buscalioni [2]

[1] Laboratory for Molecular Modeling, National Institute of Chemistry, Ljubljana, Slovenia

[2] Departamento Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain

We present Open Boundary Molecular Dynamics (OBMD) simulation of a melt of star polymers, i.e. molecules composed of several linear polymeric chains attached to the central monomer. The simulation box is open in one direction, enabling the exchange of mass and momentum with the surroundings. The simulations are run under fixed normal load, which is, together with shear flow, imposed to the system as a boundary condition at the open ends. We study rheological and structural properties of the sheared melt under fixed normal load and compare them with the ones obtained from simulations under constant volume, in which the shear flow is introduced by modification of the equations of motion and boundary conditions. The results indicate that in equilibrium the melt under constant load exhibits grand-canonical behavior. Furthermore, the density of the melt decreases with the increase of the strength of shear flow, as opposed to the constant volume case, where it remains constant. The two cases also yield some different rheological properties of the melt, while the results coincide in the majority of the structural ones.

Inertial migration of elastic capsules in poiseuille flow

Christian Schaaf[1], Kevin Irmer [1], Christopher Prohm [1], Holger Stark [1]

[1] Technische Universität Berlin, Germany

Deformable particles such as capsules, vesicles, and red blood cells assemble at fixed equilibrium positions in a microfluidic channel. This behavior can be used to separate particles with different cell properties. For example, softer cells travel closer to the center than stiffer ones. Using the lattice-Boltzmann method, we study the dynamics of single deformable particles in a microfluidic channel for intermediate Reynolds numbers. We show that particles move to different equilibrium position depending on their size and deformability. For Reynolds numbers below 100, their equilibrium positions collapse onto a single master curve depending only on the Laplace number.

The steady state of the particles is determined by the lift force profiles, which we determine for different channel aspect ratios.

The Cassie-Wenzel transition of fluids on nanostructured substrates: Macroscopic force balance versus microscopic Density-Functional Theory

Nikita Tretyakov [1], Burkhard Dünweg [1][2][3], Periklis Papadopoulos [1][4], Doris Vollmer [1], Hans-Jürgen Butt [1], Kostas Ch. Daoulas [1]

[1] Max Planck Institute for Polymer Research, Mainz, Germany

[2] Institut für Festkörperphysik, Technische Universität, Darmstadt, Germany

[3] Monash University, Melbourne, Australia

[4] Physics Department, University of Ioannina, Greece

Classical density functional theory is applied to investigate the validity of a phenomenological force-balance consideration to describe the stability of the Cassie state of liquids deposited on substrates with nanoscale corrugation. A bulk free-energy functional of third order in local density is combined with a square gradient term that describes the liquid-vapor interfacial tension. The bulk parameters are chosen to reproduce the liquid density and the compressibility of water. The interface term is adjusted to model the gas-liquid interfacial width. The influence of the substrate is taken into account via an external potential, based upon standard Lennard-Jones interactions, such that the three-dimensional corrugation geometry is explicitly modeled. The present study focuses on substrates patterned with nanostripes and square-shaped nanopillars. Using both the force-balance relation and density-functional theory, we locate the Cassie-to-Wenzel transition as a function of the corrugation parameters. We demonstrate that the force-balance relation gives a qualitatively reasonable description of the transition even on the nanoscale. However, a straightforward attempt to employ the Young contact angle quantitatively fails and smaller values have to be applied instead. These effective contact angles therefore describe not only the interplay between the hydrophobicity and the water-vapor interface but also embody the effects of line tension and the finite interface thickness. This suggestion is supported by the fact that for large periods of substrate corrugation the striped and pillared geometry yield the same effective contact angles.

Study of lipid bilayer membrane using Dissipative Particle Dynamics

Rakesh Vaiwala [1]

[1] IIT Bombay, India

Nearly four decades ago, W. Helfrich theorized the quantitative nature of steric hindrance between biomembranes, and proposed that this entropic repulsion due the thermal fluctuations of membrane decays as $1/d^3$ (where d is the distance between two biomembranes). Recently Freund's analysis on the steric interaction between biomembranes in a periodic stack concludes that the force decays as $1/d$. To resolve this contradiction, we have set up dissipative particle dynamics simulations on the system of two juxtaposed planar bilayers. Our approach is to look for an appropriate functional form of the height fluctuations in reciprocal space by introducing a distance dependent term; the parameter that decays to zero in the limit of d tending to infinity. It would bring about the thorough understanding and interpretation of the repulsion between bilayers. The work is currently in progress.

Mesosopic simulation of binary fluid mixtures using SDPD

Christian Zander [1], Manuel Hirschler [1], Ulrich Niekén [1]

[1] Institute for Chemical Process Engineering, University of Stuttgart, Germany

The processes, which determine the morphology of many porous media as for example polymer membranes, take place on very short, mesoscopic time and length scales. Simulations are a promising tool to get an understanding of the relevant processes, but should account for thermal

fluctuations to be applicable at these scales. We adapt the SPH/SDPD model for phase separating multicomponent fluid mixtures proposed in [1], which can be extended to account for thermal fluctuations. The model is applied to isothermal, binary systems, which are described by the van der Waals equation of state, and fluctuations of the momentum and the concentration are included. We study fluctuations in an ideal mixture at thermodynamic equilibrium and investigate the effect of fluctuations on the spinodal decomposition of a binary mixture after a temperature quench.

[1] C. Thieulot, L.P.B.M Janssen and P. Espanol, *Phys. Rev. E* 72, 016713 (2005)

Force-assisted desorption of a polymer chain grafted to an attractive surface: first-order transition with slow dynamics and large fluctuations

Shuangshuang Zhang [1], Shuanhan Qi [1], Friederike Schmid [1]

[1] Johannes Gutenberg University, Mainz, Germany

Using Brownian Dynamics simulations, we investigated the static and dynamic properties of an adsorbed polymer chain tethered at one end to a solid structureless surface with a pulling force applied to the other end. The competition between extension and adsorption gives rise to a first-order transition in the thermodynamic limit [1][2][3]. Interestingly, from the point of view of statics the first-order transition has some unusual features: instead of a bimodal curve, the distribution of the order parameter is flat and metastable states are completely absent. Due to the absence of an excess interfacial energy, all the conformations with different phase composition have approximately the same free energy, and strong fluctuations arise. Besides static unusual behavior, the dynamic process also shows unconventional features like second-order critical slowing down. Anomalous slowing down of the large scale relaxation time and substantial fluctuations of the lateral conformation arise. The characteristic relaxation time and the dispersion of the order parameter show a remarkable peak in the vicinity of the transition point, and demonstrate an anomalous pre-transitional growth according to a power law with chain length.

[1] A. A. Gorbunov, A. M. Skvortsov, *J. Chem. Phys.* 98, 5961 (1993).

[2] S. Bhattacharya, V.G. Rostkashvili, A. Milchev, T.A. Vilgis, *Phys. Rev. E* 79, 030802(R) (2009)

[3] A. M. Skvortsov, L. I. Klushin, A. A. Polotsky, and K. Binder, *Phys. Rev. E* 85, 031803 (2012).

Nanodroplet evaporation of pure liquids and nanoparticle suspensions on solid surfaces

Jianguo Zhang* [1], Frédéric Leroy [1], Florian Müller-Plathe [1]

[1] Technische Universität Darmstadt, Darmstadt, Germany

(*Now in Max-Planck Institute for Polymer Research, Mainz, Germany)

The evaporation of nanodroplets of pure liquids and nanoparticle suspensions on solid surfaces has been studied by Molecular Dynamics (MD) simulation. For the pure liquid case, the relationship between contact line pinning and surface heterogeneities is addressed in detail at the nanoscale [1]. It is found that the droplet evaporation is a direct signature of the typical size of the surface heterogeneity. The contact angle both at equilibrium and during evaporation could be predicted from a local Cassie-Baxter equation in which the interactions within a distance of seven fluid-particle diameters around the contact line were considered, indicating the local nature of the interactions that drive the wetting behavior (e.g. the contact angle) of droplets. At the same time, we propose a nanoscale explanation of pinning during evaporation. Pinning should be interpreted as a drastic slowdown of the contact line dynamics rather than a complete immobilization of it during a transition between two contact angle boundaries. For the nanoparticle suspension evaporation, our results show that the evaporation rate, the interaction parameters between different components and the shapes of the nanoparticles are all very important for the final deposit pattern after complete evaporation [2].

1. Jianguo Zhang, Florian Müller-Plathe and Frédéric Leroy, *Langmuir*, 2015, 31 (27), pp 7544–7552.

2. Jianguo Zhang, Frédéric Leroy, Florian Müller-Plathe, *In preparation*.

5 Participant List

Organizers

Duenweg, Burkhard - Max Planck Institute for Polymer Research, Mainz, Germany
Jagadeeshan, Ravi Prakash - Monash University, Melbourne, Australia
Schmid, Friederike - Institute of Physics, Johannes Gutenberg University, Mainz, Germany

Alcanzare, Maria Michiko - Aalto University, Finland
Alexeev, Dmitry - ETH Zurich, Switzerland
Alidadi Soleymani, Fatemeh - Forschungszentrum Jülich, Germany
Amabili, Matteo - University of Rome "La Sapienza", Italy
Ball, Robin - Dept of Physics, University of Warwick, United Kingdom
Belardinelli, Daniele - Department of Physics and INFN, University of Rome Tor Vergata, Italy
Ciccotti, Giovanni - University of Rome "La Sapienza", Italy
Daddi Moussa Ider, Abdallah - Bayreuth University, Germany
Delgado-Buscalioni, Rafael - Autonomous University of Madrid, Spain
Dlugosz, Maciej - University of Warsaw, Centre of New Technologies, Poland
Donev, Aleksandar - Courant Institute, New York University, USA
Dyer, Oliver - University of Warwick, United Kingdom
Ellero, Marco - College of Engineering, University of Swansea, United Kingdom
Español, Pep - National University of Distance Education, Spain
Faure, G r me - CEA, France
Fielding, Suzanne - Durham University, United Kingdom
Gallo, Mirko - Universita di Roma "La Sapienza", Italy
Garcia, Alejandro - Department of Physics, San Jose State University, California, USA
Graham, Mike - Dept. of Chemical and Biological Engr., Univ. of Wisconsin-Madison, USA
Halifa Levi, Raz - Tel Aviv University, Israel
Han, Minsub - Incheon National University, South Korea
Heidari, Maziar - Max Planck Institute for Polymer Research, Mainz, Germany
Hirschler, Manuel - University of Stuttgart, Institute for Chemical Process Engineering, Germany
Ihle, Thomas - North Dakota State University, USA
Jung, Gerhard - Institute of Physics - Johannes Gutenberg Universit t Mainz, Germany
Ladd, Tony - University of Florida, Gainesville, USA
Lauricella, Marco - Istituto per le Applicazioni del Calcolo, Rome, Italy
Maggs, Anthony C. - ESPCI, France
Mima, Toshiki - Toyota Central R&D Labs., Japan
Narayanan, Kiran - KAUST, Saudi Arabia
Noh, Chanwoo - Seoul National University, South Korea
Park, Sang-Won - Seoul National University, South Korea
Park, Gun Woo - DICMaPI University of Naples Federico II, Italy
Paul, Subhajit - Jawaharlal Nehru Centre for Advanced Scientific Research., India
Praprotnik, Matej - National Institute of Chemistry, Slovenia
Sabli c, Jurij - Laboratory for Molecular Modeling, National Institute of Chemistry, Ljubljana, Slovenia
Schaaf, Christian - Technische Universit t Berlin, Germany
Shaqfeh, Eric S. G. - Institute of Computational and Mathematical Engineering, University of Stanford, USA
Stark, Holger - Technische Universit t Berlin, Germany

Szymczak, Piotr - Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Poland

Tretyakov, Nikita - Max Planck Institute for Polymer Research, Mainz, Germany

Vaiwala, Rakesh - Indian Institute of Technology Bombay, India

Wagner, Alexander - North Dakota State University, USA

Zander, Christian - University of Stuttgart, Institute for Chemical Process Engineering, Germany

Zhang, Jianguo - Max Planck Institute for Polymer Research, Mainz, Germany

Zhang, Shuangshuang - Johannes Gutenberg University, Mainz, Germany