School cum Workshop

Fluid-Structure Interactions in Soft-Matter Systems: From the Mesoscale to the Macroscale

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Book of Abstracts

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1 School: Invited Lectures

Numerical Investigations of Coarse-Graining across Time and Length Scales for Soft-Matter Systems

A. A Louis
Rudolf Peierls Centre for Theoretical Physics,
University of Oxford, 1 Keble Road, Oxford OX1 3NP, UK

In soft matter we routinely rely on coarse-graining techniques that make our problems tractable while still (we hope) retaining the essential physics. In this talk I will discuss in some detail a number of "no free lunch" theorems that should be kept in mind when deriving coarse-graining schemes. Techniques and principles for coarse-graining across time-scales to include the combined effects of Brownian motion and hydrodynamic interactions will be emphasised.

The Micromechanics of Colloidal Dispersions

John F. Brady
Chemical Engineering, California Institute of Technology,
Pasadena, CA 91125

What do corn starch, swimming spermatozoa, DNA and self-assembling nanoparticles have in common? They are all (or can be modeled as) "particles" dispersed in a continuum suspending fluid where hydrodynamic interactions compete with thermal (Brownian) and interparticle forces to set structure and determine properties. These systems are "soft" as compared to molecular systems largely because their number density is much less and their time scales much longer than atomic or molecular systems. In this talk I will describe the common framework for modeling these diverse systems and the essential features that any hydrodynamic modeling must incorporate in order to capture the correct behavior. Actually computing the hydrodynamics in an accurate and efficient manner is the real challenge, and I will illustrate past successes and current efforts with examples drawn from the diffusion and rheology of colloids to the "swimming" of catalytic nanomotors.

Introduction to Homogeneous Non-equilibrium Molecular Dynamics Simulation Methods, Part 1

Peter Daivis
School of Applied Sciences, RMIT University,
GPO Box 2476, Melbourne Vic. 3001, Australia

We begin with a discussion of the underlying theory of homogeneous non-equilibrium molecular dynamics (NEMD) simulation methods for single component fluids [1-3]. The balance equations for mass, momentum and internal energy are introduced and the entropy production is derived, and the linear constitutive equations for viscous flow and heat transport are presented. It is shown how methods for simulating rheological flows (the SLLOD algorithm) and heat flow (the Evans heat flow algorithm) in single component fluids follow naturally from these basic equations. Specialised implementations of periodic boundary conditions for rheological flows are illustrated [3]. A treatment of non-linear response theory due to Williams and Evans [4] is outlined and applied to shear flow. The basic ideas behind the various fluctuation theorems are discussed and the main results are summarised [5]. Applications of non-equilibrium molecular dynamics simulation algorithms to shear and elongational flows of simple models of polymer melts and other complex fluids are described [3].

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Introduction to Homogeneous Non-equilibrium Molecular Dynamics Simulation Methods, Part 2

Peter Daivis
School of Applied Sciences, RMIT University,
GPO Box 2476, Melbourne Vic. 3001, Australia

Part 2 begins with a discussion of the concept of temperature from both the macroscopic and microscopic viewpoints, followed by a discussion of homogeneous thermostats for non-equilibrium molecular dynamics simulations [1,2]. The difficulties that can arise due to incorrectly formulated thermostats are pointed out and illustrated with examples [3]. Deviations from local equilibrium for systems that are far from equilibrium and their effect on non-linear properties are discussed [4]. The balance equations and entropy production for two component systems are introduced, followed by a discussion of the relevant linear transport coefficients. Equilibrium and non-equilibrium molecular dynamics methods for computations of the thermal conductivity, mutual diffusion coefficient and thermal diffusion coefficient in two component fluids are introduced [5], and the methods for computing the related thermodynamic quantities are briefly summarised [6].

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Fluctuating Hydrodynamics and the Lattice Boltzmann Method

R. Adhikari
The Institute of Mathematical Sciences
CIT Campus, Taramani, Chennai 600113, India

Local conservation laws imply that changes in momentum in any small volume of fluid must be due to currents from the volume boundary. In addition to currents produced by advection, pressure and velocity gradients, spontaneous thermal fluctuations produce momentum currents. While these are often neglected in large scale flows, they become increasingly important at small scales where, for example, they produce Brownian motion of particles and conformational fluctuations of polymers. The fluctuating lattice Boltzmann equation (FLBE) provides an accurate and computationally efficient method of solving the Landau-Lifshitz equations of fluctuating hydrodynamics. I will describe, together with short numerical examples, the construction and use of the FLBE for solving problems in fluctuating hydrodynamics. I will provide a self-contained introduction to stochastic differential equations, emphasising the fluctuation dissipation relation, followed by the fluctuating Boltzmann equation, from which the fluctuating lattice Boltzmann equation can be derived directly by a discretisation of velocity space. I will briefly describe how external objects can be coupled to the fluctuating fluid and the tests used to verify that both fluid and coupled objects are in (fluctuating) Gibbsian equilibrium.

Numerical Methods for Fluid-Structure Interactions

M. Lukáčová-Medvid'ová
Institute of Mathematics, University of Mainz,
Staudingerweg 9, 55099 Mainz, Germany

In this lecture we give an overview of different numerical techniques used for numerical simulations of fluid-structure interactions. We describe the monolithic and partitioned schemes as well as loosely and strongly coupled schemes. Furthermore we will explain the sources of the so-called added mass effects and their consequences in numerical instabilities of the whole FSI algorithms, see, e.g., [1-4] for further details.

In order to track moving domains different techniques such as the immersed boundary methods, the Lagrangian methods as well as the Arbitrary Eulerian-Lagrangian techniques may be used. In the present talk we will mainly concentrate on the Arbitrary Eulerian-Lagrangian methods and point out the role of the geometric conservation law in order to obtain stable coupling between the fluid and structure. For a particular loosely coupled scheme, the so-called kinematic coupling, we will demonstrate theoretically as well as experimentally its stability.

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A Boundary Integral Method for Deformable Drops

P. Anderson
Eindhoven University of Technology
Eindhoven, The Netherlands

A three-dimensional boundary integral method for deformable drops in viscous flows at low Reynolds numbers is presented. The method is based on a new nonsingular contour-integral representation of the single and double layers of the free-space Green's function. The contour integration overcomes the main difficulty with boundary-integral calculations: the singularities of the kernels. It also improves the accuracy of the calculations as well as the numerical stability. A new element of the presented method is also a higher-order interface approximation, which improves the accuracy of the interface-to-interface distance calculations and in this way makes simulations of polydispersed foam dynamics possible. Moreover, a multiple time-step integration scheme, which improves the numerical stability and thus the performance of the method, is introduced. To demonstrate the advantages of the method presented here, a number of challenging flow problems is considered: drop deformation and breakup at high viscosity ratios for zero and finite surface tension; drop-to-drop interaction in close approach, including film formation and its drainage; and formation of a foam drop and its deformation in simple shear flow, including all structural and dynamic elements of polydispersed foams.

Immersed Boundary Method – Overview and Applications

Aaron Fogelson
University of Utah
Salt Lake City, USA

In many biological systems, a moving fluid interacts with deformable elastic objects so that the motions of the fluid and the objects are coupled. Peskin introduced a hybrid Eulerian-Lagrangian computational method, now known as the Immersed Boundary method, for studying one such system, blood flow in the heart, and the method has been extended by him and others to deal with a wide range of biofluid dynamics problems. In this talk I will introduce the Immersed Boundary method, discuss some of the numerical issues still under active research, and describe a number of problems to which the Immersed Boundary method has been applied.

How to Analyse Boundary Conditions in LBE Schemes

Irina Ginzburg
Irstea, Antony Regional Centre, HBAN,
1 rue Pierre-Gilles de Gennes CS 10030,
92761 Antony cedex, France

A kinetic-type boundary condition replaces an outgoing population with the solution for incoming one. This sets a closure relation for each individual link cut by the solid wall. Each closure relation presents a specific linear combination of equilibrium and non-equilibrium components, inter-connected via Chapman-Enskog expansion. Our purpose is to fit them to a macroscopic boundary rule. This analysis becomes especially elegant in the frame of two-relaxation-time (TRT) collision operator [1], where general methodology for Dirichlet boundary conditions, either for velocity or pressure, is developed with symmetry argument in hand.

The analysis is first demonstrated for the well-known bounce-back and anti-bounce-back boundary conditions. The bounceback boundary closure relation is explored in most details to prescribe the exact location of solid walls in straight and diagonal, Couette and Poiseuille-Hagen channel flows. We show that the effective width of the parabolic flow depends on the specific (free-tunable) combination of two relaxation rates Λ [2], which also controls any steady solution of the TRT scheme [3]. However, within the BGK subclass [4] of the TRT model, the Λ varies as a square of the transport coefficient, and this completely destroys boundary accuracy for their large numerical values. This second-order boundary error becomes crucial for modest grid resolutions in pore space or for highly non-linear ADE problems, such as solute infiltration into dry soil [5]. The TRT model in combination with the bounce-back is then most efficient LBE scheme for flow and transport in reconstructed images of porous media, e.g.[6].

However, for any collision operator, when the channel walls are not parallel to grid axes, the bounce-back rule cannot set exactly either linear or parabolic profile. Multi-reflection (MR) boundary schemes [7] make it possible for arbitrary-shaped walls. We will show that there is an infinite numbers of MR schemes with equal, second or third-order, formal accuracy. Further choices can be guided by the wish to improve their stability or to guarantee

proper parametrization of the modeled solutions by non-dimensional physical numbers. We also show that linear interpolations [8,9] can be improved to achieve this goal. For example, it allows for viscosity independent estimates of soil permeability. Finally, we touch upon a proper definition of macroscopic variables in the presence of sources, an appearance of the accommodation boundary layers beyond the Chapman-Enskog expansion, and local mass conservation by boundary rules.

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Using Dissipative Particle Dynamics as a Tool to Study Mesoscale Flow Phenomena

Friederike Schmid
Institut für Physik, Universität Mainz
Staudingerweg 7-9, 55128 Mainz, Germany

In the first part of the tutorial, a general introduction into the simulation method of Dissipative Particle Dynamics (DPD) will be given, focussing especially on applications in fluid dynamics. The statistical physics background will be discussed and the method will be compared with other mesoscale simulation methods, such as multiparticle collision dynamics and Lattice Boltzmann. Furthermore, we will also discuss the issue of implementing suitable hydrodynamic boundary conditions.

In the second part, we will consider specifically DPD methods for studying electrohydrodynamic phenomena. Mesoscale simulations of electrokinetic phenomena are challenging due to the long range nature of both hydrodynamic and electrostatic interactions. In solutions of high ionic strength, the electrostatic interactions are partly screened, but the ions in solution still influence the hydrodynamic flows. Several methods have been proposed in recent years to deal with this problem.

Smoothed Particle Hydrodynamics

M. Ellero
Lehrstuhl für Aerodynamik und Strömungsmechanik,
Technische Universität München, 85747 Garching, Germany

The goal of this lecture is to review Smoothed Particle Hydrodynamics (SPH), a Lagrangian particle-based method developed more than thirty years ago for the approximate numerical solution of continuum hydrodynamics equations [1-3]. In SPH particles can be viewed as moving fluid elements on which a suitable set of ordinary differential equations is solved. In particular, in the case of the Navier-Stokes equations, a Lagrangian weak form approximation can be derived by replacing derivatives with integral operators discretized on a set of particle positions through an interpolation process. The method does not require any connectivity among fluid elements, as in standard grid-based techniques but, being based on a meshless interpolation, a sufficient number of neighbors for every particles must be ensured [4]. This problem is strictly connected to the issue of accuracy in SPH, indeed the presence of two typical numerical scales, associated respectively to the particle spacing and smoothing interpolation length, produces two different discretization errors. As analyzed recently theoretically [5] and numerically [6], both errors must go to zero in order to ensure convergence in a strict sense. These topics will be critically discussed.

A fundamental issue in SPH is also represented by the efficiency of the time stepping. Particularly, incompressible formulations [7] as well as implicit solvers [8] can allow a significant increase of the maximal time step allowable in the simulations. I will review some recent achievements in these areas.

In the second part of the talk I will focus on application and extension of the SPH method with specific emphasis to the description of complex fluids. In particular, I will show how the method can be extended to smaller mesoscales by incorporating thermal fluctuations on the hydrodynamics quantities. This has been done in [9,10] in a thermodynamically consistent way, that is by satisfying a fluctuation-dissipation theorem exactly, not only in the continuum limit but at the discrete particle level too. The corresponding SPH extension, denoted as Smoothed Dissipative Particle Dynamics (SDPD) can be viewed as a Lagrangian discretization of the *fluctuating hydrodynamics*. Connection to another mesoscopic method, namely Dissipative Particle Dynamics (DPD) will be also discussed.

Extensions of SPH to the study of complex continuum fluids described by general *viscoelastic* constitutive equations will be also reviewed and results in transient flows and complex geometries showed [11-13]. Finally, the application of SPH for describing structures of arbitrary shape and size suspended in a fluid, namely colloidal and non-colloidal *particle suspension* [14], will be discussed highlighting advantages and possible limitations.

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2 Workshop: Invited Talks

Stochastic Thermodynamics for Non-Equilibrium Steady States

Udo Seifert
II. Institut für Theoretische Physik, Universität Stuttgart
Pfaffenwaldring 57 / III, 70550 Stuttgart, Germany

Stochastic thermodynamics provides a framework for describing systems embedded in a heat bath and externally driven to non-equilibrium such as colloidal particles in time-dependent optical traps or in shear flow. Non-equilibrium steady states (NESSs) are characterized by time-independent driving [1].

After briefly introducing the general concepts, I will focus on our recent work concerning (i) the role of slow hidden degrees of freedom in the fluctuation theorem [2], and (ii) the form of the fluctuation- dissipation theorem for such NESSs [3,4]. In the first system, we have analyzed entropy production for two coupled colloidal particles. The second system allows to discuss the emergence of an "effective temperature" in a sheared colloidal suspension.

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Molecular Spin and Rotational-Translational Coupling in Nanofluidic Flows

P. J. Daivis[1], J. S. Hansen[2], B. D. Todd[3], S. De Luca[3]
[1]School of Applied Sciences, RMIT University,
GPO Box 2476, Melbourne Vic. 3001, Australia
[2]DNRF Center (Glass and Time), IMFUFA, Department of Science,
Systems and Models, Roskilde University, DK-4000, Roskilde, Denmark
[3]Mathematics, Faculty of Engineering and Industrial Sciences,
and Centre for Molecular Simulation, Swinburne University of Technology,
Melbourne, Victoria 3122, Australia

Molecular spin angular momentum is usually assumed to have no effect on the velocity profile in conventional hydrodynamics. This assumption is valid provided that certain conditions are fulfilled, but it can be shown that this is no longer the case for nanofluidic flows [1]. In fact, an accurate prediction of the velocity profile and flow rate for water flowing in a nano channel requires the coupling between rotational and translational velocities to be explicitly taken into account. In this presentation, the basic equations governing the coupling between molecular spin angular momentum and the translational momentum are described, and the consequences of this coupling are discussed for several topical examples in nanofluidics, and illustrated by results of non-equilibrium molecular dynamics simulations. Finally, it is demonstrated that this coupling can be used to drive a nanofluidic flow by applying a rotating electric field to a liquid of polar molecules in which the spin is then converted into translational motion. It is concluded that a net flow can be achieved if one side of the channel has a slip boundary condition and the other has a stick boundary condition [2].

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Shearing in Nanoconfined Fluids

Debra J. Searles[1,2,3], Stefano Bernardi[1,3],
Sarah J. Brookes[3], Denis J. Evans[4]
[1]Australian Institute for Bioengineering and Nanotechnology,
University of Queensland, Brisbane, Qld 4072, Australia
[2]School of Chemistry and Molecular Biosciences,
University of Queensland, Brisbane, Qld 4072, Australia
[3]Queensland Micro- and Nanotechnology Centre,
Brisbane, Qld 4011, Australia
[4]Research School of Chemistry, Australian National University,
Canberra, ACT 0200, Australia

In many cases lubrication occurs at high strain rates and under high confinement where the properties of the lubricant show nonlinear behaviour. We use nonlinear response theory [1] and nonequilibrium molecular dynamics techniques to evaluate the response of a fluid in a nanopore to the application of shear (also see [2]). The shear is induced by movement of the boundaries in opposite directions and the viscous heat generated is removed by a thermostat applied to the walls, leaving the dynamics of the fluid as realistic as possible. To establish a link with nonlinear response, the dissipation occurring inside the system is determined. It is time correlated with a phase variable of interest (e.g. pressure) to obtain its response. Until recently this theory has only been applied to homogeneous fluids whose equations of motion were coupled to a mechanical field and a thermostat. In our system, dissipation is generated by a boundary condition rather than a mechanical field. The theory is applied to these realistic confined systems, and we compare the shear stress response that is obtained with that of homogeneous systems at equivalent state points. We also consider the effects of the structure of the wall and the type of fluid on the results.

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Interface Problems for Two-fluid Mixtures

Aaron Fogelson
University of Utah
Salt Lake City, USA

Many biological problems involve interaction between two materials (e.g., a polymer network and a solvent) that can move relative to one another. One approach to modeling these interactions is with mixture models in which both materials can co-exist at each point in space. In such a model, the volume fraction of each material is tracked as a function of space and time, and momentum equations for both materials are used to determine their velocities. In many applications, the situation is further complicated by the presence of interfaces – either free-surfaces that separate a region with both materials from a region with just solvent, or physical barriers (e.g. cell membranes) that separate two regions containing the mixed materials. I will discuss approaches to solving both of these types of interface problems. For the free-boundary situation, the challenge is that the partial differential equations become degenerate in the pure-solvent region. I will introduce an interface-capturing method based on regularizing the mixture equations so as to be able to solve them throughout the domain. For the other situation, I will consider a deformable elastic boundary and introduce a new Immersed Boundary method that allows both materials to satisfy a no-slip condition on the boundary. I will discuss application of this new method to swimming in or peristaltic pumping of two-material mixtures will be discussed.

This is joint work with B. Guy, G. Wright, J. Du, and J. Keener.

A Ternary Model for Double-Emulsion Formation in a Capillary Microfluidic Device

P. Anderson
Eindhoven University of Technology
Eindhoven, The Netherlands

To predict double-emulsion formation in a capillary microfluidic device, a ternary diffuse-interface model is presented. The formation of double emulsions involves complex interfacial phenomena of a three-phase fluid system, where each component can have different physical properties. We use the Navier-Stokes/Cahn-Hilliard model for a general ternary system, where the hydrodynamics is coupled with the thermodynamics of the phase field variables. Our model predicts important features of the double-emulsion formation which was observed experimentally by Utada et al. [1]. In particular, our model predicts both the dripping and jetting regimes as well the transition between those two regimes by changing the flow rate conditions. We also demonstrate that a double emulsion having multiple inner drops can be formed when the outer interface is more stable than the inner interface.

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Diffuse Interface Simulations of Partial Drop Coalescence

T. Lee, L. Baroudi
Department of Mechanical Engineering,
City College of City University of New York,
New York, NY 10031, USA

Numerical simulations have been performed using a Galerkin Finite Element Lattice Boltzmann Method (FELBM) for an incompressible binary fluid based on the Cahn-Hilliard diffuse interface approach to study partial coalescence of liquid drops with a body of the same liquid. Under certain conditions, the merging between the drop and the bulk is not completed at once but goes through many cycles of partial coalescence, which is observed for systems of low viscosity. We investigate the effects of initial conditions on the early stages of inertial coalescence. The simulation results will be compared with the existing benchmark calculations and experimental results with gas or liquid as a surrounding fluid. The critical Ohnesorge number will be determined as a function of Bond number, and density and viscosity ratios of the drop and the surrounding fluid.

Segregation Phenomena in Flowing Suspensions of Deformable Particles: Toward an Understanding of Cell and Particle Dynamics in Blood Flow

Michael D. Graham
Department of Chemical and Biological Engineering,
University of Wisconsin-Madison
3010 Engineering Hall, 1415 Engineering Drive,
Madison, WI 53706-1691, USA

Blood is a suspension of particles of various shapes, sizes and mechanical properties and the distribution of these particles during blood flow is important in many contexts. Red blood cells (RBCs) tend to migrate toward the center of a blood vessel, leaving a so-called cell-free layer at the vessel wall, while white blood cells (WBCs) and platelets are preferentially found near the walls, a phenomenon called margination that is critical for the physiological responses of inflammation and hemostasis. Potential beneficial effects on hemodynamics arise from addition of high molecular weight long-chain polymer molecules known as drag-reducing additives (DRAs) to blood; one effect of these additives is the reduction of the cell-free-layer thickness. Additionally, the segregation properties of WBCs, platelets, and RBCs can be employed for their separation or detection in microfluidic devices. Finally, drug delivery particles in the bloodstream will also undergo segregation phenomena - 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 of flowing suspensions. Two specific issues are addressed here: (1) the effect of DRAs on the formation of the cell-free layer and (2) the origin of the margination phenomenon and its dependence on the relative properties of the different types of suspended particles in a mixture. In the case of polymer additives, the experimentally observed thinning of the cell-free layer is reproduced in the simulations and the mechanism underlying it is described. The study of margination reveals that this phenomenon is strongly affected by the nature of pair collisions between different types of particles during flow. Having in hand an understanding of

the mechanisms underlying these phenomena now allows more rational approaches to development of quantitative models of them and processes that exploit them. This knowledge will also lead to a better understanding of the consequences of these phenomena in physiology and medicine.

Mesoscale Modeling of Red Blood Cell Traversal Through a Microfluidic Device

D. A. Fedosov, G. Gompper
Theoretical Soft Matter and Biophysics,
Institute of Complex Systems and Institute for Advanced Simulation,
Forschungszentrum Jülich, 52425 Jülich, Germany

Microfluidic devices have a wide range of applications including the analysis of a microsample, the detection of rare solutes, cell sorting, etc. One type of microfluidic devices is called bumper arrays [1], which employs various obstacles of different geometry and structure. Complex geometry results in an intricate fluid flow within a device, whose properties may be exploited, for instance, to sort various solutes [2]. Design optimization of such devices may be quite complex, since the number of possible geometrical structures is very large. Realistic flow modeling provides excellent opportunities to better understand flow properties of various solutes through bumper arrays. We employ the Dissipative Particle Dynamics method to model flow behavior of red blood cells (RBCs) in a bumper arrays device. RBCs are modeled as deformable cells represented by a viscoelastic spring-network which incorporates appropriate mechanical and rheological cell-membrane properties [3]. We will illustrate the use of complex flow geometries to separate cells of different sizes and the application of blood flow simulations to optimize the device performance.

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Approaches to Multiscale Flows via Kinetic / Atomistic Simulations

S. Melchionna[1], U. M. B. Marconi[2], M. Bernaschi[3], S. Succi[3]
[1]IPCF-CNR, Consiglio Nazionale delle Ricerche,
Dipartimento di Fisica, Universita' Sapienza,
P.za A. Moro 2, 00185 Rome, Italy
[2]Scuola di Scienze e Tecnologie, Università di Camerino,
Via Madonna delle Carceri, 62032 , Camerino, Italy,
INFN, sez. di Perugia, Italy
[3]IAC-CNR, Consiglio Nazionale delle Ricerche,
Via dei Taurini 19, 00185 Rome, Italy

Complex systems demand for multiscale and multiphysics hierarchical approaches to the involved degrees of freedom in order to handle the different scales/models in a coherent manner. The bottom-up perspective provides the most solid, yet the most demanding route to complex flows, whereas the top-down is simpler but depends on some effective model, therefore it is more apt for multi-physics computing. In this talk, we will illustrate different cases where the two approaches can be used in specific contexts where the involved elements are at the edge between microscopic and macroscopic scales, such as: i) the mechanical and frictional/electroviscous response of composite DNA-electrolyte systems, ii) the unfolding of the VWF protein under shearing conditions, iii) the motion of red blood cells in complex hemodynamics flows. In each circumstance, the level of fidelity of the computational approach will be discussed.

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Modelling and Simulation of Some Non-Newtonian Fluids with Application in Hemodynamics

M. Lukáčová-Medvid'ová, A. Hundertmark, G. Rusnáková
Institute of Mathematics, University of Mainz,
Staudingerweg 9, 55099 Mainz, Germany

We will present our recent results on mathematical modelling and numerical simulation of non-Newtonian flows in compliant two-dimensional domains having applications in hemodynamics, cf. [1], [2], [3]. For the macroscopic models of the shear-thinning non-Newtonian fluids the power-law Carreau model and the logarithmic Yeleswarapu model will be considered. We will also address further aspects of blood flow concerning the viscoelasticity. For the structural model the generalized string equation for radially symmetric tubes will be generalized to stenosed vessels and vessel bifurcations. The arbitrary Lagrangian-Eulerian approach is used in order to take into account moving computational domains. In order to realize loose coupling between the structure and the fluid we use the kinematic-splitting algorithm and analyze its stability. Numerical experiments for the Carreau and the Yeleswarapu model, comparisons of the non-Newtonian and Newtonian models and the results for hemodynamical wall parameters; the wall shear stress and the oscillatory shear index will be presented as well.

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Density Functional Theory, Hydrodynamics, and Boundary Conditions

P. Español[1] and R. Delgado-Buscalioni[2]
[1] Dept. Física Fundamental, UNED
Senda del Rey, 9, 28040 Madrid, Spain
[2] Dept. Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid,
Campus de Cantoblanco, 28049 Madrid, Spain

We present a derivation of the coupled dynamics of a spherical particle with a simple fluid starting from first principles. The framework of non-equilibrium statistical mechanics [1] (aka, the Theory of Coarse-Graining) is used in order to derive the equations of motion for the mass and momentum density fields and the position and momentum of the sphere. The reversible part of the dynamics is generated by the derivatives of a free energy functional, while the irreversible part contains the coarse-grained interaction between the fluid and the particle. This interaction appears in the equations as additional terms that are highly localized near the surface of the particle. These terms contain additional transport coefficients related to the slip coefficient, for which Green-Kubo expressions are provided [2]. In the limit where the hydrodynamic disturbances vary smoothly, it is possible to interpret the interaction between the fluid and the particle in terms of boundary conditions.

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Inertial Coupling Method for Point Particle Hydrodynamics in Compressible Fluids

R. Delgado-Buscalioni[1], F. Balboa-Usabiaba[1], I. Pagonabarraga[2]
[1] Departamento de Física Teórica de la Materia Condensada,
Universidad Autónoma de Madrid, Madrid 28049, Spain
[2]Departament de Física Fonamental, Universitat de Barcelona,
Carrer Martí i Franqués 1, 08028-Barcelona, Spain

I will present a method for particle hydrodynamics based on an mixed Eulerian-Lagrangian approach. The particle dynamics are solved in continuum space while the fluid equations are solved in an Eulerian mesh using finite volume fluctuating hydrodynamics. The particle-fluid coupling force is obtained by imposing zero relative average velocity at the particle domain ("no-slip"). In doing so the particle-fluid momentum exchange takes place instantaneouly and both fluid and particle inertia are fully taken into account. For instance, the transfer of fluctuating fluid momentum to the particle is enough to thermalize the particle velocity to the fluid temperature. I will derive the equations of motion for the particle, hereby described by a minimal model: a single position vector and a kernel function of compact support. The kernel properties are essential for physical consistency: ensuring that the momentum balance is similar in Eulerian and Lagrangian variables and providing the particle effective volume and hydrodynamic properties (radius). The near velocity field around the particle is properly captured and the drag force consistently increases above the Stokes expression with the Reynolds number. In compressible fluids at low Mach number, acoustic forces measured under imposed ultrasound standing waves result in excellent agreement with the theoretical expressions.

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Coupling an Incompressible Fluctuating Fluid with Suspended Structures

A. Donev[1], F. B. Usabiaga[2], R. Delgado-Buscalioni[2], B. E. Griffith[3]
[1]Courant Institute of Mathematical Sciences,
New York University, New York, NY 10012
[2]Departamento de Fisica Teorica de la Materia Condensada,
Universidad Autonoma de Madrid, Madrid 28049, Spain
[3]Leon H. Charney Division of Cardiology, Department of Medicine,
New York University School of Medicine, New York, NY 10016

Bidirectional coupling of immersed structures, such as colloidal particles or polymer chains, to the surrounding fluid flow has been studied extensively; however, thermal fluctuations in the fluid equations are not usually considered even though they are responsible for Brownian motion. Achieving discrete fluctuation-dissipation balance in the coupled fluid-structure system is not trivial and requires special care in both the fluid solver and the fluid-structure coupling. I will describe an extension of the Inertial Coupling Method [1] developed for compressible flow by Usabiaga Balboa, Delgado Buscalioni and Pagonabarraga Mora to incompressible flow. The method allows for bidirectional coupling of inertial blob particles with a fluctuating fluid. Our algorithm is based on techniques used in the Immersed Boundary Method [2] and recently-developed finite volume schemes for fluctuating hydrodynamics [3]. We develop a temporal discretization that strictly conserves momentum and is limited in stability only by advection, and reproduces the correct spectrum and dynamics of the thermal fluctuations at both short and long times.

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Diffuse Reflection Boundary Conditions and Lattice Boltzmann Models for Microfluidics

V. Sofonea, V. E. Ambrus
Center for Fundamental and Advanced Technical Research
Romanian Academy
Bd. Mihai Viteazul 24, 300223 Timisoara, Romania

Lattice Boltzmann (LB) models are derived from the Boltzmann equation using a simplified version of the collision operator, as well as a discrete set of vectors in the two-dimensional (2D) or three-dimensional (3D) momentum space. Derivation of the LB models using Gauss quadratures, as well as the implementation of diffuse reflection boundary conditions are discussed. Numerical simulations conducted with various values of the Knudsen number show that the LB models can accurately capture specific microfluidics effects near the walls: the velocity slip, the temperature jump, the thermal creep and the longitudinal heat flux that is not driven by a temperature gradient.

Simulations of Soft Matter Interfaces

J. Harting[1,2], S. Frijters[1], F. Günther[1], B. Kaoui[1], T. Krüger[1]
[1]Department of Applied Physics,
TU Eindhoven, Eindhoven, The Netherlands
[2]Institute for Computational Physics,
University of Stuttgart, Stuttgart, Germany

First, we focus on fluid interfaces stabilized by colloidal particles. Modern simulation algorithms based on a multicomponent lattice Boltzmann model to describe the fluids combined with a molecular dynamics solver to describe the suspended particles allow to tune numerous relevant parameters of the system, such as particle size, shape, wettability and surface tension between the fluids. We focus on the adsorption of single or few particles to a flat interface and study the effect of local particle ordering. Finally, the transition from a so-called bijel to a Pickering emulsion in dependence on particle properties and the ratio of the fluid contents is presented [1-3].

In the second part of the presentation we investigate the dynamics of a single viscous vesicle under confining shear. Here, we utilize a lattice Boltzmann solver for the flow together with an immersed boundary algorithm to describe the deformable membrane. The transition from tank-treading to tumbling motion of the vesicle can be triggered by the ratio between internal and external fluid viscosities. We show that the transition can be induced solely by reducing the confinement, keeping the viscosity contrast constant. The possibility to trigger the tumbling-to-tank-treading transition either by geometry or viscosity contrast alone opens attractive possibilities for microrheological measurements as well as the detection and diagnosis of diseased red blood cells in confined flow [4,5].

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Advantages and Disadvantages of the Two-Relaxation-Times Lattice Boltzmann Scheme

Irina Ginzburg
Irstea/Cemagref, Antony Regional Centre, HBAN,
1 rue Pierre-Gilles de Gennes CS 10030,
92761 Antony cedex, France

The two-relaxation-times (TRT) symmetrized Lattice Boltzmann model is examined for consistency, stability and accuracy in bulk, boundaries and interfaces [1-9]. The TRT model employs two different relaxation rates for symmetric and anti-symmetric collision modes, restoring the simplest LBGK model [10] when their values are the same. However, exact analysis of the equivalent (recurrence) equations of the TRT operator undoubtedly shows that the TRT is the minimal collision configuration which allows to fully control *steady* solutions by the non-dimensional *physical* numbers, providing that the specific ("magic") combination Λ of two rates is fixed when the transport coefficient varies. Unlike with the LBGK model, this results in the expected *viscosity-independent* permeability, when modeling porous flow with the Stokes or Brinkman equations in combination with the bounce-back no-slip rule. The obtained permeability values depend on Λ but they lie in a reliable interval when Λ does not exceed much its exact (straight/diagonal Poiseuille flow) values, which are $\Lambda = \frac{3}{16}$ and $\Lambda = \frac{3}{8}$, respectively.

In the transient regime, the stability of the TRT depends on two relaxation rates separately. However, the TRT *isotropic or anisotropic advection-diffusion schemes* may easily remove their second-order numerical diffusion and keep the same stable velocity amplitude for any Peclet value when $\Lambda = \frac{1}{4}$ (optimal subclass). In turn, the non-negativity of the equilibrium guarantees stability for the LBGK and optimal subclasses. However, this property is not retained by the TRT model in general. Furthermore, the two relaxation rates alone are not sufficient to eliminate the entire, advection-diffusion fourth-order error, because of the *fourth-order* numerical diffusion. Heuristic arguments allow to link this truncated corrections and stability, in agreement with the exact (one-dimensional) and numerical (multi-dimensional) von Neumann stability analysis. This linear analysis works reasonably well even for highly non-linear problems, such as the pollutant transport in variably saturated Darcy's underground flow [11], but only providing that the

two relaxation rates lie sufficiently far from their *opposite* bounds when Λ is set.

A related topic is the available anisotropy range. The TRT model builds anisotropic diffusion entries via an anisotropic symmetric equilibrium distribution. Then the optimal subclass may tolerate negative anisotropic equilibrium weights, extending the available range beyond the diagonal-dominant diffusion tensors. However, the equilibrium weights then become discontinuous when the anisotropy changes abruptly, as it happens to hydraulic conductivity in heterogeneous soils. The alternative, anisotropic and velocity-dependent multi-relaxation matrix gets anisotropy-independent solvability conditions for isotropic equilibrium, and allows to describe fully anisotropic tensors with the minimal (coordinate) velocity sets [12,13]. Yet, these necessary bounds do not guarantee the effective stability, and the the optimal TRT accuracy or stability is difficult to attain for large eigenvalue scattering. Finally, when the simplest link-wise symmetric component is replaced by the multiple-relaxation-type collision, which is more stable for hydrodynamic problems, the stable diffusion equilibrium parameter space may slightly grow but may also drastically narrow for improper choice of the free, symmetric modes eigenvalues. Altogether, an adequate choice of the free-tunable parameters enables the TRT to gain in efficiency against the forward-time central finite-difference schemes and in performance against the LBGK model. However, unsuitable choices may result in quite unstable and/or inaccurate schemes.

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Roles of Many-body Hydrodynamic Interactions in Colloid Dynamics and Ordering

Hajime Tanaka[1], Akira Furukawa[1], Takeaki Araki[2], and Yusuke Goto[1]
[1]Institute of Industrial Science, Univ. of Tokyo, Muguro-ku, Tokyo, Japan
[2]Department of Physics, Kyoto Univ., Sakyo-ku, Kyoto, Japan

Dynamics of colloidal suspensions are seriously affected by hydrodynamic interactions between particles. However, hydrodynamic effects are quite difficult to deal with because of the long-range nature and the resulting strong nonlocal couplings among all the relevant degrees of freedom of colloidal suspensions. To get rid of this difficulty, we developed a new simulation method, which we call Fluid Particle Dynamics (FPD) method [1]. By applying this method, we studied dynamic couplings between colloid motion and additional degrees of freedom in the surrounding complex liquids through the flow field. They include the gel formation of attractive colloidal particles [2], electrophoretic motion of charged colloidal suspensions [3], aggregation phenomena of charged colloids, and interactions between colloidal particles immersed in a nematic liquid crystal [4] or in a critical binary mixtures, and hydrodynamic ordering of active colloids. We discuss some of these interesting phenomena, focusing on dynamic couplings between colloid position, velocity fields, and additional degrees of freedom in the surrounding complex liquids through the flow field.

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Direct Numerical Simulations of Hydrodynamically Interacting Colloids and Self-Propelling Particles

Ryoichi Yamamoto, John Molina
Department of Chemical Engineering
Kyoto University, Kyoto 6158510, Japan

Using the smoothed profile method (SPM) method [1,2] developed for direct numerical simulations (DNS) of colloidal dispersions, we studied several dynamical problems of particle dispersions, including sedimentation, diffusion, coagulation, rheology, tumbling motion in shear flow, and electrophoresis in AC/DC electric field. Recently, two major extensions have been made for the SPM. The first extension is for compressible host fluids [3], and the second extension is for self-propelled particles. The latter is done by introducing active slip boundaries at the fluid/particle interface. Dynamical behaviours of the hydrodynamically interacting self-propelled particles are studied with fully resolving the hydrodynamics of the host fluid [4].

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On Lattice Fokker Planck for Dilute Polymer Dynamics

Santosh Ansumali
Engineering Mechanics Unit, JNCASR, Jakkur, Bangalore 560064, India

Lattice Boltzmann model is quite successful as an approximate solver of Boltzmann BGK equation for hydrodynamics as well as gaseous microflows [1,2]. Recently, this method was extended for solving other kinetic equations such as Fokker-Planck equation[3,4].

I will be describing this new approach in context of the Smoluchowski equation governing the probability density of polymer configurations. The method is benchmarked by comparing the bulk rheological properties for shear flow as well as extensional flow with those obtained using Brownian dynamics simulations [5]. Furthermore, access to the full distribution function in this formulation will be utilized to explore the validity of closures such as FENE-P model. Finally, some priliminary results which extends the method to the non-homogeneous polymer dynamics will be described.

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Simulation of Passive Microrheology Using Particle Methods

A. Vázquez-Quesada[1,2], M. Ellero[2], P. Español[3]
[1]Departamento de Física Teorica de la Materia Condensada,
Universidad Autonoma de Madrid, 28049 Madrid, Spain
[2] Lehrstuhl für Aerodynamik und Strömungsmechanik,
Technische Universität München, 85747 Garching, Germany
[3]Departamento de Física Fundamental, Universidad Nacional de Educacion a Distancia,
Apartado 60141, 28080 Madrid, Spain

In this talk I will present a particle method based on smoothed particle hydrodynamics for passive microrheology simulations of polymeric fluids [1]. The viscoelasticity of the solvent is modeled via a standard Oldroyd-B model and thermal fluctuations, inherently present at the microscopic scale, are incorporated into the particle framework by application of the GENERIC formalism, ensuring the strict fulfillment of the Fluctuation-Dissipation theorem at the discrete level [2]. Rigid structures of arbitrary shape suspended in the viscoelastic solvent are modeled by freezing SPH particles within a given solid domain and letting them interact with the solvent particles [3]. The rheological properties of the Oldroyd-B fluid, namely frequency-dependent storage and loss moduli, are extracted via macroscopic deterministic simulations under small amplitude oscillatory (SAOS) flow and, alternatively, through standard micro-rheological simulations of a probe particle suspended in the same Brownian viscoelastic medium, by assuming the validity of a generalized Stokes-Einstein relation (GSER). We check that good agreement with the analytical theory for the Oldroyd-B model is found in the deterministic SAOS flow over the entire regime of frequencies investigated. Concerning the micro-rheological measurements, good agreement is observed only up to a maximal frequencies corresponding to time scales considerably larger than the viscous time of the probe particle where the diffusive regime is fully established. At larger investigated frequencies, a crossover between diffusive and ballistic behavior for the MSD of the probe is observed and validity of the GSER is questionable. The model presented here provides an optimal computational framework to complement experimental observations and to analyse quantitatively the basic assumptions involved in the theory of microrheology.

Future directions will be also outlined in this talk. In particular we are currently working on the development of a refined version of the GSER including the effect of fluid inertia and compressibility, which might extend the applicability of microrheology to larger frequencies. To this aim, we have recently derived a generalization of Faxén's theorem to the non-steady motion of a sphere through a compressible linear viscoelastic fluid in arbitrary flow [4]. The relevance of the theorem to microrheology will be discussed.

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Manipulating Flow and Transport in Microchannels by Structured Surfaces

Friederike Schmid, Jiajia Zhou, Alexey Belyaev, Olga Vinogradova,
Sebastian Meinhardt, Ralf Eichhorn, Jens Smiatek
Institut für Physik, Universität Mainz
Staudingerweg 7-9, 55128 Mainz, Germany

Structuring is an efficient tool to modulate the hydrodynamic boundaries at surfaces. In the first part, we present the results of Dissipative Particle Dynamics simulations of flow past superhydrophobic striped surfaces in microchannels, and demonstrate how anisotropic surface patterning results in an anisotropic slip tensor. The simulation results are in excellent agreement with theoretical predictions. In the second part, we discuss as an application, how microchannels with variable surface slip can be used to separate enantiomeric particles by chirality.

Hydrodynamics of Air Entrainment by Moving Contact Lines

F. Toschi[1], T. S. Chan[2], S. Srivastava[1], A. Marchand[3], B. Andreotti[3], L. Biferale[4], and J. H. Snoeijer[2]
[1]Department of Physics and of Mathematics & Computer Science Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands
[2]Physics of Fluids Group, Faculty of Science and Technology University of Twente, 7500AE Enschede, The Netherlands
[3] PMMH UMR 7636 ESPCI - CNRS - Univ. Paris Diderot - Univ. P. M. Curie, 10 rue Vauquelin, 75005 Paris, France
[4]Department of Physics and INFN, University of Tor Vergata Via della Ricerca Scientifica 1, 00133 Rome, Italy

When a plate is immersed in a viscous fluid the drag generated deforms the air-fluid interface. For plate velocities below a critical threshold the meniscus equilibrates at a new position, some distance Δ below the free surface. When the velocity is above the threshold air entrainment can take place. The problem is the symmetric counterpart of the celebrated Landau-Levich deep coating problem, where a plate is pulled out from a viscous fluid bath. We discuss the numerical modeling used to investigate the problem, which is based on the Lattice Boltzmann method, furthermore comparison against lubrication theory is presented and discussed.

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Bridging the Scales via the Lattice Boltzmann Method: From Non-ideal Fluids to Fluid-Structure Interactions

Fathollah Varnik[1,2], Markus Gross[1], Timm Krüger[3],
Dierk Raabe[2], Ingo Steinbach[1]
[1]ICAMS, Ruhr-University Bochum, Bochum, Germany
[2]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
[3]Department of Applied Physics, Eindhoven University of Technology, Eindhoven, Netherlands

Modelling physical phenomena across the scales is a veritable challenge for scientific computing. Due to the complexity of the problems involved, rigorous and predictive bottom-up approaches are quite rare and largely remain a task for future research. In this context, it is of great interest to develop models which allow to efficiently incorporate the essential effects originating from a large number of interactions at a smaller scale in a description of the system behavior at a larger scale. In this talk, we present two of such approaches which may serve to study a large variety of physical phenomena. In the first part of the talk, a model based on the lattice Boltzmann (LB) method is developed that allows to simulate a non-ideal, van-der-Waals-like fluid including thermal fluctuations [1,2]. It is shown in detail how a Langevin theory of a non-ideal fluid LB model can be constructed that respects all basic laws of equilibrium statistical mechanics. The heart of the proposed theory constitutes a fluctuation-dissipation theorem derived at the kinetic level that ensures accurate thermalization of all lattice Boltzmann degrees of freedom, including the non-hydrodynamic ones. This theorem is obtained by first transferring the Onsager's regression hypothesis to the discrete Boltzmann equation for non-ideal fluids in the moment space and then deriving from it the desired LB model [1]. The theory is general and can be applied to any existing deterministic lattice Boltzmann model. To demonstrate this, two of the most widely used LB models for non-ideal fluids are extended and successfully benchmarked by a study of the equipartition theorem, static structure and capillary fluctuations. The method is then applied to a variety of physical phenomena such as spreading of nanodrops (where a cross-over from nano- to macroscale behavior is observed by tuning thermal fluctuations), surface roughening and static and dynamic critical fluctuations [3].

The second part of the presentation deals with modelling of fluid-structure interactions in the case of soft objects embedded in a fluid such as, e.g., red blood cells and capsules. The approach combines, via the immersed boundary method, the lattice Boltzmann method –which solves the fluid dynamical equations– with the finite element method for the membrane dynamics. The method is implemented and successfully benchmarked in the case of a single cell under simple shear [4]. It is then applied to the study of particle stress in a dense suspension, where a new approach for accurate determination of local stress is proposed and tested [5]. Moreover, using this hybrid method, the collective dynamics of dense suspensions of red blood cells is investigated uncovering the onset of tank-treading even in highly dense suspensions upon an increase of the suspension stress [6].

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Theory of Fluctuating Lattice Boltzmann Methods

A. J. Wagner and G. Kaehler
Department of Physics, North Dakota State University,
1121 Albrecht Blvd., Fargo, ND 58108, USA

The fluctuating lattice Boltzmann was first introduced by Ladd [1] by introducing a fluctuating stress tensor. His original implementation was then improved upon by Adhikari [2] by introducing noise in all moments, not just the stress moments. Duenweg [3] justified this new implementation by relating it to the fundamental statistical mechanics of lattice gases. Gross [4] justified the Adhikari implementation for ideal gases by relating it to the original Fox/Uhlenbeck [5] treatment of the fluctuating Boltzmann equation. We show here that in order to truly derive the fluctuation dissipation theorem in full analogy to the Fox/Uhlenbeck treatment a new fluctuating lattice Boltzmann method is required. In this treatment the collision matrix becomes velocity dependent [6]. We show that for an example D2Q9 implementation the new method shows significant improvements, particularly for non-zero mean velocities and low densities.

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Mesoscopic Simulations of Active Droplets

M. E. Cates, E. Tjhung, D. Marenduzzo
School of Physics, University of Edinburgh
James Clerk Maxwell Building, Kings Buildings,
Edinburgh EH9 3JZ, United Kingdom

The continuum hydrodynamic equations for self-propelled active matter with polar and/or nematic order are simulated using lattice Boltzmann (LB). The polar case is relevant for describing subcellular actomyosin gels, in which a polymerization-depolymerization (p-dp) process of the actin filaments can cause cells to crawl. LB simulations of a droplet of polar active material however show in addition a second mechanism, more like swimming than crawling, leading to motility even when the p-dp process is switched off. This second mechanism involves spontaneous breaking of the symmetry (that arises only in the absence of p-dp) between states of opposite polarity.

Chemical Swimming

John F. Brady
Chemical Engineering, California Institute of Technology,
Pasadena, CA 91125

The design of nanoengines that can convert stored chemical energy into motion is an important challenge of nanotechnology, especially for engines that can operate autonomously. Recent experiments have demonstrated that it is possible to power the motion of nanoscale and microscale objects by using surface catalytic reactions — so-called catalytic nanomotors. The precise mechanism(s) responsible for this motion is (are) still debated, although a number of ideas have been put forth. Here, a very simple mechanism is discussed: A surface chemical reaction creates local concentration gradients of the reactant (the fuel) and product species. As these species diffuse in an attempt to re-establish equilibrium, they entrain the motor causing it to move. This process can be viewed either as osmotic propulsion or as self-diffusiophoresis or more figuratively as "chemical swimming". The concentration distributions are governed by the ratio of the surface reaction velocity to the diffusion velocity of the reactants and/or products. For slow reactions the reaction velocity determines the self-propulsion. When surface reaction dominates over diffusion the motor velocity cannot exceed the diffusive speed of the reactants. The implications of these features for different reactant concentrations and motor sizes are discussed and the predictions are compared with Brownian Dynamics simulations. We also show that chemically active particles can attract or repel each other through long-range "Coulomb-like" interactions. And suspensions of active particles can exhibit Debye-like screening and phase behaviors analogous to those of a one-component plasma.

Mesoscale Simulations of Active Particle Suspensions

Gerhard Gompper
Theoretical Soft Matter and Biophysics,
Institute of Complex Systems and Institute for Advanced Simulation
Forschungszentrum Jülich, D-52425 Jülich, Germany

Complex fluids under shear flow are the classical example of stationary non-equilibrium behavior. However, there are also many systems, where an intrinsic non-equilibrium behavior arises from the active motion of their constituent particles. Examples are mostly biological systems — like suspensions of bacteria, sperm and algae, and mixtures of biopolymers and motor-proteins —, but also synthetic systems — like self-propelled bimetallic nanorods or janus colloids.

Mesoscale simulation techniques are essential in order to obtain a detailed understanding of the structure formation and dynamics of such complex active systems. We focus on the Multi-Particle Collision Dynamics (MPC) approach, which has been shown previously to capture hydrodynamic interactions and thermal fluctuations in a variety of complex fluid flows very well [1].

Several examples will be discussed to demonstrate the unusual properties of active particle suspensions: (i) Interactions between squirmers (spherical swimmers with a prescribed surface velocity field), which show the interplay between hydrodynamic attraction and thermal motion [2], (ii) interaction between sperm cells and a wall, which illustrate effective surface adhesion [3], (iii) the synchronization and bundling of bacterial flagella, which shows the interplay of hydrodynamics and elasticity [4], and (iv) the structure formation in mixtures of semi-flexible filaments and motor proteins, which illustrates the collective behavior of many active particles [5,6].

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Emergent Patterns in Suspensions of Self-Propelling Particles

I. Pagonabarraga[1]
[1]Departament de Física Fonamental
Facultat de Física, Universitat de Barcelona
Carrer Martí i Franqués 1, 08028 Barcelona, Spain

There exist a variety of colloidal size objects which have the ability to self propel in a suspending fluid medium. Heterogeneous colloids with catalytic sites, or appropriately charged colloids can move as a result of the reactions which take place on parts of their surface. Also natural microorganisms, such as certain bacteria, can also swim as a result of their internal metabolism. In all these situations there is no external force which drives the objects. Nonetheless, since they displace in a viscous medium, the objects induce a flow which decays slowly and hence affect the motion of other suspended particles. Therefore, even the free motion of ensembles of such objects will exhibit peculiar features which arise from the dynamic correlations induced by the embedding medium.

I will introduce model systems that account effectively for the mechanism of self-propulsion, rather than attempting at understanding the microscopic details that control intrinsic motion of small sel-fpropelling individuals. Such an approach will help us to focus on the features that characterize collective motion and pattern formation in these type of model systems driven by internal forcings. I will discuss how gravity affects the sediment formation of self-propelling suspensions and the role of hydrodynamically induced fluid flows.

Stokesian Hydrodynamics of Active Filaments

R. Adhikari
The Institute of Mathematical Sciences
CIT Campus, Taramani, Chennai 600113, India

The conversion of chemical energy into mechanical stresses is essential to the function of many biological and biomimetic systems. When such conversions occur in a fluid environment the mechanical stresses produce flows which, thereby, couple the structures on which the conversions take place. We have developed a general model for those situations where active energy conversion takes place on an elastic filament. This model contains, in addition to monopolar singularities familiar from the Zimm model, dipolar singularities which account for the active conversion of chemical energy to mechanical stress. We present two striking results obtained from simulations. First, at sufficiently large ratios of elasticity to activity, a free, straight filament can spontaneously bend and self-propel. Secondly, a filament clamped at one end can spontaneously oscillate in a fashion reminiscent of cilia. We outline the many unexplored aspects of this model and suggest experimental tests of our predictions in both biological and biomimetic systems.

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Lattice Boltzmann Models with Competing Interactions: Theory and Simulations

M. Sbragaglia[1], R. Benzi[1], M. Bernaschi[1], S. Succi[1,2]
[1]Department of Physics and INFN, University of Rome Tor Vergata,
Via della Ricerca Scientifica 1, 00133 Rome, Italy
[2]Istituto per le Applicazioni del Calcolo CNR,
Viale del Policlinico 137, 00161 Roma, Italy

A multicomponent lattice Boltzmann model able to describe some dynamical behaviors of soft-glassy materials is theoretically analyzed [1]. Due to the competition between short-range attractive and mid/long-range repulsive forces, the model is shown to give rise to a very rich configurational dynamics promoting a host of non-trivial collective effects. Most notably, whenever the self-species attraction and repulsion effects come close to an exact balance, low surface tension is achieved, thus producing a large interface between the two fluids. The equilibrium analysis [2] allows us to determine such surface tension and the resulting disjoining pressure, developing in a thin film when two interfaces overlap. This disjoining pressure is used to stabilize droplets and bubbles against coalescence and offers the possibility to study colloidal systems as foams and emulsions with their rheological properties in confined geometries. Issues regarding the non-locality of the rheology under confinement are then investigated for planar Couette flows and pressure driven flows [3].

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Modeling Water-Like Fluid with a 3d Lattice Boltzmann Approach

N. Moradi[1], F. Rao[1], A. Greiner[1], S. Melchionna[2], S. Succi[1,3]
[1]Freiburg Institute for Advanced Studies, Freiburg, Germany
[2]Istituto Processi Chimico-Fisici, CNR, Roma, Italy
[3]Istituto Applicazioni del Calcolo, CNR, Roma, Italy

We present a three-dimensional lattice Boltzmann model, accounting for directional interactions between water-like molecules, based on the so-called Ben-Naim (BN) potential. The water molecules are represented as rigid tetrahedra, with two donors and two accepters at the corners, sitting on fixed lattice sites and interacting with neighbors through a lattice formulation of the BN angular potential. The angular momentum of the water molecules evolves in time under the drive of the torque resulting from the angular potential and it is solved by means of a quaternion technique. Solving the corresponding advection-diffusion-reaction equation for the quaternion components, via the LB method, the orientation and the velocity of the water-like molecules are updated after each LB collision-propagation step. By adding thermal fluctuations to the torque equation, the model is shown to reproduce some microscopic features of real water, such as a number of hydrogen bonds (HBs) between 3 and 4. Future goals and prospective applications of the current 3D model to biofluidic problems are outlined and commented upon.

3 Workshop: Posters

Coarse Graining in Time For Molecular Simulations

Jinwoo Lee
Department of Mathematics, Kwangwoon University,
Seoul 139-701, Korea

We suggest a new scheme for molecular simulations. It is a coarse graining in time version of usual molecular dynamics methods. Instead of considering every detail of particle trajectories, we deal with the average position of the particles and the probability distribution function of the locations. A unique feature is that the effect of high frequency motions of particles is represented as a short-range repulsive potential function. We will show how crystallization of hard spheres system can be illustrated elegantly under this scheme.

Linear and Nonlinear Density Response Function for a Simple Atomic Liquid

B. A. Dalton[1], P. J. Daivis[1], B. Todd[2], I. K. Snook[1]
[1]School of Applied Science, RMIT University,
Melbourne 3001, Australia
[2]Faculty of Engineering and Industrial Sciences,
Swinburne Institute of Technology, Hawthorn 3122, Australia

Using molecular dynamics simulations we investigate the linear and nonlinear density response of a simple atomic liquid. We introduce the Sinusoidal Longitudinal Force (SLF) method for determining the wave vector dependent density profile of liquids in an external field. In the SLF method a position dependent force is applied to each atom in an unconfined liquid system. The magnitude of the force is a sinusoidal function of the atoms position in the y dimension only. The direction of the force is also in the y dimension only. Thus using the SLF method we can control the Fourier components of the static density inhomogeneities in unconfined liquids. The form of the density response kernel is determined using a grand canonical ensemble average of the microscopic single particle density [1,2]. A Taylor series expansion of the external field contribution to the grand canonical distribution function produces terms containing a first order contribution by the external field to the single particle density, and terms containing second order contributions. We show that for small external field amplitudes the density profile is a linear functional of the external field. In the linear regime we use variations in the wavelength of the external field to produce the homogeneous liquid structure factor. We confirm this liquid structure factor using the Fourier transform of the radial distribution function. We also show that for large external field amplitudes nonlinear modes are excited in the density profile. The amplitudes of the higher modes have a nonlinear dependence on the amplitude and wavelength of the external field. We provide results showing the Fourier modes present in density profiles produced by large amplitude external fields.

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Computer Simulations of Mixed Shear and Elongational Flow

Stefano Bernardi[1], R. Hartkamp[2], T. Hunt[3], D. Searles[1], B. D. Todd[2]
[1]Australian Institute for Bioengineering and Nanotechnology,
University of Queensland, Brisbane, Qld 4072, Australia
[2]Mathematics, Faculty of Eng. & Industr. Sci., & Centre for Molec. Simul.,
Swinburne Univ. of Technology, Hawthorn, Victoria 3122, Australia
[3]Comput. Biophysics, Univ. of Twente, 7500 AE Enschede, Netherlands

Computer simulations have been widely applied to study the rheology of simple and complex fluids subject to shear or elongational forces. In this work we derive new Periodic Boundary Conditions (PBCs) [1] to be used in nonequilibrium molecular dynamics (NEMD) simulations in order to study the behavior of fluids under a combination of these flows (*e.g.* mixed flow) which is likely to occur in realistic systems. These PBCs allows the simulation to be performed for an indefinite amount of time potentially eliminating the issue of relaxation typical of complex molecules and highly viscous fluids.

Because the strain and elongation rates accessible in direct NEMD simulations is much higher than that in controlled experiments, we also show how the transient-time correlation function (TTCF) method can be applied to calculate the nonlinear response of homogeneous fluids close to equilibrium [2].

We compare the TTCF response of the pressure tensor and of the generalized viscosity to that obtained by directly averaged NEMD simulations and discuss the consequence of noise in simulations with small external fields. TTCF is far more efficient than NEMD direct averaging and can therefore be applied to small rates of deformation comparable to experiments, and in principle can be used to study the rheology of polymer melts in industrial processes.

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The Microscopic Origin of Boundary Conditions in Heat Conduction

P. Español, M. Meléndez
Dpto. Física Fundamental, Universidad Nacional de Educación a Distancia,
Apdo. 60141 E-28080, Madrid, Spain

We derive the equation for heat transport in a solid by means of a projection operator technique [1]. The interaction of this solid with a surrounding medium at its boundaries is explicitly included in the derivation. This leads to surroundings modelled by source terms in the dynamic equations instead of boundary conditions. The source terms contain transport coefficients, like the Kapitza resistance [2], for which Green-Kubo expressions are calculated. The connection between these source terms and the equivalent boundary conditions is discussed.

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Free Energy Models in a Nonlinear Fluctuating Diffusion Equation

J. A. de la Torre[1], Pep Español[1], Daniel Duque[2]
[1]Dept. Física Fundamental, UNED,
Senda del Rey 9, 28040 Madrid, Spain
[2]Dept. Enseñanzas Básicas de la Ing. Naval, UPM,
Arco de la Victoria SN, 28040 Madrid, Spain

The inclusion of thermal fluctuations may be something tricky in many hydrodynamics problems. Moreover, multi-scale hydrodynamics often needs irregular grids (with a *fine grain* in specific locations of the mesh). How to include thermal fluctuations in these irregular regions is nowadays a matter of discussion.

We propose a formal definition of some discretization and continuation operators, which can be used in any regular or irregular mesh. If they verify some properties (we say that they have to be *local operators* with *linear consistency*) we can apply them to a paradigmatic non-linear stochastic diffusion equation:

$$\frac{\partial c(\mathbf{r},t)}{\partial t} = \nabla\mu(c(\mathbf{r},t))\nabla\frac{\delta\mathcal{F}}{\delta c(\mathbf{r},t)}\left[c(\mathbf{r},t)\right] + \nabla\tilde{J}\,. \tag{1}$$

This equation is paradigmatic not only because it captures an exact conservation of the number of particles, but it also satifies an H-theorem. The inclusion of thermal fluctuations is then straightforward using the fluctuation-dissipation theorem. This non-linear stochastic diffusion equation needs to be modelled with a free energy functional and a mobility coefficient. Taking the latter as a constant, we can freely explore free energy functionals $\mathcal{F}[c(\mathbf{r},t)]$: an ideal gas, a Gaussian model and a Ginzburg-Landau functional.

In our current work [1] we study the role of thermal fluctuations in the diffusion equation, performing simulations for the three functionals given. We obtain cross correlation curves and equilibrium probability distributions, which can be used to check our numerical simulations with the theoretical behaviour, extending the regular case previously studied [2].

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Collective Dynamics in Large Suspensions of Active Particles

E. Lushi[1,2], A. Donev[2], C. S. Peskin[2], M. J. Shelley[2]
[1]Department of Mathematics, Imperial College London, UK
[2]Courant Institute, New York University, USA

I will outline a novel mathematical and computational model to trace the dynamics of a large number of motile or active particles or micro-swimmers that interact directly and also via the fluid in which they are suspended and can affect due to their locomotion. I will highlight the differences in the macroscopic structures emerging in the collective particle dynamics and the generated flow fields and how they depend on the volume fraction, propulsion mechanism and particle shape. A few applications of the method will be mentioned, as well as how particle interactions, direct or via the fluid, affect overall flow properties like transport, speed, viscosity.

Collective Hydrodynamics of Active Particles

J. J. Molina[1], Y. Nakayama[2], R. Yamamoto[1]
[1] Department of Chemical Engineering, Kyoto University,
Nishikyo-ku, Kyoto 615-8510, Japan
[2] Department of Chemical Engineering, Kyushu University,
Fukuoka 819-0395, Japan

The possibility of designing active (self-propelled) colloidal particles, that can mimic the work peformed by complex molecular motors present in biological systems, has led to many recent theoretical and experimental studies. The three main questions that must be answered are the following: How can such a motion be (continuously) generated? Can it be guided to perform useful work? and finally, what is the emerging dynamics of a system composed of many such particles? Self-phoretic mechanisms, by which the particle generates the field gradients responsible for the surface effects which drive it, are currently the simplest option to realise such a system[1]. Recent experimental work on catalytic[2] and laser-irradiated[3] janus particles, driven by self-generated concentration and temperature gradients, respectively, has shown how general this approach is. However, the issue of how to extract useful work from an ensemble of these self-propelled particles remains an open question. To describe the motion of such a system at the relevant length scales (nano to micro) one must take into account both the hydrodynamic (and inter-particle) interactions as well as their Brownian motion. As such, the modelling of these systems presents a considerable computational challenge. The first numerical studies were therefore limited to systems of two particles[4], at zero Reynolds number, from which the pair interaction was obtained and used to study the collective motion of larger systems. In our work, we solve the Newton and Navier-Stokes equations, by using the smooth-profile method[5,6], in order to fully resolve the hydrodynamic interactions of a system of self-propelled colloids. As a first step, we ignore the mechanism responsible for the motion, and consider a system of motors (constant force along a preferential axis) or swimmers (constant slip velocity profile at the solid-fluid interface), in order to study how the hydrodynamic interactions help/hinder the collective motion. Finally, we consider the specific phoretic mechanism recently introduced by Córdova-Figueroa and Brady[7], the diffuso-phoretic motor consisting of a catalytic janus particle driven by a solute concentration gradient, to study the coupling between the hydrodynamic interactions and the solute advection-diffusion.

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Simulation of Floating Objects in Free Surface Flows

Simon Bogner[1,2], Ulrich Rüde[1]
[1]Lehrstuhl für Systemsimulation, Universität Erlangen-Nürnberg,
D-91058 Erlangen, Germany
[2]simon.bogner@informatik.uni-erlangen.de

The lattice Boltzmann method (LBM) has grown a popular approach for the simulation of complex fluids. We present an algorithm for the simulation of particles in free surface flows (liquid-gas-solid flows) – i.e., a *volume of fluids* interface capturing method using an LBM for the liquid flow is enhanced with freely floating and moving rigid obstacles.

In contrast to common LBM multiphase approaches, the free surface lattice Boltzmann method [1] only simulates the fluid region and neglects the gas phase. Being a free boundary approach, the problem of the large density difference between liquid and gas is circumvented. Rigid particle suspensions have been introduced to the lattice Boltzmann context in [2] using a so-called momentum exchange approach. Based on the same principle we facilitate simulations of floating bodies in free surface flows [3]. The combination free surface lattice Boltzmann and fluid structure interaction relies on an algorithm tracking the state of the lattice cells and handling state transitions by a set of dynamic cell conversion rules.

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Towards a Lattice Boltzmann Model for Water-like Fluids

N. Moradi[1], F. Rao[1], A. Greiner[1,2],
S. Melchionna[3], S. Succi[1,4]
[1]Freiburg Institute for Advanced Studies, University of Freiburg, Albertstrasse 19, 79104, Freiburg, Germany
[2]Department of Microsystems Engineering, University of Freiburg, Georges-Köhler-Allee 103, 79110 Freiburg, Germany
[3]IPCF-CNR, Piazzale A. Moro, 5, 00185, Roma, Italy
[4]IAC-CNR, via dei Taurini 9, 00185, Roma, Italy

A lattice Boltzmann approach is developed to account for directional interactions between water-like molecules. We simulate the rotation of water molecules to reproduce the onset and decay of hydrogen bonds. Each lattice site features additional degrees of freedom, which consist of the orientational angles of the water molecules at this specific site. These internal degrees of freedom interact with the respective orientational degrees of freedom of the neighboring sites, through a suitable lattice pseudo-potential. This interparticle potential is given in terms of the orientation of each single molecule with respect to its neighbors [1,2]. Introducing a vector order parameter P, which fully determines the orientation of the water molecule, the interparticle potential gives rise to a torque in the hydrodynamic equations for the order parameter P. Here, focusing exactly on this issue for a 2D case, some results of a recent study by Mazzitelli and coworkers [3] are presented and various aspects of this approach are discussed. Preliminary results of an ongoing extension to 3D are shown and prospective applications at a microscopic level are highlighted.

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Towards a New Algorithm for Multiphase Lattice Boltzmann Simulations

Jasna Zelko[1] and Burkhard Dünweg[1,2]
[1]Max Planck Institute for Polymer Research,
Ackermannweg 10, 55128 Mainz, Germany
[2]Department of Chemical Engineering, Monash University,
Melbourne, VIC 3800, Australia

A new lattice Boltzmann method (LBM) for simulating multiphase flows is developed. Essentially we follow the Swift-Yeomans route, i. e. we adjust the LBM such that its continuum limit is the Navier-Stokes equation, with a driving derived from the Cahn-Hilliard free energy. In contrast to previous work, however, we decouple the bulk and interface terms, the former being incorporated into the model through the local equilibrium populations, and the latter through a forcing term. In the present work, we focus on gas-liquid phase equilibria. The equation of state can be an arbitrary function of the density, however with the strong restriction that all the weight coefficients for the equilibrium populations must remain positive.

The most novel aspect of our approach is a systematic Chapman-Enskog (CE) expansion up to the third order. Due to the third-order gradient in the interface forcing term, this is needed to obtain an LB model that is fully consistent with both hydrodynamics and thermodynamics, in the limit of small flow velocities and small lattice spacing. It is argued that the concept of small Mach number is not useful for the present system, since the Mach number diverges at the critical point.

For the bulk relaxation we confine ourselves, for simplicity, to the single relaxation time (BGK) model. A proper design of additional terms in the collision operator then enables us to cancel all spurious terms in the continuum equations, as derived via the third-order CE formalism. The price of such a consistent model are many velocity shells needed for its construction, i. e. 21 velocities in 2D and 59 velocities in 3D. The commonly noticed inconsistency of the existing models is thus traced back to their insufficient number of degrees of freedom. Therefore, the gain of the new model is in its clear derivation, full thermo-hydrodynamic consistency, and expected complete elimination of spurious currents in the continuum limit, combined with an increase of computational complexity that is expected to be only one order of magnitude (at most two), or even less.

Critical Dynamics of Isothermal Compressible Fluids

Markus Gross
ICAMS, Ruhr-University Bochum
Stiepeler Str. 129, 44801 Bochum, Germany

While the behavior of a conventional fluid at its critical point is well understood [1], the critical dynamics of an isothermal non-ideal fluid has received much less attention so far. However, an isothermal fluid is a useful description for monolayer films [2,3], which are important in industry and biology and whose critical properties might even have some relevance for the physiology of cells [4]. While the static critical properties of conventional and isothermal fluids are both described by the Ising universality class (see [5] and references in there), their dynamics is crucially different due to the isothermal condition [6]. In particular, it is found that the order-parameter dynamics of the isothermal fluid reduces to the so-called model A [1] in the critical, low-frequency limit, characterized by a divergence of the bulk viscosity. The shear viscosity, in contrast, remains finite. The theoretical predictions are well supported by Lattice Boltzmann simulations of the full fluctuating hydrodynamic equations in two dimensions.

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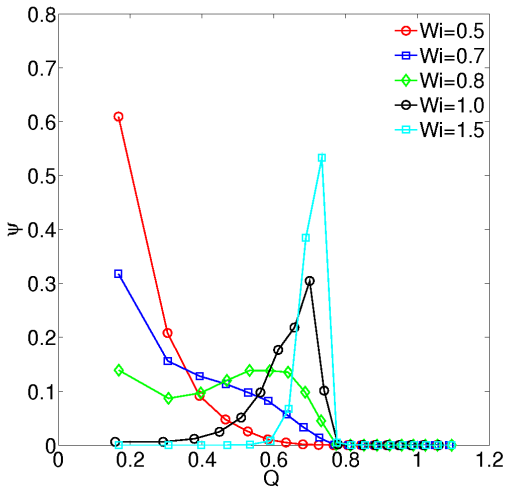
A Lattice Boltzmann Method for Dilute Polymer Solutions

Shiwani Singh, Santosh Ansumali
Engineering Mechanics Unit, JNCASR, Jakkur, Bangalore 560064, India

Recently, a lattice Boltzmann type formulation for simulating polymer dynamics at the kinetic level has been proposed [1,2]. The key idea behind these methods is to exploit the phase space dynamics on a lattice to yield the solution for the configuration probability density associated with a polymer molecule. This fact was used to develop a lattice Boltzmann methodology for polymer dynamics. We benchmarked this formulation by comparing the bulk rheological properties for shear flow as well as extensional flow with those obtained using Brownian dynamics simulations [3]. One of the important rheological property of extensional flow is the coil-stretch transition which is well captured by the present scheme as shown in the figure. In order to further validate the present scheme, we consider the dynamics of a passive scalar in a Taylor-Green vortex cell. Finally, the present scheme is used to study the coupled system of the polymer and the flow.



Probability density $\psi(\mathbf{Q})$ at steady state with different Wi (Wi is a measure of the flow strength in units of the polymer relaxation time) showing the coil-stretch transition. Here, $\mathbf{Q}$ is the end-to-end distance of the dumbbell.

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Lattice Boltzmann Simulations of Mass Transport in Soft Biomaterials

T. Gebäck, A. Heintz
Department of Mathematical Sciences and SuMo Biomaterials,
Chalmers University of Technology,
SE-412 96 Göteborg, Sweden

Within the SuMo Biomaterials research center [1], the goal is to design new materials with specific mass transport properties for a range of applications, including hygiene products and controlled release of drugs. One important step towards this goal is predicting and computing mass transport given material data, such as geometry and chemical properties.

We perform Lattice Boltzmann simulations of flow, diffusion and advection-diffusion in geometries obtained from microscopy data from real materials. Flow patterns and mass transport properties are computed from the results of the simulations, and are analyzed and compared to experimental data obtained using different techniques, including μPIV. We have also developed novel boundary conditions for the Lattice Boltzmann (advection-) diffusion equation in order to solve these equations in complex geometries [2].

Our results show in general good agreement with experimental data and can be used for prediction of mass transport properties. However, major challenges remain taking surface and structure interactions into account, as they can greatly influence mass transport in the materials in question. Some steps in this direction have been taken.

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Competition of Inertia and Deformability: Motion of Deformable Particles in Channel Flow

T. Krüger[1], B. Kaoui[1], J. Harting[1,2]
[1]Department of Applied Physics, Eindhoven University of Technology,
Den Dolech 2, 5612 AZ Eindhoven, The Netherlands
[2]Institut für Computerphysik, Universität Stuttgart,
Pfaffenwaldring 27, 70569 Stuttgart, Germany

The motion of deformable particles in a planar Poiseuille flow has not been entirely understood. On the one hand, it is known that the deformability of particles (expressed by the capillary number, Ca, the ratio of viscous fluid and elastic particle stresses) promotes a migration towards the centerplane of the flow in the absence of inertia (zero Reynolds number, Re = 0) [1]. On the other hand, inertia effects are responsible for an outward migration of rigid particles (Ca = 0) close to the centerplane [2]. We present 3D simulation results for systems with both finite Ca and Re at intermediate volume fractions and discuss the interplay of inertia and deformability effects on the lateral particle distributions and apparent viscosity.

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Nanoparticles and Surfactant on the Interface of a Droplet in Shear Flow

S. Frijters[1], F. Günther[1], J. Harting[1,2]
[1]Department of Applied Physics, Eindhoven University of Technology, Den Dolech 2, NL-5600MB Eindhoven, The Netherlands
[2]Institute for Computational Physics, University of Stuttgart, Pfaffenwaldring 27, D-70569 Stuttgart, Germany

Three-dimensional numerical simulations have been performed to investigate similarities and differences between surfactants and nanoparticles as additives at a fluid-fluid interface [1]. We subject a fluid droplet to shear and explore the deformation properties of the droplet, its inclination angle relative to the shear flow, the dynamics of the particles at the interface, and the possibility of breakup. Particles do not affect the surface tension of the interface, but they do change the interfacial free energy. The particles do not remain homogeneously distributed over the interface, but form clusters in preferred regions. These clusters are stable for as long as the shear is applied. However, although the overall structure remains stable, individual nanoparticles roam the droplet interface. Their frequency of revolution is highest in the middle of the droplet interface, normal to the shear flow, and the frequency increases with capillary number. The effect of surfactant is captured in the capillary number, but the inertia of adsorbed massive particles increases deformation at higher capillary number and eventually leads to easier breakup of the droplet.

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How does DNA Change the Conductivity of Nanopores? Blockade vs. Enhancement

S. Kesselheim, C. Holm
Institute for Computational Physics, University of Stuttgart,
Pfaffenwaldring 27, 70569 Stuttgart, Germany

We investigate the electrical conductivity of nanopores in the presence of DNA molecules by means of computer simulations and electrokinetic theory. Our simulations show that the concentration dependence of the bulk electrolyte conductivity can well be reproduced by hybrid Lattice Boltzmann/Molecular Dynamics simulations with point coupling[1]. This method is applied to study the conductivity of nanopores in the presence of DNA molecules. We find that — consistent with experiments — the conductivity is reduced by DNA only at high salt concentrations, whereas it is increased at low salt concentration. We formulate a modified electrokinetic theory that agrees well with the simulation data and also show a comparison to atomistic simulations.

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GPU Implementation of an Electrokinetics Solver as Proposed by Capuani, Pagonabarraga and Frenkel

G. Rempfer, A. Arnold, C. Holm
Institute for Computational Physics, University of Stuttgart,
Allmandring 3, 70569 Stuttgart, Germany

In 2004 Capuani, Pagonabarraga and Frenkel proposed an algorithm to solve the full set of electrokinetic equations [1]. It mainly consists of a lattice-Boltzmann algorithm coupled to a solver for the convection-diffusion equation. They demonstrated that electro-osmotic flow and the sedimentation of charged spheres can be treated with this method. We implement this method to be executed by GPUs as part of ESPResSo [2], the Extensible Simulation Package for Research on Soft Matter Systems.

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Simulations of Arterial Boundary with Lattice BGK

Xiaoyang Lu[1], Huabing Li[2]
[1]Guangdong Institute of Public Administration,
Guangzhou 510631, China
[2]Department of Computational Science and Applied Physics,
Guilin University of Electronic Technology,
Guilin 541004, China

An aneurysm may occur when the arterial wall is weakened due to the atherosclerosis or congenital biochemical factors, and loses its structural integrity and thus results in dilatation by the pulsatile intraluminal pressure[1]. The abdominal aorta is one of the primary arteries of the body that supplies the lower half of the body with blood. The diameter of the abdominal aorta ordinarily lies between 15-20 mm [2]. This diameter can dilate into a balloon like bulge referred to as an abdominal aortic aneurysm (AAA). Once the AAA develops, tension in the arterial wall increases, and thus it exhibits abnormal deformations. Very high shear stresses near the throat of the stenosis can activate platelets and thereby induce thrombosis, which can totally block blood flow to the heart or brain[3]. To date, researchers have focused on determining stress states within the aortic walls, and investigating the relationship between the bulge shape and maximal diameter of the aneurysm and the structures present in the flow[4].

In this paper, the lattice Boltzmann method[5] is applied to study the flow in elastic blood vessels. Steady flow in elastic aneurysm models has been examined for several aneurysm sizes. The overall features of the flow and the stresses on the aneurysm walls in steady flow are discussed. The wall shear stress magnitude in the recirculation zone is about ten times less than in the entrance tube. Both wall shear stress and wall normal stress profiles exhibit large magnitude peaks near the reattachment point at the distal end of the aneurysm.

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Cell-Cell Interaction Effect in Mural Thrombosis: A Dissipative Particle Dynamics Approach

S. Muhammad R. Hassani, Nasser Fatouraee
Biological Fluid Mechanics Research Laboratory,
Department of Biomedical Engineering,
Amirkabir University of Technology (Tehran Polytechnic),
Tehran, Iran 15914

Mural thrombosis, due to its highly complex physiological process and its pathological significance, has gained great attention through mathematical modeling with different methods and different models. One crucial aspect of this phenomenon is the effect of cell-cell interactions (CCI) in the development of mural clot, which is inherited from the complexity of blood via different suspended cells. In this work, we have implemented Dissipative Particle Dynamics to model the flow of plasma, biconcave RBCs, and platelets, in the proximity of a $24r_c$ mural lesion in the middle of a 2D micro-channel of $150r_c \times 80r_c$ with a parabolic inlet. The CCI is mainly gained through grouping of DPD particles within each cell which interact with the fluid particles and other cells in addition to the use of elastic collision theory [1,2]. To emphasize the CCI effect we have compared two models of thrombosis: one including only platelets flow, and in the other RBCs and platelets are both included. In this comparison, the effect of RBC-platelet interaction is vivid in both increasing the rate of aggregation and the proximal fraction of the aggregated platelets along the lesion which agree well with the previous in-vitro and numerical studies [3,4]. As a concluding remark, the explicit modeling of suspended cells in blood flow helps in gaining better view on the clot formation process.

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Dissipative Particle Dynamics Simulation of a Charged Colloid under AC Fields

Jiajia Zhou, Friederike Schmid
Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany

We study the dielectric response of spherical charged colloids under alternating electric fields (AC-fields) by mesoscopic simulation methods, accounting in full for hydrodynamic and electrostatic interactions. Specifically, we systematically investigate the effect of frequency and amplitude of the AC-fields, the ionic strength of the solution, and the bare charge of the colloids. A coarse-grained molecular dynamics approach is taken to model the fluid, in which the solvent particles are simulated using Dissipative Particle Dynamics (DPD). The electrostatic interaction between all charges are calculated explicitly using the Particle-Particle-Particle Mesh (P3M) method.

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A Mesoscale Simulation Method for Polyelectrolytes at High Salt Concentrations

S. Medina[1,2], F. Schmid[1]
[1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 7, 55128 Mainz, Germany
[2]Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany

In mesoscale simulations of electrolyte solutions it is the long range character of electrostatics and hydrodynamics that plays the critical role for computational efficiency and accuracy. In the past it became apparent that simulating high salt concentrations is too costly, if every salt ion is treated explicitly as a separate charged particle. On the other hand, charges are highly screened at high salt concentrations and ion-ion correlations are less important than in the low-salt limit. Therefore, we have developed a dynamic mean-field treatment of charges which is perfectly sufficient in many cases, improving the performance of such simulations. We apply the new method to several test cases and study electro-osmotic flow phenomena as well as the problem of shear flow in polyelectrolyte solutions.

The Effect of Slip on Fluid Flow

M. Pihl[1,2], B. Jönsson[1], M. Skepö[3]
[1]Department of Applied Surface Chemistry,
Chalmers University of Technology, Göteborg, Sweden
[2]Department of Biophysical Chemistry,
Lund University, Lund, Sweden
[3]Department of Theoretical Chemistry,
Lund University, Lund, Sweden

As opposed to macroscopic systems where the no slip boundary condition is applied, i.e. a zero velocity at the wall, at the micro and nano scales the slip boundary condition should be considered. This means there is a certain velocity at the wall, the slip velocity. Some of the factors affecting slip include wettability, shear rate and surface roughness.

We aim to be able to design surfaces with certain flow characteristics and here we investigate the relation between fluid flow and slip, using computer simulations and experimental flow studies. We study the effect of proportion and arrangement of slip on surfaces as well as the effect of surface roughness using the Comsol Multiphysics software.

The experimental flow studies are performed using micron resolution particle image velocimetry, μPIV. In this technique, water is seeded with fluorescent polystyrene particles and the images obtained using two laser pulses within a short time period, are correlated to give the flow velocity. The microchannels used are made of polydimethyl siloxane, PDMS, some of which are further surface-modified. The surfaces are characterised with different techniques, such as contact angle measurements and ESCA.

Rare Events, Slippage, Stratification and Flow Control in Microfluidics

E. Corvera Poiré[1,2]
[1]Departamento de Física y Química Teórica, Facultad de Química,
Universidad Nacional Autónoma de México,
Ciudad Universitaria, México D. F. 04510, Mexico
[2]Departament de Física Fonamental, Universitat de Barcelona,
Diagonal 647, E-08028 Barcelona, Spain

We demonstrate that the stochastic behavior induced by the natural roughening present in standard microchannels is so important, that the dynamics for the advancement of a water front displacing air has plenty of rare events. These ones are correctly characterized by an extreme-value distribution. We observe that for low pressure differences, the hydrophobic interactions of the water front with the walls of the microchannel, put the front close to the pinning point. This causes a burst-like dynamics, characterized by series of pinning and avalanches, that leads to a Gumble distribution for the velocity fluctuations and a non-classical time exponent for the advancement of the mean front position [1].

We make an analytical study of the non-steady flow of Newtonian fluids in microchannels. We consider the slip boundary condition at the solid walls with Navier hypothesis and calculate the dynamic permeability, which gives the system's response to dynamic pressure gradients. We find a scaling relation in the absence of slippage that is broken in its presence. We discuss how this might be useful to experimentally determine whether slippage exists or not in a system, the value of the slip length, and the validity of Navier hypothesis in dynamic situations [2].

We present a mechanism in the field of microfluidics by which the stratification of a viscoelastic fluid can be induced in a channel on the microscale by applying a dynamic pressure gradient at frequencies within the range of sound. Stratification is obtained with identical layers, parallel to the channel walls, whose number can be tailored. These layers are separated by 2D zero-velocity planes. This would allow different tracer particles with small diffusion coefficients to be confined in different fluid layers within the same microchannel. We obtain analytical results that allow us to make theoretical predictions regarding the possible experimental realization of stratification in a microchannel using a biofluid [3].

Finally, we show that viscoelastic flow in a microchannel under a dynamic pressure gradient dramatically changes with the value of the apparent slip. At certain driving frequencies, the flow is orders of magnitude different for systems with and without slip, implying that controlling the degree of hydrophobicity of a microchannel can lead to the control of the magnitude of the flow. We verify this for viscoelastic fluids with very different constitutive equations. We show that for dynamic situations, slippage causes an effectively thicker channel whose effective thickness depends on frequency. We have calculated relevant quantities for blood and a polymeric fluid in order to motivate experimental studies [4].

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Curvature Distribution of Entangled Semiflexible Biopolymers

M. Lämmel, K. Kroy
Institut für Theoretische Physik, Universität Leipzig, Germany

The inside of a eukaryotic cell is a crowded world into which myriads of organelles and macromolecules are packaged. A typical filamentous protein under such conditions is subjected to highly complex and heterogeneous forces and sterical constraints. The formidable task of describing the behavior of one semiflexible polymer in such a complicated energy landscape can be tackled with the help of minimal models.

In our contribution, we address the entanglement problem in semiflexible biopolymer solutions based on the wormlike chain model. We describe the caging effect on a test filament by surrounding filaments through a cylindrical confinement potential — constituting the so-called tube [1] — that is self-consistently determined. Recent theoretical work of our group [2,3] demonstrated how a heterogeneous tube potential reflects the local packing structure of the crowded environment. The predicted tube radius distribution was validated by highly accurate experimental observations for F-actin solutions [3]. The concept of a heterogeneous tube allows us moreover to analyze the influence of the polymer meshwork's entangled microstructure on the curvature distribution of a test polymer [4]. We compare our results with MC simulations and experimental observations.

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Significance of Thermal Fluctuations and Hydrodynamic Interactions in Receptor-ligand-mediated Microparticle Adhesion

K. V. Ramesh[1,2], R. Prabhakar[2], J. Ravi Prakash[3], Rochish M. Thaokar[1]
[1]Department of Chemical Engineering,
Indian Institute of Technology, Bombay, India
[2]Department of Mechanical and Aerospace Engineering,
Monash University, Melbourne, Australia
[3]Department of Chemical Engineering,
Monash University, Melbourne, Australia

Cell adhesion is ubiquitous in biological systems. It is the process of binding of a cell to a surface, extracellular matrix or another cell using cell adhesion molecules. In vitro experiments in flow chambers are being increasingly used to understand cell adhesion. These experiments typically involve the study of interaction between protein molecules on the cell surface and the ligands coated on the bottom plate of the flow chamber. The receptors on the cell surface binds with the ligands via specific adhesion. A model to describe this whole dynamical process was suggested by Korn et al. [1, 2] that considered a receptor laden hard-sphere, moving above a planar ligand-bearing wall in a simple shear flow and subject to a deterministic attraction towards the wall, and Brownian motion. Hydrodynamic interactions of the finite-sized sphere with the wall were considered. Five different dynamic states of motion – free motion, rolling adhesion, firm adhesion and two stop-and-go rolling regimes – were identified depending on the relative values of receptor-ligand association and dissociation rates. The appearance of these states is portrayed in a state diagram. In the present work, the significance of hydrodynamic interactions of the sphere with the wall, and of Brownian fluctuations is explored with simulations.

This work firstly demonstrates that although the system is at high Peclet number, the contribution of thermal fluctuations cannot be ignored. Significant differences are observed between state diagrams obtained with and without thermal fluctuations, with changes in boundaries separating the various states of motion. Secondly, we examine how HI with the wall affects the

overall kinetics of adhesion. The mean first-passage time (MFPT) of the particle from the bulk fluid to its first encounter with a wall ligand is examined to understand the rate of approach of the particle towards the wall. Once the cell is close to the wall, we investigate whether it is possible to replace the full wall HI with an effective drag coefficient without significant changes to the state diagram.

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Dynamic Crossover Scaling in Polymer Solutions

A. Jain[1], B. Dünweg[2,1], and J. Ravi Prakash[1]
[1]Department of Chemical Engineering, Monash University,
Melbourne, VIC 3800, Australia
[2]Max Planck Institute for Polymer Research,
Ackermannweg 10, 55128 Mainz, Germany

The crossover region in the phase diagram of polymer solutions, in the regime above the overlap concentration, is explored by Brownian Dynamics simulations, to map out the universal crossover scaling functions for the gyration radius and the single-chain diffusion constant. Scaling considerations, our simulation results, and recently reported data on the polymer contribution to the viscosity obtained from rheological measurements on DNA systems, support the assumption that there are simple relations between these functions, such that they can be inferred from one another.

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A Blobology for the Rheology of Dilute and Unentangled Semidilute Polymer Solutions

R. Prabhakar
Department of Mechanical and Aerospace Engineering
Monash University,
Clayton, VIC - 3800, Australia

A unified description of the evolution of polymeric stresses in both dilute and semidilute solutions is attempted with a single-mode model in which the effect of intra- and intermolecular interactions on the evolution of the mean conformation tensor is described using the concept of "blobs". Intramolecular excluded-volume interactions are effectively accounted for through the concept of theta-blobs. A new finitely-extensible "spring" force-law is proposed in which the entropic resistance to stretching is calculated for a chain of Pincus-blobs. The mean volume pervaded by partially stretched molecules is continually tracked as molecules stretch in a flow. When the instantaneous pervaded volume fraction exceeds unity, progressive screening of excluded and hydrodynamic interactions is modeled by calculating instantaneous screening lengths such that De Gennes' correlation-blobs are space-filling. Competition between Pincus and De Gennes blobs is considered when intermolecular overlap occurs. When the dynamic pervaded volume fraction is less than unity, the effect of intra- and intermolecular (far-field) hydrodynamic interactions is modeled through an isotropic conformation-dependent friction coefficient that smoothly varies with molecular stretch from its value for equilibrium coils to that given by a Batchelor-inspired interpolation formula for a semidilute suspension of rods. When molecular overlap is significant on the other hand, the friction coefficient is calculated as the Rouse-like friction of a chain of De Gennes blobs. Kramers' expression is used to calculate the polymer stress tensor in this mean-field model. Predictions for equilibrium coil dimensions and material functions in shear and extensional flows are discussed.

The Effect of Rotational Switching of Flagella on the Dynamics of Single-tailed Microswimmers Near Walls

S. Clark, R. Prabhakar
Department of Mechanical and Aerospace Engineering,
Monash University, Clayton, Victoria, Australia

In swimming microorganisms such as many species of bacteria motility near a surface is critical to surface attachment and initiation of a biofilm. In species such as *Vibrio alginolyticus* and *Pseudomonas aeruginosa*, each cell is typically propelled by a semi-flexible helical flagellum driven by a rotary protein motor at its point of attachment to the cell body. Such cells can swim forwards or backwards by switching the rotational direction of the flagellum. Swimming near a surface is known to be strongly affected by hydrodynamic interactions between the cell and the wall. When driven forward, these interactions cause swimmers to be attracted towards and be aligned parallel to the surface, whereas reverse driving can cause repulsion and perpendicular alignment. Initial attachment to surfaces in bacteria is observed to occur either by the tip of the tail, or by the top of the head. Efficient attachment further requires functional flagellar switching.

We use Stokesian dynamics to investigate the role of rotational switching in the ability of a cell to steer effectively in the presence of a wall and bring itself into proper wall-vertical alignment to achieve close proximity of the head- or tail-end for possible attachment. A bead-spring model of a single-tailed swimmer is used along with hydrodynamic and mechanical interactions within the cell body and tail. We investigate how asymmetries in rotational switching and those caused in the shape of the semi-flexible filament under forward and reverse driving affect swimming dynamics near the wall. We use a toy model to study the optimal rotational protocol required to achieve a preferred orientation at the wall for a swimming hydrodynamic dipole, and compare results with full simulations.

Microswimmer Scattering by Soft Elastic Filaments

R. Ledesma-Aguilar, J. M. Yeomans
Rudolf Peierls Centre for Theoretical Physics, University of Oxford,
1 Keble Road, Oxford OX1 3NP, United Kingdom

The locomotion of microorganisms in the presence of elastic filaments, such as hairs and flagella, is very common in biological systems [1].

We perform a theoretical study, using a simple point-force hydrodynamic model, to analyse the scattering of a dipolar swimmer and semiflexible filaments.

Our swimmers consist of active dumbbells that undergo a non-reciprocal swimming stroke leading to locomotion. Fluid-mediated interactions with the elastic chains are modelled using Oseen-level hydrodynamics.

We explore the effect of the elasticity of the filaments on the swimmer velocity and orientation.

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Patterns, Segregation and Hysteresis in Vertically Vibrated Granular Mixtures

Mohammed Istafaul Haque Ansari, Meheboob Alam
Engineering Mechanics Unit,
Jawaharlal Nehru Centre for Advanced Scientific Research,
Jakkur P.O., Bangalore 560064, India

Granular materials under vertical shaking exhibit a variety of interesting phenomena: undulations [1], surface instabilities, oscillons [2], ripples [3], Leidenfrost state [4] and convection [5]. We have investigated these phenomena by conducting experiments on two types of equimolar *binary* granular mixtures: (i) glass and steel balls both having diameters of $d = 1.0\ mm$ and a density ratio of $\rho_s/\rho_g = 3.0$ and (ii) delrin and steel balls both having diameters of $1.0\ mm$ and a density ratio of $\rho_s/\rho_d = 5.5$. The particles are held in a quasi-two-dimensional Perspex container which is vibrated harmonically in vertical direction using an electromagnetic shaker. All the experiments are done by increasing the shaking intensity (measured in terms of the dimensionless shaking acceleration Γ) while keeping the shaking amplitude A/d fixed. We uncovered many unhitherto reported novel patterns: (i) the Leidenfrost state coexisting with a granular gas, (ii) horizontal segregation within a Leidenfrost state, (iii) granular convection with a floating particle cloud, and (iv) both vertical and/or horizontal segregation with other patterned states. We further show that the transition from the Leidenfrost state to convection in a binary mixture occurs via a hysteretic transition.

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Breath Figures: Nucleation, Growth, Coalescence, and the Size Distribution of Droplets

J. Vollmer[1,2]
[1]Max-Planck-Institut für Dynamik und Selbstorganisation (MPIDS),
37077 Göttingen, Germany
[2]Fakultät für Physik, Georg-August-Universität Göttingen,
37077 Göttingen, Germany

The analysis of the size distribution of droplets condensing on a substrate (breath figures) is a test ground for scaling theories. Recently we showed [1] that a faithful description of these distributions must explicitly address the nucleation and the growth mechanisms of the droplets. This finding establishes a gateway connecting microscopic features of droplets on surfaces to gross features of the evolution of the droplet size distribution.

Extending the work of Ref. [1], I will discuss the role of the substrate dimensionality, and address consequences on the modelling of other systems with vastly polydisperse droplet size distributions — like water droplets in clouds.

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