DY 14 Complex Fluids

Zeit: Freitag 15:30–18:30 Raum: TU H3010

DY 14.1 Fr 15:30 TU H3010

Lattice-Boltzmann simulations of the self-organisation of amphiphilic mesophases and possible microfluidic applications — •Jens Harting — Instut für Computerphysik, Pfaffenwaldring 27, 79569 Stuttgart

The dynamical self-assembly of a particular amphiphilic mesophase, the gyroid, can be modelled using the lattice Boltzmann method. This mesophase forms from a homogeneous mixture, without any external constraints imposed to bring about the gyroid geometry, which is an emergent effect of the mesoscopic fluid parameters. We report on self-assembly and dynamics studies of gyroid mesophases, where our particular interest is on the formation and behaviour of defects in the system in order to understand their influence on the mesophases' properties. Defects can be grain-boundary defects between gyroid domains, dislocations, line defects, or localised non-gyroid regions. Gyroid mesophases can be very stable and might thus be applicable as microfilters in very confined geometries. We will present results from simulations of the gyroid in microchannels.

DY 14.2 Fr 15:45 TU H3010

A mesoscopic, particle-based model for fluid flow with a non-ideal equation of state — •Thomas Ihle[1], Erkan Tuzel[1,2], and Daniel Kroll[1] — [1]Department of Physics, North Dakota State University, Fargo, ND 58105, USA — [2]School of Physics and Astronomy, 116 Church Street SE, University of Minnesota, Minneapolis, MN 55414, USA

A recently introduced stochastic model for fluid flow, called Stochastic Rotation Dynamics (SRD), is a promising tool for the coarse-grained modeling of a fluctuating solvent, particularly for colloidal, vesicle and polymer suspensions. Instead of solving Navier-Stokes equations explicitly, the fluid is modelled by "fluid"-particles with continuous velocities and efficient multi-particle collisions. It is shown how the transport coefficients can be calculated exactly and that they are in very good agreement with numerical simulations. A new extension of the model is presented where the collision rules depend on particle velocities which leads to a nonideal equation of state. These rules obey detailed-balance and an H-theorem. Transport coefficients, equation of state and speed of sound are calculated and compared with numerics.

DY 14.3 Fr 16:00 TU H3010

Shear thickening, stick-slip like flow behavior and rheo-chaos in non-linear Maxwell model fluids — •Siegfried Hess[1] and Ortwin Hess[2] — [1]Inst.f.Theoret.Physik, TU Berlin — [2]Advanced Technology Institute, School of Electronics and Physical Sciences, University of Surrey, Guildford, GU2 7XH, UK

The nonlinear Maxwell model equation for the stress tensor as introduced previously in O. Hess and S. Hess, Physica A 207 (1994) 517 to treat the shear thickenening and shear thinning behavior of fluids can also be applied for temperatures and densities where a substance shows a yield stress. The basic equations are discussed. Analytic and mainly numerical results are presented for the plane Couette flow geometyry. Depending on the model parameters and on the imposed sheat rate, a stationary state can be reached or not. In the second case periodic solutions of stick-slip like motions or irregular chaotic behavior is found. For some typical cases the shear stress, the first and second normal stress differences as well as the stress components which break the Couette symmetry are displayed as functions of the time. Different types of time dependent solutions can be distinguished by the rheological phase portraits. Some remarks are made on the entropy production associated with the viscous flow and the stress relaxation.

DY 14.4 Fr 16:15 TU H3010

Einfluss der festen Grenzfläche auf Struktur und Dynamik in komplexen Flüssigkeiten unter Scherung — •Max Wolff[1,2], Andreas Magerl[3] und Hartmut Zabel[2] — [1]Institut Laue-Langevin, BP 156, 38042 Grenoble Cedex 9, Frankreich — [2]Lehrstuhl für Festkörperphysik, Ruhr-Universität Bochum — [3]Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg

Die Struktur von kondensierter Materie nahe einer Grenzfläche kann sich von der im Volumen, die mit Neutronenkleinwinkelstreuung (SANS) zugänglich ist, unterscheiden.

Kürzlich konnten wir zeigen, dass mittels einer Kombination von SANS und Neutronenreflektometrie die Struktur von Polymerlösungen nahe Grenzflächen mit unterschiedlicher chemischer Terminierung in 3 Dimensionen gelöst werden kann [1]. Wir fanden in Abhängigkeit von Parametern wie Temperatur, Scherrate oder Zusammensetzung des Polymers einen unterschiedlichen Einfluss von hydrophilen und hydrophoben Grenzflächen.

Neutronenspektroskopie gibt zusätzlich Aufschluss über die mikroskopische Dynamik der Polymerlösung. Unter Scherung wird die Translationsdiffusion in Richtung des Schergradienten verlangsamt wenn durch die Grenzfläche strukturelle Ordnung induziert wird. Fehlt die grenzflächeninduzierte Ordnung, dann wird kein Einfluss von Scherung auf die Diffusion beobachtet [2].

[1] M. Wolff et al.: Phys. Rev. Lett. 92, 255501 (2004).
[2] M. Wolff et al.: Phys. Rev. E (submitted).

DY 14.5 Fr 16:30 TU H3010

Point force manipulation and activated dynamics of polymers adsorbed on structured substrates — •P. Kraikivski, R. Lipowsky, and J. Kierfeld — MPI für Kolloid- und Grenzflächenforschung, 14424 Potsdam

We study the activated motion of adsorbed polymers which are driven over a structured substrate by applying a localized *point* force. Our theory applies to experiments on single adsorbed polymers using, for example, force microscopy tips to drive the polymer. We consider both flexible and semiflexible polymers, and the surface structure is represented by double-well or periodic potentials. The dynamics is governed by kink-like excitations for which we calculate shapes, energies, and critical point forces. Thermally activated motion proceeds by the nucleation of a kink-antikink pair at the point where the force is applied and subsequent diffusive separation of kink and antikink. In the stationary state of the driven polymer the collective kink dynamics can be described by an one-dimensional symmetric simple exclusion process.

DY 14.6 Fr 16:45 TU H3010

Stretching of polymers on sub-Kolmogorov scales in a turbulent flow — •Jörg Schumacher — Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg

We study the stretching behaviour of polymers on scales below the viscous Kolmogorov scale in a turbulent flow. Brownian dynamics simulations of an ensemble of dumbells are combined with direct numerical simulations of Navier-Stokes turbulence that resolve sub-Kolmogorov scales very well. The role of extreme stretching events on the overall statistics is discussed. Our results are compared with recent measurements in so-called von Karman swirling flows.

DY 14.7 Fr 17:00 TU H3010

Lattice and continuous models of random heteropolymer adsorption — •Alexey Polotsky[1,2], Andreas Degenhard[1], and Friederike Schmid[1] — [1]Condensed Matter Theory, Fakultät für Physik, Universität Bielefeld — [2]Institute of Macromolecular Compounds of the Russian Academy of Sciences, St.-Petersburg, Russia

Continuous and lattice models were used to study the adsorption of a random heteropolymer chain onto homo- and heterogeneous substrates. Different approaches were employed for the averaging over the sequence/surface disorder and the computation of the conformational average. In the continuous case, these are the replica trick and the reference system approach, respectively, whereas in the case of a lattice model partial annealing (the so called "Morita approximation") in combination with the generating function approach were applied. For the continuous model simple equations for the desorption-adsorption transition line were obtained. In the lattice models, the temperature dependency with respect to different conformational characteristics of the chain above the adsorption threshold were calculated. Some of the results were tested by a comparison with numerical lattice calculations.

DY 14.8 Fr 17:15 TU H3010

Free Energy of a Charged Polymer in an Electrolyte — •Stephan Kramer[1], Reiner Kree[1], and Gert Lube[2] — [1]Institut f. Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institut f. Numerische und Angewandte Mathematik, Universität Göttingen, Lotzestr. 16-18, 37083 Göttingen

Many physical issues fit into the context of parameter identification in optimal control problems with constraints given by partial differential equations (PDE). Solving these problems is usually extremely time-consuming. One important issue to make solving such problems feasible is optimizing the discretization of the PDE constraint especially for simulations in three dimensions. This is achieved by employing *goal-oriented* error estimation in the mesh adaption which minimizes the error of some target functional of the PDE solution rather than the error in the solution itself.

As a sample problem we use the interactions between the electrostatic field in an aqueous solution of a charged, semi-flexible polymer and its conformation. The target quantity is the combined free energy consisting of the free energy of the charge distribution and the elastic energy of the molecular conformation. Now, the optimization process consists of finding a conformation and thus a charge distribution such that the total free energy is minimal.

Besides the good convergence behavior and the need for adaptivity especially in three dimensions our numerical results demonstrate the influence of the electrostatic potential on the relationship between the conformation and the free energy.

DY 14.9 Fr 17:30 TU H3010

Colloidal transport in 2d restricted geometries — •Michael Koeppl, Artur Erbe und Paul Leiderer — Universität Konstanz

Transport of electrons in two dimensions has been studied in electronic systems for decades. Typical examples are the quantum point contact or the quantum Hall effect in a semiconductor 2-dimensional electron gas (2DEG). In the non quantum mechanical regime of low densities and large structures compared to the electron wave function, colloidal systems can serve surprisingly good as a model system for electronic transport on the nanoscale. Since the fundamental interactions are not dominated by quantum effects, even systems like pedestrians show comparable dynamical behavior.

We use a videomicroscopy setup to investigate the transport of driven particles through topological restrictions and bottlenecks with sizes comparable to the particle diameter. The use of superparamagnetic colloids allows us to tune the plasma parameter of the system simply by 'turning a knob' applying an external magnetic field. We report on lane formation of the particle trajectories due to interactions. Comparison of our colloidal transport measurements with simulations of electronic systems and traffic dynamics reveals good consistency.

DY 14.10 Fr 17:45 TU H3010

Preparation and Characterization of Capped Colloids.* — •Florian S. Merkt, Artur Erbe, and Paul Leiderer — Universität Konstanz

Colloids have been used to study interparticle and particle-wall interactions on the micron scale. Here we present a technique to fabricate colloids with a large variety of surface materials. This controlled design of surface properties enables us to investigate an even broader range of interactions than was covered by previous experiments.
In particular we prepare aqueous suspensions of capped colloids in which half of the surface is covered with a metal layer. Mono- and multilayers of magnetic and unmagnetic metals are evaporated onto micron-sized Silica spheres. By adjusting the layer structure the magnitude and direction of the magnetic moments can be tuned.
The particles' magnetic properties are characterized and their behavior in light and magnetic fields is observed. Further experiments to investigate adhesion forces and interactions in close contact between colloidal and plane surfaces are proposed. Especially the detachment dynamics of colloidal particles with various surface properties sticking to a surface will be investigated.

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DY 14.11 Fr 18:00 TU H3010

The influence of particle size distribution on the solidification kinetics in colloidal hard sphere systems — •Hans Joachim Schöpe[1], Gary Bryant[2], and William van Megen[2] — [1]Johannes Gutenberg-Universität Mainz, Institut für Physik, KOMET 336, Staudinger Weg 7, D 55099 Mainz, Deutschland — [2]Department of Applied Physics, Royal Melbourne Institute of Technology, GPO Box 2476V, Melbourne 3001, Australia

A complete understanding of the solidification process (nucleation, crystal growth, ripening, vitrification) is one of the long-standing problems in solid-state physics. The use of colloidal model systems provides an ideal experimental system to reduce this lack of knowledge. A significant difference between the particles in a suspension and the atoms of a melt is that colloidal particles always have a particle size distribution (PSD). One of the least well characterized parameters in the solidification process in colloidal systems is the effect of the PSD. Here we present systematic measurements of the solidification kinetics and of the phase behaviour in dependence of the PSD of a one component system. This investigation shows that polydisperity has a significant influence to nucleation, growth velocity and the morphology and crystal structure of the resulting sample. These studies also indicate that in addition to the rate of crystallization, the crystal structure and the propensity to vitrify are also very sensitive to small variations in the particle size distribution. Surprisingly we observe a two step behaviour in the nucleation rate, which is independent of the PSD

DY 14.12 Fr 18:15 TU H3010

Why are effective potentials soft? — •Sabine H.L. Klapp — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Sekr. TC7, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin

In this contribution we focus on the question why effective potentials $\mathcal{W}(\mathcal{R})$ between interacting supramolecular are typically "soft", i.e., remain finite even for $R \to 0$ and vary much slower with R than the underlying interatomic interaction potentials. To this end we consider a number of special model systems, which can be treated semi–analytically, starting with an atom and a diatomic. However, the characteristic "softness" of *mesoscopic* effective potentials is recovered only for our most complex model, that is two "glassy disks" with liquid–like, yet frozen internal configurations of atoms. In this case $\mathcal{W}(\mathcal{R})$ varies so slowly that it can be parametrized by estimating the free energy change associated with the disk's overlap. The resulting overlap approximation behaves qualitatively like *ad hoc* effective potentials used in dissipative particle dynamics (DPD) simulations [1]. We also show that $\mathcal{W}(\mathcal{R})$ vanishes when the molecular units to be coarse–grained are *non–bonded* [2]. This sheds some doubts on the widely used procedure of coarse–graining water molecules in DPD simulations.

1) S. H. L. Klapp, D. J. Diestler, and M. Schoen, J. Phys.: Condens. Matter **16**, 7331 (2004). 2) H. Bock, K. E. Gubbins, and S. H. L. Klapp, in preparation.