CPP 8 SYMPOSIUM Nonequilibrium Phenomena in Soft-Condensed Matter

Time: Tuesday 14:00–16:45 Room: ZEU Lich

CPP 8.1 Tue 14:00 ZEU Lich

Optimal control of self-organized dynamics in cellular signaling — •Dirk Lebiedz — IWR, Im Neuenheimer Feld 368, 69120 Heidelberg

Recently, increasing experimental evidence has become available supporting the significance of self-organization and pattern formation for information processing in cellular signal transduction. The underlying complex mechanisms can only be understood by help of detailed mathematical modeling and simulation. In that context, model based control studies of self-organized dynamics are promising for two major reasons. First, to study potential dynamic regulatory mechanisms, and second, to explore possibilities for specific manipulation of biochemical system dynamics by external stimuli and targeted modifications realized for example by tailored drug application. Optimal control allows the general formulation of inverse problems with time-varying input parameters as well as specific control aims in the form of objective functionals to be minimized. We present applications of advanced numerical optimization to ordinary and partial differential equation models for cellular signal transduction systems and demonstrate how optimal control can be exploited for studying both inherent regulatory mechanisms and specific external manipulations. [1] D. Lebiedz, U. Brandt-Pollmann, Manipulation of self aggregation patterns and waves in a reaction-diffusion-system by optimal boundary control strategies, Phys. Rev. Lett. 91, 208301 (2003) [2] D. Lebiedz, S. Sager, H.G. Bock, P. Lebiedz. Annihilation of limit-cycle oscillations by identification of critical perturbing stimuli via mixed-integer optimal control, Phys. Rev. Lett., 95, 108303 (2005)

CPP 8.2 Tue 14:15 ZEU Lich

Numerical study of electrostatic colloidal interaction at interface — •Pavel Dyshlovenko[1] and Piotr Warszyński[2] — [1]Ulyanovsk State Technical University, 32 Severny Venets Street, Ulyanovsk 432027, Russia — [2]Institute of Catalysis and Surface Chemistry, ul. Niezapominajek 8, 30-239 Kraków, Poland

Electrostatic interaction of a pair of colloidal particles immersed in electrolyte in the vicinity of a charged plane is studied numerically within the framework of the non-linear Poisson-Boltzmann equation in two dimensions. Particular attention is given to the many-particle effects and non-linearity. The question under consideration is related to the important practical problem of colloidal adsorption/deposition. The relevant details of numerical procedure are briefly discussed. The results of the numerical experiments indicate that the inter-particle interaction near a charged plane differs appreciably from the interaction of free particles. For the problem considered, the repulsion of two like-charged particles weakens for large values of plane's charge, both positive and negative. In contrast, the repulsion exceeds the one of free particles when the wall is charged moderately.

CPP 8.3 Tue 14:30 ZEU Lich

Capillary Rise of Liquids in Mesoporous Silica — •Patrick Huber[1], Klaus Knorr[1], and Andriy Kityk[2] — [1]Technische Physik, Universität des Saarlandes, D-66041 Saarbrücken — [2]Institute for Computer Science, Technical University of Czestochowa, PL-42200 Czestochowa

In order to study liquid flow in restricted geometries we have investigated the capillary rise (spontaneous imbibition) of water and n-alkanes in mesoporous Vycor glass (mean pore diameter 10 nanometer). An analysis of the mass uptake of the porous monoliths versus time, $m(t)$, allows us to determine a characteristic speed of the imbibition process, v_{imb}, which gives access to the ratio of surface tension σ and viscosity η of the confined liquids: $v_{imb} \sim \sigma/\eta$. For imbibing water as well as for the n-alkanes investigated (C_8H_{18}-$C_{30}H_{62}$) we find a $\sqrt{t}$-*Lucas-Washburn* type behavior for both the mass uptake and the position of the advancing liquid front. The relative imbibition speeds of the different *nanoconfined* liquids scale as expected from the ratio of the *bulk* fluid parameters. The width of the advancing two-phase boundary as a function of time is extracted from light scattering data sets recorded during imbibition. It is discussed with regard to state-of-the art theories of kinetic roughening of such boundaries in disordered media.

[1] M. Alava, M. Dubee, M. Rost, *Imbibition in disordered media*, Adv. Phys. **53**, 83 (2004).

CPP 8.4 Tue 14:45 ZEU Lich

Phase-field description for the budding of two-component vesicles — •Roger Folch and Uwe Thiele — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany

We present a diffuse-interface or phase-field model[1] for the *dynamics* of the budding process of a vesicle induced by phase separation on its membrane. Possible two-dimensional budding mechanisms are explored in addition to known three-dimensional scenarios [2]. The model extends previous developments to simulate two-fluid flow[3] and the dynamics of a vesicle under flow[4] to include the internal dynamics of the membrane (phase-separation) and thus account for its non-static mechanical properties.

[1] R. González-Cinca, R. Folch, R. Benítez, L. Ramírez-Piscina, J. Casademunt and A. Hernández-Machado (cond-mat/0305058), in *Advances in Condensed Matter and Statistical Mechanics*, pp. 203–236, ed. by E. Korutcheva and R. Cuerno, Nova Science Publishers (New York, 2004).
[2] R. Lipowsky and R. Dimova, J. Phys. Condens. Matt. **15**, 31 (2003).
[3] R. Folch, J. Casademunt, A. Hernández-Machado and L. Ramírez-Piscina, Phys. Rev. E **60**, 1724; *ibid.* 1734 (1999).
[4] J. Beacourt, F. Rioual, T. Séon, T. Biben and C. Misbah, Phys. Rev. E **69**, 011906 (2004).

CPP 8.5 Tue 15:00 ZEU Lich

Suppression of demixing in a small gap between parallel plates: From Cahn-Hilliard to model H — •Santiago Madruga and Uwe Thiele — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany

We analyse the spinodal decomposition of a mixture in the gap between parallel plates [1]. Linear results obtained with the full transport equations for (a) solely diffusive transport described by the Cahn-Hilliard equation and (b) diffusive and convective transport described by model H consisting of coupled Navier-Stokes and Cahn-Hilliard equations [2] are compared to an effective thin film description.

Detailed results are given for the dependence of the critical gap width (below which decomposition is suppressed) on the physico-chemical properties of the bounding plates. Criteria for the validity of the thin film description are given.

[1] R. Kenzler *et al.*, Comp. Phys. Comm. **133**, 139–157 (2001).
[2] D. M. Anderson, G. B. McFadden, and A. A. Wheeler, Ann. Rev. Fluid Mech. **30**, 139–165 (1998).

CPP 8.6 Tue 15:15 ZEU Lich

The depinning transition of a driven droplet on a heterogeneous substrate — •Uwe Thiele[1] and Edgar Knobloch[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany — [2]Department of Physics, University of California, Berkeley CA 94720, USA

On non-ideal real substrates used in experiments the onset of droplet motion under driving along the substrate is strongly influenced by chemical or physical defects. A finite driving force is necessary to overcome the pinning influence of the heterogeneities occurring on a micro- or mesoscale. This is thought to be responsible, for instance, for the observed hysteresis between advancing and receding contact angles.

In the present paper we aim at understanding not only the processes that lead to pinning, but also the bifurcation that leads to depinning and the subsequent behavior of a moving droplet. We study driven droplets on a heterogeneous inclined plate using a long-wave evolution equation for the film thickness profile in two cases: (a) a periodic sinusoidal modulation of the disjoining pressure, and (b) strongly localized hydrophilic or hydrophobic 'defects'. As a result the drop may be pinned at the rear by an enhanced wetting region, or at its front by a region of reduced wettability. The results are obtained by a combination of branch following methods, linear stability theory and direct numerical simulation of the model equation.

— 15 min. break —

CPP 8.7 Tue 15:45 ZEU Lich

Transport coefficients of polymer solutions and blends near a glass and a liquid-liquid phase transition — •Werner Köhler, Albert Voit, Jürgen Rauch, and Alexei Krekhov — Physikalisches Institut, Universität Bayreuth

Transport coefficients in polymer solutions and blends can usually be written in terms of a thermodynamic (osmotic modulus) and a kinetic (friction) factor. We discuss self diffusion, collective diffusion, and thermal diffusion of dilute to concentrated polymer solutions and polymer blends in the vicinity of a glass and a liquid-liquid phase transition. The dramatic increase of local friction near T_g is accompanied by a slowing down of mass diffusion, whereas the Soret coefficient, which is a measure for the susceptibility to external temperature fields, remains unaffected by the glass transition. In sharp contrast is its divergence near a critical point which is caused by the critical slowing down of collective diffusion and an almost constant thermal diffusion coefficient. We show how this diverging susceptibility can be utilized for patterning of critical polymer blends both in the one and in the two phase regime.

[1] A. Voit, A. Krekhov, W. Enge, L. Kramer, W. Köhler. Phys. Rev. Lett. 92 (2005) 214501
[2] J. Rauch, W. Köhler. J. Chem. Phys. 119 (2003) 119777

CPP 8.8 Tue 16:00 ZEU Lich

Nonequilibrium subdiffusion of a Brownian particle in a quasicrystalline potential — •Michael Schmiedeberg and Holger Stark — Universität Konstanz, Fachbereich Physik, D-78457 Konstanz

We study the motion of a single colloidal particle in an optical lattice with two-dimensional quasicrystalline symmetry. From Brownian-dynamics simulations we find that initially the particle exhibits subdiffusional motion over several decades in time until it crosses over to pure diffusion in the long-time limit. We demonstrate that the subdiffusion is due to a temporally extended relaxation process towards thermal equilibrium where the particle then enters the diffusive regime. The duration of the transient subdiffusion increases for decreasing temperature. We observe a similar behavior for the motion of particles in random potentials which demonstrates that quasicrystalline systems are useful for studying aspects of disordered systems.

CPP 8.9 Tue 16:15 ZEU Lich

Unfolding of a globular polymer in shear flow — •Alfredo Alexander-Katz and Roland R. Netz — Physik Department, Tech. Univ. Muenchen, James-Frank Str., D-85748, Garching, Deutschland

In the process of clotting in small vessels, platelets form a plug in an injured zone only in the presence of a protein known as the von Willebrand Factor (vWF). The absence or malfunction of the vWF leads to a bleeding disorder, the so-called von Willebrand disease. It is believed that the protein is globular when released into the blood flow. In this talk, we present a study of a simple model of vWF in shear flow. Using hydrodynamic simulations, we show that a globular polymer undergoes globule-stretch transitions above a critical shear rate. Finally, we discuss the scaling of the critical shear rate with the length of the polymer, and compare it to the physiological values attainable in the body.

CPP 8.10 Tue 16:30 ZEU Lich

A Fluctuation Theorem for Wet Granular Matter — •Axel Fingerle and Stephan Herminghaus — MPI for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen, Germany

Alhough there are various formulations of fluctuation theorems extending the second law of thermodynamics, the time inversion symmetry of the equations of motion is the key principle in every derivation. Wet granular matter has been described successfully by the Minimal Capillary Model [S. Herminghaus, *Adv. Phys.*, **54**, 221 (2005)]. This dynamical system has a non-trivial time inversion map due to the hysteretic interaction by liquid bridges between grains. We present numerical results and give simple analytic arguments to determine why the exponential suppression of 'violations' of the second law remains valid even for a time inversion map that is non-local in time.