Symposium Computational Soft matter physics (SYMP)

jointly organized by
Chemical and Polymer Physics Division (CPP),
Dynamics and Statistical Physics Division (DY), and
Biological Physics Division (BP)

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Overview of Invited Talks and Sessions

(lecture room H 0105)

Invited Talks

SYMP 1.1	Thu	9:30–10:00	H 0105	**Hydrodynamic cooperativity in active fluids** — •Ignacio Pagonabarraga
SYMP 1.2	Thu	10:00–10:30	H 0105	**Hydrodynamic Effects on Molecular Motion** — •Raymond Kapral
SYMP 1.5	Thu	11:15–11:45	H 0105	**Proton transport through water-filled narrow pores** — •Christoph Dellago
SYMP 1.6	Thu	11:45–12:15	H 0105	**Role of fluctuations in the selectivity mechanism for the KcsA potassium channel** — •Michael E. Paulaitis, Dilip Asthagiri, Lawrence R. Pratt
SYMP 2.1	Thu	14:00–14:30	H 0105	**DNA mechanics and dynamics** — •Richard Lavery
SYMP 2.2	Thu	14:30–15:00	H 0105	**Charge mobility of discotic mesophases of polyaromatic hydrocarbons: a multiscale quantum/classical study** — •Denis Andrienko
SYMP 2.4	Thu	15:30–16:00	H 0105	**Simulation of coarse-grained membrane models** — •Marcus Müller
SYMP 2.5	Thu	16:00–16:30	H 0105	**Fragments of a computational cell: mesoscopic simulations of soft matter** — •Julian C. Shillcock

Sessions

SYMP 1.1–1.7	Thu	9:30–12:30	H 0105	**Computational soft matter physics**
SYMP 2.1–2.7	Thu	14:00–17:00	H 0105	**Computational soft matter physics**

SYMP 1: Computational soft matter physics

Time: Thursday 9:30–12:30 Location: H 0105

Invited Talk SYMP 1.1 Thu 9:30 H 0105

Hydrodynamic cooperativity in active fluids — •Ignacio Pagonabarraga — Departament de Física Fonamental, Facultat de Física, Martí i Franquès 1, E-08028 Barcelona, Spain

The dynamics of complex fluids leads to a rich variety of structures which emerge out of the interactions between suspended particles, as well as out of the dissipative interactions mediated by the solvent in which they are suspended. The understanding of such non-equilibrium structures requires a proper treatment of the hydrodynamic coupling at a mesoscopic level, in which suspended particles can be resolved in detail. At the same time, the solvent must be coarse grained because a fully atomistic description, in which the solvent molecules are resolved cannot reach the relevant time and length scales in which these materials evolve. I will analyze how such approaches can be developed, and will concentrate in systems which develop structures under non-equilibrium conditions. These can be achieved through external driving of the system or through internal drivings. The latter include relaxation from initial metastable states, as is the case of phase separating mixtures, or the steady states reached by the motion of active particles. I will discuss the analogies between these different situations and will analyze the properties of systems composed by active self-propellig suspended particles. These systems are intrinsically out of equilibrium and therefore display peculiar properties. I will consider the morphologies and structures they can develop at long times and the role of hydrodynamics in these systems.

Invited Talk SYMP 1.2 Thu 10:00 H 0105

Hydrodynamic Effects on Molecular Motion — •Raymond Kapral — Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Toronto, ON M5S 3H6, Canada

Modelling the dynamics of complex systems is a challenging task for computer simulation since physically relevant distance and time scales are often very long. This fact has stimulated the development of a variety of different coarse-grain molecular dynamics methods that attempt to bridge gap between short and long scales. In this talk I will discuss multiparticle collision (MPC) dynamics. MPC dynamics introduces a simple coarse grain model for collisions that retains the most important features of full molecular dynamics, namely, it conserves mass, momentum and energy, and preserves phase space volumes. Because of its simplicity, the statistical mechanics of systems with such dynamics can be analyzed in detail, the macroscopic laws can be derived and transport properties can be computed easily. MPC dynamics can be combined with molecular dynamics to study polymer, biomolecular and colloidal systems, as well as a variety of other systems, including chemically reacting systems. Since momentum is conserved, the dynamics automatically accounts for hydrodynamic interactions among the solute molecules dissolved in the MPC solvent. The following topics will be discussed using hybrid MD-MPC dynamics that combines MD of the solute molecules, interacting with the solvent molecules through intermolecular forces, with MPC dynamics for the solvent molecules: analysis of the hydrodynamic interactions between a pair of nanoparticles; hydrodynamic effects on polymer collapse; and hydrodynamic interactions in the hinge motions of proteins induced by ligand binding and product release.

SYMP 1.3 Thu 10:30 H 0105

Statistical Mechanics of the Fluctuating Lattice Boltzmann Equation — •Burkhard Duenweg[1], Ulf D. Schiller[1], and Anthony J. C. Ladd[1,2] — [1]Max-Planck-Institut fuer Polymerforschung Mainz — [2]Chemical Engineering, University of Florida, Gainesville, USA

The statistics of the occupation variables of a stochastic lattice Boltzmann simulation is analyzed in terms of a generalized lattice gas. We show that the most probable state of this model corresponds to the equilibrium distribution of the lattice Boltzmann equation. Stochastic collision rules are described in terms of a Monte Carlo process satisfying detailed balance. This allows a straightforward derivation of the discrete Langevin equation for the fluctuating modes. Detailed balance requires to thermalize all non-conserved modes. A Chapman–Enskog analysis shows that the approach is fully consistent with macroscopic fluctuating hydrodynamics.

SYMP 1.4 Thu 10:45 H 0105

Scale bridging by hybrid simulations in microfluidics — •Martin Hecht and Jens Harting — Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany

We have developed a hybrid molecular dynamics and stochastic rotation dynamics simulation method to simulate fluid flow close to walls for appplications in microfluidics. Moreover, this approach can be applied to various problems in soft condensed matter physics. Many important applications in this field deal with suspensions, membranes, macromolecules, or reacting fluids. However, the time and length scales in these mesoscopic systems are much above those which are accessible with conventional molecular dynamics simulations. Several mesoscopic simulation methods (lattice Boltzmann, stochastic rotation dynamics, dissipative particle dynamics) have been developed, which can deal with larger system sizes and larger simulation times. The prize one has to pay, to reduce the computational cost, is a simplification of the underlying processes on the molecular scale. For some applications, the details on the molecular length scale are essential in some regions of the system, whereas in other regions the resolution may be reduced. In this case, hybrid simulation techniques, which use different simulation methods for different regions of the system, are a possibility to minimize the computational costs of simulations under the constraint that in some regions the full physics has to be taken into account. In this talk we present our approach and first simulation results and discuss the key points of hybrid simulation approaches in general.

15 min. break

Invited Talk SYMP 1.5 Thu 11:15 H 0105

Proton transport through water-filled narrow pores — •Christoph Dellago — Institute for Experimental Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria

One-dimensional chains of hydrogen bonded water molecules provide excellent conductors for protonic currents through pores across membranes, a process which is fundamental to many biological systems and technological applications. In this talk, I will report on the results of computer simulations of proton transfer along water chains inside the cavity of narrow carbon nanotubes. Free energy and rate constant calculations show that protons move across the membrane diffusively along single-file chains of hydrogen-bonded water molecules. Proton passage through the membrane is opposed by a high barrier in the effective potential, reflecting the large electrostatic penalty for desolvation and reminiscent of charge exclusion in biological water channels. Inside the pore, the proton mobility along the water chain exceeds that in bulk water by a factor of 40, but is reduced if orientational defects are present. Excess protons interact with such hydrogen-bonding defects through long-range electrostatics, resulting in coupled motion of protons and defects. The effective proton-defect interaction as well as the defect-defect interactions can be understood in terms of one-dimensional lattice model, in which water molecules located at regularly spaced lattice sites interact via dipole-dipole interactions. Using canonical and grand canonical Monte Carlo simulations of this simplified model, we have studied the filling behavior of long pores and find that the water chains remain ordered up to nearly macroscopic lengths, carrying implications for long-range proton transfer and the collective behavior of water molecules in carbon nanotube bundles.

Invited Talk SYMP 1.6 Thu 11:45 H 0105

Role of fluctuations in the selectivity mechanism for the KcsA potassium channel — •Michael E. Paulaitis[1], Dilip Asthagiri[2], and Lawrence R. Pratt[3] — [1]Department of Chemical and Biomolecular Engineering, Ohio State University — [2]Department of Chemical and Biomolecular Engineering, Johns Hopkins University — [3]Department of Chemical and Biomolecular Engineering, Tulane University

The KcsA potassium channel belongs to a class of channels that is selective for K^+ over Na^+ at rates of K^+ transport approaching the diffusion limit. Selectivity is explained thermodynamically in terms of the favorable partitioning of K^+ relative to Na^+ in a narrow selectivity filter in the channel. One mechanism for this selectivity invokes the size difference between K^+ and Na^+, and the molecular complementarity of the selectivity filter with the larger K^+ ion. An alternative view holds that size-based selectivity is precluded because the conformational fluctuations of the selectivity filter are greater than the size difference between these two ions. A quasi-chemical theory implemented on the basis of molecular simulation is derived to examine these hypotheses by calculating the distribution of binding energies for Na^+ and K^+ in a model of the selectivity filter of the KcsA channel. We find that Na^+ binds strongly to the selectivity filter with a mean binding energy substantially more favorable than that for K^+. The difference is comparable to the difference in hydration free energies of Na^+ and K^+ in bulk aqueous solution. Thus, the average filter binding energies do not discriminate Na^+ from K^+ when measured from the baseline of the difference in bulk hydration free energies. Strong binding of the smaller Na^+ also constricts the selectivity filter, consistent with a negative partial molar volume of Na^+ in water in contrast to a positive partial molar volume of K^+ in water. Discrimination in favor of K^+ can be attributed to the scarcity of favorable binding configurations for Na^+ relative to K^+. That relative scarcity is quantified as enhanced binding energy fluctuations, which reflect both the energetically stronger binding of Na^+ and the constriction of the filter induced by Na^+ binding.

SYMP 1.7 Thu 12:15 H 0105

Escape transition of grafted polymer chains from a cylindrical tube — •Hsiao-Ping Hsu[1], Kurt Binder[1], Leonid I. Klushin[2], and Alexander M. Skvortsov[3] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]American University of Beirut, Department of Physics, Beirut, Lebanon — [3]Chemical-Pharmaceutical Academy, St. Petersburg, Russia.

A grafted polymer chain confined in a finite cylindrical tube of length L and diameter D undergoes an abrupt transition when the number of monomers in the chain, N, reaches a critical value. This problem has the merit that it is potentially very relevant for experiments and application such as the problem of polymer translocation through pores in membranes. In order to check the theoretical prediction based on the Landau free energy approach, we study $3d$ single polymer chains with one end grafted at the inner wall of a cylindrical tube, by simulating self-avoiding walks on a simple cubic lattice with finite cylindrical confinement. A biased sequential sampling algorithm with re-sampling, similar to the pruned-enriched Rosenbluth method (PERM) is used. The difficulty of obtaining correct samplings for the first-order phase transition is solved by pulling the free chain end with different strength of force out from the tube, and reweighting the biased configuration. We estimate the free energy, the end-to-end distance, the number of imprisoned monomers, the order parameter, and its distribution. It is shown that in the thermodynamic limit, there is a very pronounced jump in several average characteristics. All simulation results are in good agreement with the analytical theory.

SYMP 2: Computational soft matter physics

Time: Thursday 14:00–17:00 Location: H 0105

Invited Talk SYMP 2.1 Thu 14:00 H 0105

DNA mechanics and dynamics — •Richard Lavery — Institut de Biologie et Chimie des Protéines, CNRS UMR 5086 / Université de Lyon, France

The DNA double helix is easily deformable, both on a local level, in response to changes in base sequence or to interactions with other species, and on a global level, in response to external constraints such as supercoiling or stretching. We are using molecular mechanics and dynamics to study these properties of DNA and to relate them to the biological behavior of this vital biomacromolecule. Our studies have enabled us both to examine the extreme deformations of the double helix which can be induced during single molecule experiments and the more subtle deformations which are vital in protein-DNA recognition processes. We are also investigating how different base sequences influence DNA dynamics and can impact on processes such as energy transfer.

S.B. Dixit *et al.*, Biophys. J. **89**, 3721 (2005).
E. Emanuele *et al.*, J. Phys. Chem. **109**, 16109 (2005).
R.A. O'Flanagan *et al.*, Bioinformatics **21**, 2254 (2005).
T. Lionnet *et al.*, Phys. Rev. Lett. **96**, 178102 (2006).
F. Lankas *et al.*, Structure **14**, 1527 (2006).

Invited Talk SYMP 2.2 Thu 14:30 H 0105

Charge mobility of discotic mesophases of polyaromatic hydrocarbons: a multiscale quantum/classical study — •Denis Andrienko — MPI for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Discotic liquid crystals form columnar phases, where the molecules stack on top of each other and the columns arrange in a regular lattice. The self-organization into stacks results in the one-dimensional charge transport along the columns. Combining atomistic molecular dynamic simulations, Kinetic Monte Carlo, and Marcus-Hush approaches we study the effect of the side chain substitution on the transition temperatures as well as molecular ordering in the mesophases. Our study rationalizes the differences in charge carrier mobilities in the herringbone and hexagonal mesophases which is predominantly due to the change of the overlap integral between the neighboring molecules. We are able to reproduce the trends and magnitudes of charge mobilities as measured by pulse-radiolysis time-resolved microwave conductivity technique. The proposed multiscale approach can readily be generalized to study conductive properties of conjugated polymers and disordered molecular crystals.

SYMP 2.3 Thu 15:00 H 0105

Viscoelasticity and primitive path analysis of entangled polymer liquids: From f-actin to polyethylene — Nariya Uchida[1], Gary S. Grest[2], and •Ralf Everaers[3] — [1]Department of Physics, Tohoku University, Sendai 980-8578, Japan — [2]Sandia National Laboratories, Albuquerque, NM 87185, USA — [3]Université de Lyon, Laboratoire de Physique, École Normale Supérieure de Lyon, CNRS UMR 5672, 46 allée d'Italie, 69364 Lyon Cedex 07, France

We combine computer simulations and scaling arguments to develop a unified view of polymer entanglement based on the *primitive path analysis* (PPA) of the microscopic topological state. Our results agree with experimentally measured plateau moduli for three different polymer classes over a wide range of reduced polymer densities: (i) semidilute theta solutions of synthetic polymers, (ii) the corresponding dense melts above the glass transition or crystallization temperature, and (iii) solutions of semi-flexible (bio)polymers such as f-actin or suspensions of rodlike viruses. Together these systems cover the entire range from loosely to tightly entangled polymers. In particular, we argue that the primitive path analysis renormalizes a loosely to a tightly entangled system and provide a new explanation of the successful Lin-Noolandi packing conjecture for polymer melts.

R. Everaers *et al.*, *Science 303*, 823-826 (2004)
N. Uchida, G.S. Grest and R. Everaers, *J. Chem. Phys.*, in press.

15 min. break

Invited Talk SYMP 2.4 Thu 15:30 H 0105

Simulation of coarse-grained membrane models — •Marcus Müller — Institut für Theoretische Physik, Georg-August Universität, Göttingen

Collective processes in membranes – like pore formation in membranes under tension or fusion of two apposed bilayers – exhibit a large degree of universality, i.e., similar phenomena are observed in systems that significantly differ in their microscopic interactions. Since these phenomena involve length scales of micrometers and time scales of milliseconds, they are difficult to study by atomistic simulations, but minimal coarse-grained models can provide detailed and direct insights into the molecular mechanisms.

An advantage of coarse-grained models is the calculation of free energies of self-assembled structures. This can be accomplished either by mapping the model onto molecular field theories and using the mean field approximation or by special simulation techniques. In the latter case, applying an external, ordering field, one imposes a pre-defined structure onto the fluid in the disordered phase (e.g., at high temperature). This structure closely resembles the self-assembled structure (at low temperature, in the absence of an ordering field). Subsequently, one gradually switches off the external, ordering field and, in turn, increases the control parameter (temperature) that drives the self-assembly. The free energy difference along this reversible path is obtained via thermodynamic integration or expanded ensemble simulation techniques.

Invited Talk SYMP 2.5 Thu 16:00 H 0105

Fragments of a computational cell: mesoscopic simulations of soft matter

— •Julian C. Shillcock — MEMPHYS - Center for Biomembrane Physics, University of Southern Denmark, Odense, Denmark

As computer power increases, it becomes possible to build complex and realistic computational models of cellular processes. Vesicle fusion has recently been intensively studied using a variety of simulation techniques ranging from atomistic Molecular Dynamics to self-consistent field theory. Whereas continuum models of the fusion pathway assume that the membranes pass through known shapes and transitions, simulations allow the membranes to adopt whatever shapes and structures minimise their free energy. Quite distinct techniques, such as Monte Carlo and Molecular Dynamics simulations, have revealed common features in the fusion process, giving confidence that the observed molecular rearrangements are not simply artifacts of the models. Having established that vesicle fusion can be observed in simulations, the next stage is to extend the models to capture more features of biological systems. Computational membrane models are now sophisticated enough to allow the "sculpting"of membranes into crypts or microvilli, to study the diffusion and reactions of particles diffusing within these confined volumes, and to follow the translocation of rigid nanoparticles across a membrane. In the latter process, which may be important for investigating the toxicity of nanomaterials, the shape and interactions of the nanoparticles determine the efficiency of the translocation process. We present results showing that computational models of membranes are not only structurally similar to biological membranes, but can also be used to study dynamic processes such as fusion, endocytosis, invagination, and the interactions of synthetic nanoparticles with membranes.

SYMP 2.6 Thu 16:30 H 0105

Non-cubic bicontinuous space partitions: transformation pathways between cubic lyotropic phases and possible equilibrium structures

— •Gerd E Schröder-Turk — Inst. für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen

Triply-periodic minimal surface families that contain the cubic Gyroid (G), Diamond (D) and Primitive (P) surfaces are studied in terms of their global packing and local curvature properties. These properties are central to understanding the formation of mesophases in amphiphile molecular systems. The surfaces investigated are the tetragonal, rhombohedral and hexagonal tD, tP, tG, rG, rPD and H surfaces. These non-cubic surfaces furnish topology-preserving transformation pathways between these cubic surfaces. We introduce 'packing homogeneity', defined as the standard deviation Δd of the distribution of the channel diameter throughout the labyrinth; the channel diameter d is determined from the medial surface skeleton centered within the domains. Curvature homogeneity is defined similarly as the standard deviation ΔK of the distribution of Gaussian curvature. We demonstrate that the cubic G and D surfaces are the most homogeneous members of these families. We show that the tetragonal pathway between the cubic phases to be more homogeneous than the rhombohedral one, relevant to pressure-induced phase transitions between these phases. We discuss the possibility of bicontinuous hexagonal equilibrium phases.

SYMP 2.7 Thu 16:45 H 0105

Reproducibility of single particle-dynamics. The Hori-type generalized Langevin equation

— •Jörg R. Silbermann[1], Sabine H. L. Klapp[1,2], and Martin Schoen[1] — [1]Stranski-Lab für Physikalische und Theoretische Chemie, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin — [2]Institut für Theoretische Physik, Technische Universität Berlin, Strasse des 17. Juni 124, 10623 Berlin

We consider the dynamics of a single tagged particle of mass M in a 2D Lennard-Jones (LJ) system. Employing the Mori-Zwanzig projector operator formalism, one can derive [1] an effective equation of motion of the form of a generalized Langevin equation (GLE). The "random force" $F_0^r(t)$ appearing in the GLE is in general unknown. For a harmonic solid, however, one can derive a GLE where $F_0^r(t)$ coincides with the total force $F_0^*(t)$ acting on the tagged particle in a "reference system", where the mass is changed from M to an arbitrary mass m^*. We study to what extent this GLE is still able to capture the dynamics of the tagged particle under conditions where the harmonic approximation is no longer justified. To this end we compute typical time-autocorrelation functions for the tagged particle in molecular dynamics simulations for the full LJ system and compared those with the ones from the GLE. We find excellent agreement at low temperatures and a surprisingly good reproduction of the dynamics even in the high-temperature liquid phase.

[1] K. Wada, J. Hori, Prog. Theor. Phys. **49**, 129, (1973).