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 PAGO-NABARRAGA — 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.