

CPP 11: Modelling and Simulation of Soft Matter

Time: Monday 15:00–18:15

Location: ZEU 255

CPP 11.1 Mon 15:00 ZEU 255

Scalable and fast concurrent multiscale molecular simulation with predictive parallelization schemes — ●HORACIO VARGAS GUZMAN¹, CHRISTOPH JUNGHANS², KURT KREMER¹, and TORSTEN STUEHN¹ — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — ²Computer, Computational, and Statistical Sciences Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Concurrent multiscale simulation enables the study of molecular systems with different resolutions in specific subdomains of a simulation box. Modeling soft-matter and biological systems in the context of multiscale simulations are challenging research avenues which drive the permanent development of new simulation methods and algorithms. In computational terms, those methods require parallelization schemes that make productive use of computational resources for each simulation and from its genesis. Here, we introduce the dual resolution domain decomposition algorithm that is a combination of a resolution sensitive spatial domain decomposition with an initial sliding subdomain-walls procedure. The algorithm modeling is presented for dual resolution systems in terms of scaling properties as a function of the size of the low-resolution region and the high to low resolutions ratio. The algorithm competences are validated within adaptive resolution simulations, by comparing its scalability and speedup to a spatial domain decomposition. Two representative adaptive resolution simulations have been employed in this work, namely, a biomolecule solvated in water and water in an ideal gas reservoir.

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Controlling the Distance of Core-Shell Nanostructures via Star Polymers — ●QIYUN TANG¹, CHRISTIAN ROSSNER², MARCUS MÜLLER¹, PHILIPP VANA², and OTTO GLATTER³ — ¹Institute für Theoretische Physik, Georg-August-Universität, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — ²Institute für Physikalische Chemie, Georg-August-Universität, Tammannstrasse 6, D-37077 Göttingen, Germany — ³Institute für Anorganische Chemie, Technische Universität Graz, Stremayrgasse 9/V, A-8010 Graz, Austria

Recent experiments have demonstrated that the star polymers can be used to precisely control the distance of core-shell nanostructures, which are formed by a single, large and multiple, small gold nanoparticles. Here we use a Monte Carlo simulation based on a coarse-grained bead-spring model to systematically study the distance scaling behaviour of this core-shell nanostructure. Our results show that these distances are mainly controlled by the position of free arm ends of star polymers, and the simulation results are in good agreement with the small-angle X-ray scattering (SAXS) results of core-shell nanostructures dispersed in solution. Interestingly, we found that the scaling of core shell distances for 2-arm, 3-arm, and 6-arm star polymers approaches one master curve as a function of the arm length of star polymers. We also found that increasing the arm number of star polymers could increase the density of free arm end groups, and therefore grab more small gold nanoparticles. Our results show the feasibility to precisely control the core-shell structures at the nanoscale.

CPP 11.3 Mon 15:30 ZEU 255

Formation of multicore structures in single dendritic-linear copolymers — ●MARTIN WENGENMAYR^{1,2}, RON DOCKHORN^{1,2}, and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Germany — ²Technische Universität Dresden, Germany

Dendritic polymers gain attention for promising applications in drug delivery purposes or as catalysts. Usually the dendritic part will be rather hydrophobic and has the tendency to collapse in aqueous environment. Hydrophilic chains attached to the terminal groups form a corona being reminiscent to a polymer micelle. We investigate the conformational and thermodynamic properties of these molecules by analytical models and computer simulations. A mean-field model applying the Daoud-Cotton approach and a surface tension argument is presented and suggests the splitting of the unimolecular single-core structure into a multicore structure with increasing dendrimers generation and decreasing solvent selectivity. Monte Carlo simulations utilizing the bond fluctuation model with explicit solvent are performed which show the formation of multicore structures for trifunctional codendrimers. These findings are aimed to understand the physics

of spontaneous self-assembly of co-dendrimers in various well-defined macro-conformations under change of environmental conditions.

CPP 11.4 Mon 15:45 ZEU 255

Controlled Fabrication of Nanoparticles through Rapid Solvent Exchange — ●TATIANA MOROZOVA and ARASH NIKOUBASHMAN — JGU, Mainz, Germany

Polymeric nanoparticles are widely sought after for scientific and technological applications, but large-scale fabrication techniques are still at an early development stage. Recently, a new technology to form monodisperse polymer nanoparticles through rapid micromixing of polymers in solution (tetrahydrofuran, THF) with a nonsolvent (water) was developed. The general applicability of this technique for the large scale fabrication of monophasic and biphasic Janus nanoparticles has been demonstrated recently [1,2], but the underlying self-assembly mechanisms are still largely unknown. To elucidate this behavior, we performed united atom molecular dynamic (MD) simulations of a single polystyrene (PS) chain in THF-water mixtures with variable mixing ratios. Depending on the mole fraction of water, the mixture is either a good or a bad solvent for PS and the polymer coil collapses into a globule. We developed appropriated force fields for these complex systems and analyzed systematically the polymer radius of gyration depending on solvent quality. These detailed simulations will allow us to develop a physically informed coarse grained model, which can be used to perform simulations with multiple chains.

[1] A. Nikoubashman, V.E. Lee, C. Sosa, R.K. Prud'homme, R.D. Priestley and A.Z. Panagiotopoulos, ACS Nano 10, 1425 (2016)

[2] C. Sosa, R. Liu, C. Tang, F. Qu, S. Niu, M.Z. Bazant, R.K. Prud'homme, R.D. Priestley, Macromolecules 49, 3580 (2016)

CPP 11.5 Mon 16:00 ZEU 255

Polymer bottlebrushes in solution: A combined theory and simulation study — JAROSLAW PATUREJ, ●TORSTEN KREER, and JENS-UWE SOMMER — Leibniz-Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden

We present a theoretical model for polymer bottlebrushes in solutions, where the branched chain is considered as a sequence of cylindrical blobs. Our approach delivers a consistent description of backbone and side-chain scaling under variation of concentration, providing power-laws in different concentration regimes. Upon increasing concentration, we envision a hierarchical screening: First, there is screening by the cylindrical blobs of different chains. Further increase of the concentration leads to screening inside the overlapping cylinders and, finally, amongst the side chains of different brushes. Our analytical predictions are tested via molecular dynamics simulations, which reveal very good agreement with the theory.

CPP 11.6 Mon 16:15 ZEU 255

Depleted depletion drives polymer swelling in poor solvent mixtures — ●DEBASHISH MUKHERJI¹, CARLOS MARQUES², TORSTEN STUEHN¹, and KURT KREMER¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Institut Charles Sadron, CNRS, Strasbourg, France

Macromolecular solubility in solvent mixtures often strike as paradoxical phenomena [1]. In a system where all particle interactions are repulsive, chains can nevertheless collapse, due to increased repulsive monomer-solvent interactions that lead to an effective attraction between monomer units also known as depletion induced attraction. While it is well understood why a polymer can collapse in a purely repulsive solvent, polymer swelling at intermediate mixing ratios of two repulsive solvents still lacks a microscopic explanation. Here, for binary solvent mixtures, we combine computer simulations and theoretical arguments to unveil the microscopic, generic origin of this collapse-swelling-collapse scenario. We show that this phenomenon naturally emerges at constant pressure in mixtures of purely repulsive components when a delicate balance of the entropically driven depletion interactions is achieved [2]. [1] D. Mukherji, C. M. Marques, and K. Kremer, Nature Communications 5, 4882 (2014). [2] D. Mukherji, C. M. Marques, T. Stuehn, and K. Kremer, arXiv:1609.09839 (2016).

15 min break

CPP 11.7 Mon 16:45 ZEU 255

The stretching behaviour of a single tethered polymer in pressure-driven flow — •KAI SZUTTOR¹, TAMAL ROY², STEFFEN HARDT², CHRISTIAN HOLM¹, and JENS SMIATEK¹ — ¹Institute for Computational Physics, Stuttgart, Germany — ²Centre of Smart Interfaces, Darmstadt, Germany

We incorporate mesoscopic molecular dynamics (MD) simulations to investigate the stretching behaviour of a tethered polymer in a confined geometry. In particular we are interested in the connection between fluid flow characteristics and the force on the polymer chain. In addition, the comparison to analytical predictions show that hydrodynamic interactions (HIs) are crucial for the observed stretching behaviour. However, the comparison also shows that the general scaling behaviour for the stretching is not strongly influenced by HIs. Simulation results agree with recent experimental results for λ -DNA stretching in micro scale channels.

CPP 11.8 Mon 17:00 ZEU 255

Dynamics of polymer chains in active fluids — •JAEHO SHIN and VASILY ZABURDAEV — Max Planck Institutes für Physik komplexer Systeme, Dresden, Germany

While the dynamics of polymer chains in viscous fluids are well understood, the dynamics in active fluids, which are common in living systems, can be very different. Here we study the dynamics of polymer chains in fluids that contain active Brownian particles (ABPs) in 2D by using Brownian dynamics simulations. The ABPs can be trapped in concave regions of the polymer contour and thus can strongly affect the propulsion of the polymer. The polymer center of mass shows super-diffusive motion at short times and above the capturing time of the ABPs, it goes to normal diffusion with the diffusivity much larger than in the case of a passive viscous medium. Interestingly, the long time diffusivity shows a non-monotonous behavior as functions of both the chain length n and the bending stiffness κ . We analyze the chain conformation by looking at its Fourier modes and find that at the optimal length/ stiffness, the chain has preferentially bent conformations. Finally, we consider the barrier crossing of polymer chains in a double-well potential. The crossing times show a non-monotonous behavior as a function of n and κ due to the non-monotonous diffusivity. These findings can be instrumental for efficient sorting of polymer chains by their length and elastic properties.

CPP 11.9 Mon 17:15 ZEU 255

An improved dissipative coupling scheme for a system of Molecular Dynamics particles interacting with a Lattice Boltzmann fluid — •NIKITA TRETYAKOV¹ and BURKHARD DUENWEG^{1,2,3} — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Institute for Solid State Physics, Technical University of Darmstadt, Germany — ³Department of Chemical Engineering, Monash University, Australia

We consider the dissipative coupling between a stochastic Lattice Boltzmann (LB) fluid and a particle-based Molecular Dynamics (MD) system, as it was first introduced by Ahlrichs and Duenweg (J. Chem. Phys. 111 (1999) 8225). The fluid velocity at the position of a particle is determined by interpolation, such that a Stokes friction force gives rise to an exchange of momentum between the particle and the surrounding fluid nodes. For efficiency reasons, the LB time step is chosen as a multiple of the MD time step, such that the MD system is updated more frequently than the LB fluid. In this situation, there are different ways to implement the coupling: Either the fluid velocity at the surrounding nodes is only updated every LB time step, or it is updated every MD step. It is demonstrated that the latter choice, which enforces momentum conservation on a significantly shorter time scale, is clearly superior in terms of stability and accuracy, and nevertheless only marginally slower in terms of execution speed. The second variant is therefore the recommended implementation.

CPP 11.10 Mon 17:30 ZEU 255

Modeling Structure Formation of Twin Polymerization via a

reactive Bond Fluctuation Model — •JANETT PREHL and CON- STANTIN HUSTER — Technische Universität Chemnitz, Chemnitz, Deutschland

Utilizing twin polymerization the formation of nanostructured organic-inorganic hybrid materials is possible in only one single reaction process. These hybrid materials consist of an interweaved organic polymer with an inorganic network. Both materials exhibit nanoporous structures at 0.5-3nm, which is a desirable property for i.e. gas storage- or fuel cell media.

Although a huge class of twin monomers triggering twin polymerization are identified and first quantum chemical calculations are performed, the structure formation process leading to the nanoporous materials as well as influence factors defining the porosity are still not known in detail. However, this knowledge would help to design customized materials for future applications.

To gain insights into the structure formation process and the resulting morphology we develop a Monte-Carlo-based reactive bond fluctuation model for twin polymerization. After introducing our model and explaining the obtained results we will also compare them with experimental data.

CPP 11.11 Mon 17:45 ZEU 255

The Wang-Landau Reaction Ensemble Method: Simulation of Weak Polyelectrolytes and General Acid-Base Reactions — •JONAS LANDSGESELL — ICP Uni Stuttgart, Stuttgart, Deutschland

We present a novel method for the study of weak polyelectrolytes and general acid-base reactions in molecular dynamics and Monte Carlo simulations. The approach combines the advantages of the reaction ensemble and the Wang-Landau sampling method. Deprotonation and protonation reactions are simulated explicitly with the help of the reaction ensemble method while the accurate sampling of the corresponding phase space is achieved by the Wang-Landau approach. The combination of both techniques provides a sufficient statistical accuracy such that meaningful estimates for the density of states and the partition sum can be obtained. With regard to these estimates, several thermodynamic observables like the heat capacity or reaction free energies can be calculated. We demonstrate that the computation times for the calculation of titration curves with a high statistical accuracy can be significantly decreased when compared to the original reaction ensemble method. The applicability of our approach is validated by the study of weak polyelectrolytes and their thermodynamic properties.

CPP 11.12 Mon 18:00 ZEU 255

Studying multicomponent polymer solutions with a particle-based model linked to simple density functional theory — •JIANGUO ZHANG, DEBASHISH MUKHERJI, KURT KREMER, and KOSTAS DAOULAS — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Multicomponent polymer solutions are fascinating systems for polymer physics, due to complex structural, thermodynamic, and rheological properties. Molecular-level mechanisms controlling these properties are only partially understood, which complicates technological applications, e.g. coating processes. This knowledge gap motivates our study, where we investigate ternary (polymer, solvent, cosolvent) mixtures using a mesoscopic particle-based model. Polymers and (co)solvent molecules are described [1] as worm-like chains and single beads, respectively. Non-bonded interactions are introduced through a polynomial functional, which is third order in local component densities. Analytical mean-field results for equations-of-state and compressibility facilitate the parameterization of the model. The functional-based definition serves as a framework for Monte Carlo simulations using a simple particle-to-mesh scheme. Different scenarios for polymer solubility in solvent and cosolvent are considered. In the dilute regime, the model reproduces co-non-solvency behavior observed previously with a generic microscopic model [2]. Conformational and structural properties at different concentrations are studied, modeling polymer films exposed to solvent-cosolvent vapor at different partial pressures. [1] Zhang et al, EPJ SP 2016. [2] Mukherji et al, Nat Commun 2014.