CPP 71: Modelling and Simulation of Soft Matter II (joint session CPP/DY)

Time: Wednesday 15:00–16:45   Location: ZEU 255

CPP 71.1   Wed 15:00   ZEU 255

Machine Learning Inter-Atomic Potentials Generation Driven by Active Learning: A Case Study for Amorphous and Liquid Hafnium dioxide — •Anand Narayanan Krishnamoorthy[1,2], Ganesh Sivaraman[3], Matthias Baur[1], Christian Holm[1], Chris Benmore[6], Marius Stan[4], Gabor Csanyi[5], and Álvaro Vázquez–Mayagoitia[7] — [1]Institute for Computational Physics, University of Stuttgart — [2]Helmholtz Institute Muenster — [3]Leadership Computing Facility, Argonne National Laboratory - USA — [4]Applied Materials Division, Argonne National Laboratory, USA — [5]Department of Engineering, University of Cambridge, UK — [6]X-ray Science Division, Argonne National Laboratory, USA — [7]Computational Science Division, Argonne National Laboratory, USA

We propose a novel active learning scheme for automatically sampling a minimum number of uncorrelated configurations for fitting the Gaussian Approximation Potential (GAP). We apply this scheme to a Hafnium dioxide (HfO2) dataset generated from a melt-quench ab initio molecular dynamics (AIMD) protocol. Our results show that the active learning scheme, with no prior knowledge of the dataset is able to extract a configuration that reaches the required energy fit tolerance. Further, molecular dynamics (MD) simulations performed using this active learned GAP model on 6144-atom systems of amorphous and liquid state elucidate the structural properties of HfO2 with near ab initio precision and quench rates (ie 1.0 K/ps) not accessible via AIMD.

CPP 71.2   Wed 15:15   ZEU 255

BoltzmaNN: Heuristic inverse design of pair potentials using neural networks — •Fabian Berressem, Mihir Khadilkar, and Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University Mainz, Germany

In this work, we investigate the use of neural networks (NNs) to devise effective equations of state from a given isotropic pair potential using the virial expansion of the pressure. We train the NNs with data from molecular dynamics simulations, sampled in the NVT ensemble at densities covering both the gas- and liquid-like regime. We find that the NNs provide much more accurate results compared to the analytic estimate of the second virial coefficient derived in the low density limit. Further, we design and train NNs for computing the potential of mean force from the radial pair distribution function, $g(r)$, a procedure which is often performed for coarse-graining applications. Here, we find that a good choice for the loss function is crucial for an accurate prediction of the pair potentials. In both use cases, we study in detail how providing additional information about forces and the density impacts the performance of the NNs. We find that including this additional information greatly increases the quality of the predictions, since more correlations are taken into account. Further, the predicted potentials become smoother and are in general much closer to the target potential.

CPP 71.3   Wed 15:30   ZEU 255

Prediction of iSCFT chemical potentials via machine learning — •Lucia Milena Wesenberg, Ludwig Schneider, and Marcus Müller — Institute for Theoretical Physics, Georg-August University Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

We explore the use of machine learning to enhance the simulation of polymeric nanostructures. Self-assembly of symmetric diblock copolymers is the chosen testing system for this purpose. Such polymers consist of two equally long blocks of different monomer types. As the two monomer types are incompatible but linked in the center of each polymer, microphase separation occurs.

Simulations of such systems often pose a challenge for particle-based models as large systems and concomitantly long time scales need to be simulated. Thus, continuum models are employed, where the dynamics can be conceived as the relaxation towards the local minimum of a free-energy basin and jumps between such basins. These models reduce the degrees of freedom by integrating out the molecular degrees of freedom. The most detailed continuum model investigated here is the Self-Consistent Field Theory (SCFT). Unfortunately, dynamic SCFT requires the chemical potential of a non-equilibrium morphology that is computationally expensive to obtain. The SCFT potential calculation is an iterative process, and the stability of the algorithm depends

heavily on the starting conditions. Our machine learning approach provides suitable initial conditions for the algorithm. The predicted starting conditions reduce the computational effort considerably.

CPP 71.4   Wed 15:45   ZEU 255

PolyEC - an event-chain framework — •Tobias A. Kampmann, David Müller, and Jan Kierfeld — TU Dortmund University, Germany

PolyEC is a MC event chain framework suitable for simulation of various colloidal systems. We focus on modularity and extensibility to simulate heterogenous systems. In event-chain simulations only one particle is active and interactions can be treated independently by factorization, which allows for a highly modular approach for particle-based simulations. Albeit ECMC is a monte-carlo method, a single event-chain is deterministic (although there are modifications where this is not true). One crucial feature of this method is that each state a piece-wise deterministic event-chain visits between events are properly (Boltzmann-) weighted. This opens the possibility to measure observables like pressure or the distribution of energy *on the fly*. As examples we show needle-colloid mixtures and an active particle system.

CPP 71.5   Wed 16:00   ZEU 255

Analytical and computational study of advection-diffusion-reaction processes in catalytic fibrous membranes — •Gabriel Sitaru and Stephan Gekle — Biofluid Simulation and Modeling, Theoretische Physik VI, Universität Bayreuth

We investigate the efficiency of multi-step catalytic systems where a reactant species is flown through a set of fibrous catalytic membranes. The complexity of such systems arises from the interplay of three different time scales: advection, diffusion and reaction. A theory based on infinitely long cylindrical catalytic sites is developed for the steady-state of an advection-diffusion limited reaction. Additionally, the time-dependent concentration profiles are computed using a Lattice-Boltzmann based solver for both the advection-diffusion-reaction and the Navier-Stokes equations. The comparison shows a good agreement between the theory and the numerical results, our model breaking down only in the very low-Péclet regime (i.e. diffusive flow). Both methods can be easily used to predict the efficiency of a multi-step catalysis in fibrous membranes with various geometries.

CPP 71.6   Wed 16:15   ZEU 255

The stability field of the chiral CO2 water hydrate from molecular dynamics simulations — •Marcello Sega[1], Jakob Michl[2], and Christoph Dellago[2] — [1]Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Germany — [2]Faculty of Physics, University of Vienna, Austria

Recent experimental evidence[1] shows that the water network characterizing the high-pressure CO2 hydrate[2] is, in fact, ice XVII, which possesses open helicoidal channels giving the structure a chiral nature. The question of the stability field boundaries of this hydrate is still open, and we report on recent molecular dynamics simulations[3] in which we found that the CO2-filled ice XVII is more stable than the sI clathrate and than the mixture of ice VI and dry ice at pressure values ranging from 6 to 18 kbar and in a wide temperature range. We propose a phenomenological correction to take into account the limitation of the model potentials, suggesting that the stability should more realistically range from 6.5 to 13.5 kbar. Our simulation results support the current hypothesis that the chiral CO2 hydrate is stable at temperatures above the melting curve of ice VI.

[1]L. Del Rosso, M. Celli, and L. Ulivi, Nat. Comm. 7, 13394 (2016)
[2]H. Hirai, K. Komatsu, M. Honda, T. Kawamura, Y. Yamamoto, and T. Yagi, The J. Chem. Phys. 133, 124511 (2010)
[3]J. Michl, M. Sega, and C. Dellago, J. Chem. Phys. 151, 104502 (2019)

CPP 71.7   Wed 16:30   ZEU 255

Mechanics of shape-shifting droplets — •Ireth Garcia-Aguilar[1], Piermarco Fonda[1], Eli Sloutskin[2], and Luca Giomi[1] — [1]Instituut-Lorentz, Universiteit Leiden, The Netherlands — [2]Department of Physics and Institute of Nanotechnology & Advanced Materials, Bar-Ilan University, Ramat-Gan, Israel

It has been long understood that dispersed liquid droplets are spherical in order to minimize the tension at their interface. Surprisingly, oil emulsion droplets in water have been observed to spontaneously deform into polyhedral shapes when cooling down the system. The equilibrium shape of a droplet at some temperature depends on its initial volume but all deformations take place below the freezing point of the surfactant monolayer, while the bulk oil and water remain liquid. The frozen interface forms an hexagonal lattice which is topologically constrained to accommodate defects. These produce large stresses that induce in and out-of-plane deformations in the crystal which in turn are opposed by the interfacial tension between oil and water. Initially, it was thought that this competition determines the droplet shape; however, this alone can not explain the size dependence of the deformations. By modeling the interface as a 2D elastic surface and studying its equilibrium geometry, we found a mechanism that explains the size-scaling behaviour. Interestingly, crystalline defects are not the only peculiarity playing a role in shaping the droplets.