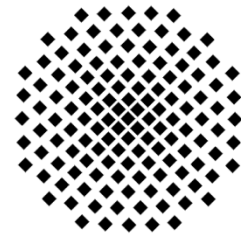


Stuttgarter Physikalisches Kolloquium

Fachbereich Physik, Universität Stuttgart
Max-Planck-Institut für Festkörperforschung
Max-Planck-Institut für Intelligente Systeme

Ansprechpartner: Prof. Harald Giessen
E-Mail: giessen@physik.uni-stuttgart.de
Telefon: 0711 - 685-65111



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Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart-Vaihingen

Gastgeber: Prof. Alejandro Muramatsu, Universität Stuttgart, Telefon: 0711 - 685-65204

Computational Soft Matter: bridging time and length scales

Axel Arnold

ICP, Universität Stuttgart - *Antrittsvorlesung*

Abstract

Many properties of soft matter, for example polymers or colloids, arise on mesoscopic time and length scales between the atomistic and continuum scale. On these scales, a description in terms of individual units like monomers or colloids is still necessary, but a fully atomistic resolution is inaccessible to simulations, even for future generations of supercomputers. Therefore, we use specific mesoscopic particle models in order to investigate soft matter computationally. Our software ESPResSo, the Extensible Simulation Package for RESearch on Soft matter, is specifically designed for coarse grained models of soft matter. In this talk, I will present recent algorithmic developments that help ESPResSo to reach new time and length scales in mesoscopic simulations, plus one application.

On the mesoscopic scale, hydrodynamic interactions often play an important role, but are neglected in simulations due to the high computational costs. Our lattice Boltzmann solver for graphics cards overcomes this barrier by speeding up the calculations by almost two orders of magnitude. In order to be able to reach the long time scales associated with rare events like translocation or crystallization, I present our FRESH framework that allows to bias a simulation to undergo a transition without biasing the statistics like transition rates.

As an example of mesoscopic modeling I will talk about computer simulations of DNA segregation in bacteria. Our simulations showed that in confined geometries such as a bacterium, DNA segregates solely due to entropic reasons. This is an important step towards understanding the origin of primitive bacteria, since it shows that an active mechanism for DNA segregation is not necessary, in contrast to what is commonly believed in the biological community.