Karlsruhe Institute of Technology

IAM
Institut für Angewandte Materialien

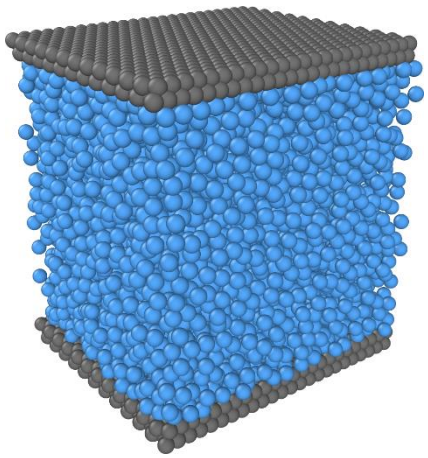
Master Thesis
Fluctuations and Transport Properties of Confined Fluids

Background

Lubricated friction determines human interaction with the environment as well as function and reliability of machinery. In the so-called boundary lubrication regime, the contacting bodies are separated only by a few layers of molecules and therefore, the confined fluid often behaves differently than in the bulk. However, macroscopic properties of the lubricated contact are typically measured under entrainment conditions which are out of reach with molecular length and time scales. To address this multiscale problem, within the *Research Training Group 2450 – Tailored Scale-Bridging Approaches To Computational Nanoscience*, we develop new simulation methods to predict energy dissipation and deformation in these systems. We use classical molecular dynamics (MD) simulations to obtain local stress states in the fluid which enter mesoscale simulations. On the other hand, conserved variables are evolved in time and control the boundary conditions of the MD ensemble.

Tasks

You will perform MD simulations of fluid systems at equilibrium. Starting with a bulk system, you will further investigate the influence of solid walls confining the fluid which is expected to change the correlations of equilibrium fluctuations. Your results will be used to validate a continuum hydrodynamics solver considering thermal fluctuations.



Simulation of liquid Argon in a slab geometry

Requirements

- Basic knowledge of the classical MD method
- Basic programming skills (e.g. in Python)

Contact

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