Karlsruhe Institute of Technology

IAM
Institut für Angewandte Materialien

Bachelor Thesis:
Active Learning From Molecular Simulation Data

Background

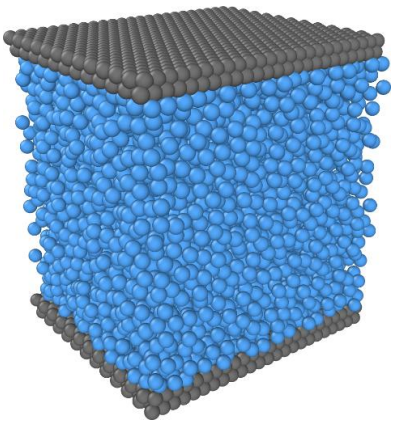
Lubricated friction determines human interaction with the environment as well as function and reliability of machinery. In the so-called boundary lubrication regime, the contacting bodies are separated only by a few layers of molecules and therefore, the confined fluid often behaves differently than in the bulk. However, macroscopic properties of the lubricated contact are typically measured on length and time scales much larger than molecular ones.

To address this multiscale problem, we develop tools to predict energy dissipation and deformation in these systems by combining molecular and continuum simulation methods with the help of machine learning.

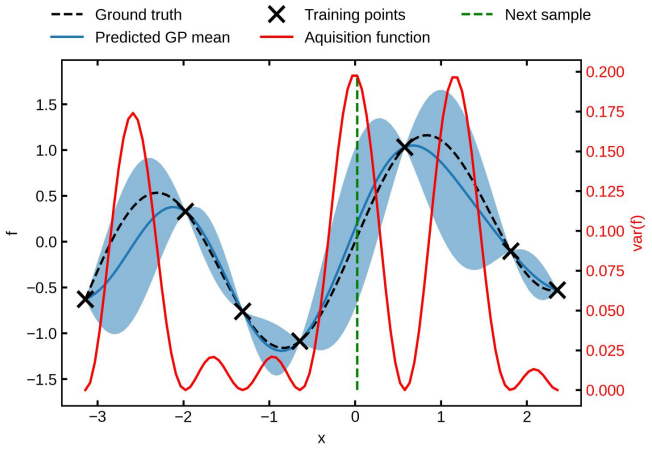
Tasks

A first step towards a data-driven surrogate model may be the exploration of an equation of state in a predefined parameter space (temperature and density) or the shear-thinning behavior of a model lubricant. The outline of the thesis can be adjusted to the candidate but may look as folllows:

- Literature review on Gaussian Processes and Active Learning
- Acquaintance with the molecular dynamics simulation package LAMMPS
- Implementation of the simulation/learning workflow in Python
- Evaluation of the implemented scheme on model systems



Snapshot of MD simulation: Lennard-Jones fluid confined between rigid walls.



Graphical representation of an active learning step using Gaussian process regression.

Requirements

- Interest in numerical simulation and machine learning
- Basic programming skills are beneficial but not required

Contact

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