

Accelerated Molecular Dynamics for Rare Event Sampling

Most scientific phenomena across various fields, from life sciences to engineering, are multiscale due to an interplay of disparate spatial and temporal scales. In the Multiscale Modeling of Fluid Materials group, we focus on tackling such problems with multiscale modeling and simulations.

State-of-the-art approaches to speed up Molecular Dynamics simulations require detailed knowledge about the slow processes of a system. Neural Networks (NNs) are powerful models to extract knowledge from high-fidelity data. Therefore, the thesis aims to leverage NN models to discover slow modes in Molecular Dynamics simulations.

Your thesis will consist of the following tasks:

- Researching state-of-the-art approaches from the literature
- Implementing approaches into our chairs' framework
- Validating implementation on benchmark systems

If you are interested in the thesis, please reach out to paul.fuchs@tum.de with a short introduction and your transcript of records.

