Professorship of Multiscale Modeling of Fluid Materials
TUM School of Engineering and Design
Technical University of Munich

High-Throughput DFT Calculations for the Development of Machine Learning Force Fields

Project Description:
Multiscale modelling is essential for understanding complex phenomena in fields ranging from life biochemistry to materials engineering. A promising research area in this area is the development of machine learning potentials (MLPs), particularly those based on Graph Neural Networks (GNNs), which have emerged as a powerful tool for bridging the gap between quantum-mechanical accuracy and classical molecular dynamics efficiency.
This thesis focuses on developing high-throughput Density Functional Theory (DFT) datasets and training GNN-based MLPs. These datasets will serve as the foundation for developing accurate and transferable force fields that can be applied to large-scale molecular dynamics simulations. The project will involve generating and curating DFT data, training GNN models, and evaluating their performance in predicting interatomic forces and energies.

Objectives

1. **High-Throughput DFT Dataset Generation:** Use high-throughput DFT calculations to generate a diverse and comprehensive dataset of atomic structures, energies, and forces for training MLPs.
2. **GNN Model Development:** Research and implement state-of-the-art GNN architectures for learning interatomic potentials from the generated DFT data.
3. **Training and Validation:** Train the GNN models on the DFT dataset and validate their accuracy in predicting energies and forces for unseen structures.
4. **Performance Evaluation:** Benchmark the trained GNN potentials against traditional force fields and ab initio methods in terms of accuracy and computational efficiency.

Requirements

- **Machine Learning Practice:** Experience with training and evaluating machine learning models, particularly neural networks is advantageous.
- **Programming Experience:** Proficiency in Python. Familiarity with machine learning frameworks (e.g., PyTorch, JAX)
- **Quantum Chemistry Knowledge:** Understanding of DFT and quantum chemistry calculations is advantageous.

What We Offer

- Access to a GPU cluster for resource-intensive computations.
- An opportunity to work on a cutting-edge project with potential applications in materials science, chemistry, and beyond.

Application Process

If you are interested in this project or have further questions, please send a short email to m.sanocki@tum.de with the following:

1. A brief introduction about yourself (background, interests, and motivation).
2. Your transcript of records.