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

Hyperparameter Optimization and Benchmarking of Machine Learning Potentials for Molecular Dynamics Simulations

Project Description
Machine learning potentials (MLPs) have revolutionized molecular dynamics (MD) simulations by providing a bridge between the accuracy of quantum-mechanical methods and the efficiency of classical force fields. However, the performance of MLPs heavily depends on the choice of hyperparameters, such as network architecture, learning rate, and training data composition. Systematic hyperparameter optimization and benchmarking are essential to ensure that MLPs are accurate, transferable, and computationally efficient.
This thesis focuses on the hyperparameter optimization and benchmarking of developed MLPs, particularly those based on Graph Neural Networks (GNNs). The project will involve designing and implementing a framework for hyperparameter tuning, evaluating the performance of optimized MLPs on diverse datasets, and benchmarking their accuracy and efficiency against traditional force fields and ab initio methods.

Objectives

1. **Training and Validation:** Train MLPs with optimized hyperparameters and validate their performance on diverse datasets, including energies, forces, and molecular properties.
2. **Benchmarking:** Compare the accuracy and computational efficiency of optimized MLPs against traditional force fields and ab initio methods.
3. **Performance Analysis:** Analyze the impact of hyperparameters on MLP performance and provide guidelines for future development.

Requirements

- **Machine Learning Practice:** Experience with training and evaluating machine learning models, particularly neural networks.
- **Programming Experience:** Strong proficiency in Python. Familiarity with machine learning frameworks (e.g., PyTorch, JAX)
- **Molecular Dynamics Knowledge:** Basic understanding of MD simulations and force fields is advantageous but not mandatory.

What We Offer

- Access to high-performance computing resources for training and benchmarking MLPs.
- 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.