Freie Universität Berlin

A fast implementation of deep neural-network potentials for molecular dynamics simulations of alloys

by

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Master Thesis in Computational Science

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Abstract

A concise 200–300 word summary of:

- Motivation (accelerating atomistic simulations using neural network potentials)
- Goal (integrating DeepMD potential calculation into HALMD)
- Method (extracting weights, replicating inference in C++/CUDA)
- Key results and performance (accuracy vs. speed trade-off)
- Conclusions

Contents

1 Introduction

1.1 Motivation

1.2 Objectives and Scope

1.3 Structure of the Thesis

This thesis is organized into six main sections, each addressing a distinct aspect of the integration of deep neural-network potentials into the HALMD simulation framework for binary alloy systems.

Section 1: Introduction presents the motivation for employing machine-learned interatomic potentials in molecular dynamics, highlighting the limitations of traditional analytical models and the potential of deep learning to achieve *ab initio*-level accuracy at a fraction of the computational cost. The objectives and scope of the work are defined, followed by an outline of the thesis structure.

Section 2: Background introduces the theoretical and computational foundations of the work. It provides an overview of the HALMD software, describing its modular design, GPU acceleration, and classical molecular dynamics formulation. The section also discusses the Deep Potential Molecular Dynamics (DeepMD) framework, including the principles of neural-network potentials, descriptor construction, and the overall architecture of the Deep Potential model for multi-species systems such as alloys.

Section 3: Methodology details the integration process of the DeepMD potential into HALMD. It explains the extraction of model parameters (weights, biases, and descriptors) from a trained DeepMD model, the reconstruction of the descriptor pipeline (R and G matrices), and the implementation of the neural network inference and force computation within HALMD. Special attention is given to the treatment of multiple atomic species and the efficient GPU-based execution of the potential evaluation.

Section 4: Results presents the outcomes of the integration. This includes validation of the energy and force predictions against reference DeepMD-kit calculations, performance benchmarks of the HALMD implementation on GPU hardware, and case studies of binary alloy systems. The accuracy, scalability, and computational efficiency of the implementation are systematically analyzed.

Section 5: Discussion interprets the results, addressing the accuracy–performance trade-offs, sources of deviation between HALMD and DeepMD outputs, and the numerical stability of the approach. It also highlights the implications of using neural-network potentials in multi-component systems.

Section 6: Conclusions and Future Work summarizes the key contributions of the thesis and discusses possible directions for future development. Potential extensions include optimized GPU kernels, support for additional descriptor types, and extension of the implementation to more complex alloy systems beyond binaries.

Overall, the structure of the thesis is designed to guide the reader from the motivation and theoretical foundations through the detailed implementation and validation of a high-performance, machine-learned potential within the HALMD framework.