Materials Science and Engineering Dissertation Defense

Enhancing SLUSCHI Through the Optimization of Computational Methods for Calculating Melting Temperature Via the Incorporation of Machine Learning

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Abstract

Two approaches for integrating machine learning into the Solid and Liquid in Ultra Small Coexistence with Hovering Interfaces package (SLUSCHI) are presented to improve the efficiency of first-principles melting simulations. Accurate melting temperature pre-diction requires computationally expensive density functional theory (DFT) calculations, limiting system size and timescale. First-principles methods are limited by high computational cost and require a trade-off between speed and accuracy when determining melting temperatures. Those limitations are further demonstrated through high-pressure simulations of Fe. Many simulations were performed exploring a wide range of parameters affecting calculated melting temperatures. Additional simulations were conducted to explore potential methodological sensitivities including carbon contamination, Brillouin zone sampling, and DFT-dependent variables. To address the computational cost of DFT simulations, machine learning methods are incorporated into SLUSCHI. The first approach incorporates on-the-fly machine-learning force fields into SLUSCHI using the Vienna Ab initio Simulation Package (VASP). This enables VASP to build machine-learning force fields trained on first-principles data generated during simulation. This method maintains accuracy comparable to DFT and experimental results. However, computational cost increases because additional iterative simulations needed are required to resolve phase behavior. A second approach integrates the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) into SLUSCHI to replace computationally expensive DFT calculations. By utilizing machine-learning potentials from the Large-scale Atomistic Simulation with neural network Potential (LASP NN) in conjunction with LAMMPS, computational time was significantly reduced, and melting temperature calculations remained within one standard deviation of DFT results. This enhanced method was further expanded to determine melting behavior of high-pressure Y_2O_3, producing a pressure-temperature phase diagram and identifying thermodynamic features at elevated pressures. These results demonstrate that the integration of machine learning substantially im-proves the efficiency and scalability of SLUSCHI while maintaining quantitative accuracy, providing a framework for extending SLUSCHI through development, validation, and ap-plication to complex systems. The resulting methodology has potential applications in high-throughput materials modeling, materials design, and geophysical modeling.

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