Deep-learning-based Molecular-Dynamics Simulations of Iron in Planetary Core Conditions

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Introduction

- To understand the behavior of materials compressed to extreme conditions, it would be desirable to perform large-scale molecular dynamics (MD) simulations. However, the high-fidelity simulation results still rely on high-accuracy force field.
- DF-QMD is helpful but fails to work efficiently with a larger scale of extreme condition atom data.
- This study takes advantage of recent developments in machine learning (i.e., DeepMD-kit[1]) in recent years and aims at developing potential models with *ab initio* accuracy to study materials at extreme conditions.
- Application of deep-learning potentials for MD simulations of iron at planetary-core conditions (temperatures T=6000~8000K and pressure P= 300~400GPa).
- Simulation reviews high accuracy the deep-learning potential compares to *ab initio* MD potential model.
- Simulation shows cooperative diffusion along <111> directions of body-centered cubic iron, a special state of iron near melting that has many geophysical implications[2].

Training and Simulation

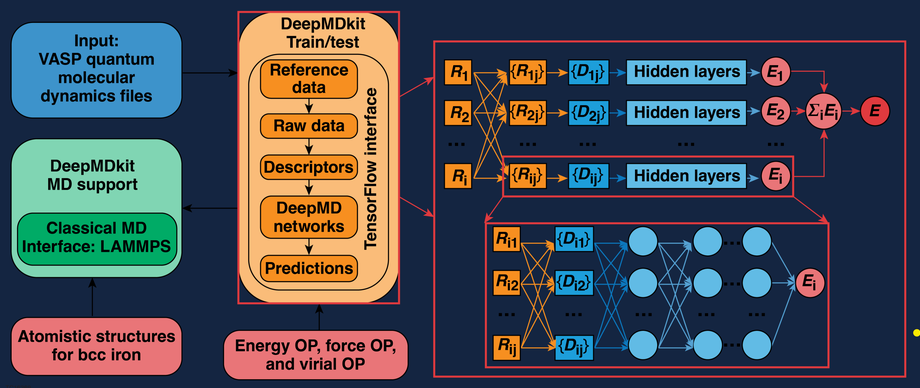

Fig.1 Workflow of training and pre-simulation process

- The reference data are generated from quantum molecular dynamics (QMD) simulations based on Kohn-Sham-Mermin density functional theory. These simulations are for BCC iron at various temperatures along a 13.9-g/cm^3 isochore. The calculations are based on 128-atom cell, 2x2x2 k mesh, with NVT ensembles generated by using a Nosé–Hoover thermostat[2].
- The data are passed and mapped into descriptors *Di* with translational, rotational, and permutational symmetries preserved.
- A feedforward network in which descriptor data flows from the input layer as *Di*, through multiple hidden mapping layers, to the output layer and generates the atomic energy *Ei*. The mathematical equation for this process is $E_i = L_i^{out} \cdot L_i^h \cdot L_i^{h-1} \cdot L_i^{h-2} \cdot \cdots \cdot L_i^1 \cdot D_i$.Here the *Li* is the mapping layers, which is a composition of a linear transformation and a non-linear transformation.
- The final prediction data are then calculated (i.e., The force on the ith atom is computed by taking the negative gradient of the system energy with respect to its position) and generate a potential model,
- The potential will be used with atomistic BCC iron structure file as input for LAMMPS[3] NVT and NPT simulations.

Results

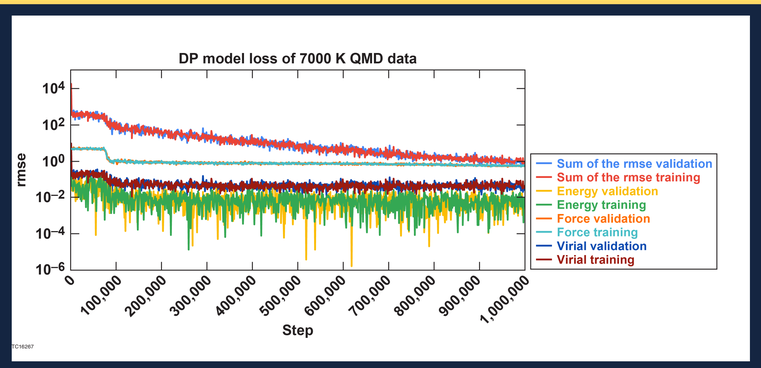

Fig.2 Loss figure of 7000K potential model generated by DeepMD-kit

- The loss is defined as a sum of different mean square errors of the DNN predictions by $L(P_\epsilon, P_f, P_\xi) = \frac{P_\epsilon}{N}\Delta E^2 + \frac{P_f}{3N}\sum_i |\Delta F_i|^2 + \frac{P_\xi}{9N}\|\Delta\Xi\|^2$, where ΔE, ΔF_i and $\Delta\Xi$ denote root mean square (RMS) error in energy, force, and virial, respectively. And P_ϵ, P_f, P_ξ are perfectors.
- The RMSE of energy, force and virial (per 2000-atom cell and units are eV, eV/Å and eV, respectively) in both training and validation sets decrease significantly after 1,000,000 steps of training.
- Dataset consist of 5000 snapshots (3000 for training and 2000 for validation), the total time of 1,000,000 steps of training is ~24h.

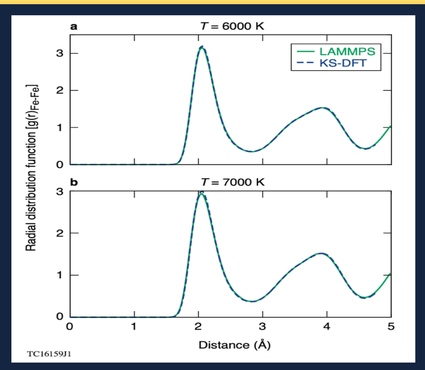

Fig.3 Comparison of radial distribution function between data generated by LAMMPS and KS-DFT

- In both 6000K and 7000K, the radial distribution function lines of LAMMPS simulation results match those of KS-DFT's.
- The preferable match of both simulation results reveal a high accuracy of the deep-learning based potential model.

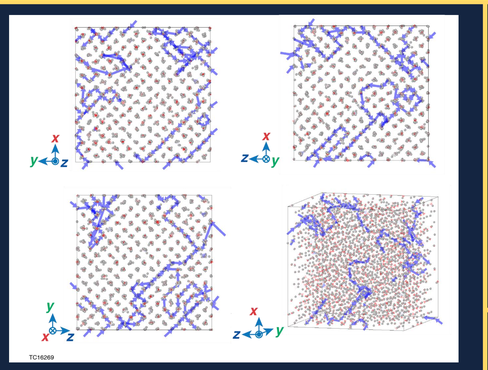

Fig.4 Cooperative diffusion along <111> direction from LAMMPS simulation

- Our 2000-atom machine-learning MD simulations reconfirm our QMD findings that cooperative diffusion of iron occurs along <111> directions in bcc iron.

Future Work

- Continue the training with a different temperature QMD data to get a universal potential model for BCC iron in high accuracy, this model can thus be used to start accurate simulation at 9000K+ temperature condition. And help understanding and answering some open questions in planetary science (i.e., how planet core form).

References

1. H. Wang, L. Zhang, J. Han, W. E, "DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics", Comp. Phys. Comm. 208 (2018).
2. M. Ghosh, S. Zhang, L. Hu, S.X. Hu., "Cooperative Diffusion in Body-Centered-Cubic Iron at Earth and Super-Earth's Inner Core Conditions," submitted to Nature Communications.
3. A. P. Thompson, *et al., "*LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales", Comp Phys Comm, 271 (2022) 10817.

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