Homework

1.1. (1 point) Actively train MTPs of different levels (4,6,8,10,12) for the Nb system during molecular dynamics at T=300 K for 100 ps with the time step of 1 fs. Start with a dataset containing one configuration (train_init.cfg from https://gitlab.com/ashapeev/mlip-2-tutorials/-/wikis/Tutorial-2/Home).

1.2. (1 point) Plot the dependence of energy RMSE and force RMSE on the number of MTP parameters. Make conclusions.

1.3. (1 point) Plot the dependence of the number of the selected configurations on the number of MTP parameters. Make conclusions.

1.4. (1 point) Starting from the MTP of 12^{th} level and the dataset obtained in 1.1 at T=300 K, actively train this MTP sequentially at the temperatures T = 800 K, 1300 K, and 1800 K. To that end you should start from the database and the potential obtained from the previous (lower) temperature for the next (higher) temperature. Provide a table with four columns: temperature, number of configurations in the database, energy RMSE, force RMSE. Make conclusions.

1.5. (1 point) Actively train MTP of 12^{th} level starting with a dataset containing one configuration at T=1800 K. Do the same as in 1.4, but decrease the temperature: T = 1300 K, 800 K, and 300 K. Provide the table with the same four columns as in 1.4. Make conclusions.

1.6. (5 points) Actively train MTP of 12^{th} level starting with a dataset containing one configuration at T=1800 K for 100 ps with the time step of 1 fs. Save the fitted potential and the training set. Conduct molecular dynamics simulations at T=1800 K for 1 ps with the time step of 1 fs using the EAM potential as the interatomic interaction model. Save the configurations for each step in the LAMMPS dump-file. As a result, we have 1000 configurations. Convert the dump-file to .cfg MLIP-2 format (write your own script for converting). Take every 50-th of these 1000 configurations, calculate energies and forces for them using EAM, train MTP of 12^{th} level on these 20 configurations. Create the active learning state for the MTP trained on 20 configurations, select the configurations from 1000 configurations, calculate energies and forces for the selected configurations with the EAM potential, update the training set, re-train MTP. We refer this potential to as “pre-trained” MTP. Actively train the “pre-trained” MTP during molecular dynamics at T=1800 K for 100 ps. Save the fitted potential and the training set. Compare the number of configurations in the resulting training set obtained when starting from the potential fitted on one configuration in the training set and the “pre-trained” potential. Make conclusions.