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calorine: A Python package for constructing and sampling neuroevolution potential models

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Summary

Molecular dynamics (MD) simulations are a key tool in computational chemistry, physics, and materials science, aiding the understanding of microscopic processes but also guiding the development of novel materials. A MD simulation requires a model for the interatomic interactions. To this end, one traditionally often uses empirical interatomic potentials or force fields, which are fast but inaccurate, or ab-initio methods based on electronic structure theory such as density functional theory, which are accurate but computationally very expensive (Müser et al., 2023). Machine-learned interatomic potentials (MLIPs) have in recent years emerged as an alternative to these approaches, combining the speed of heuristic force fields with the accuracy of ab-initio techniques (Unke et al., 2021). Neuroevolution potentials (NEPs), implemented in the `GPUMD` package, in particular, are a highly accurate and efficient class of MLIPs (Fan et al., 2021, 2022; Fan, 2022). NEP models have already been used to study a variety of properties in a range of materials, with recent examples including radiation damage in tungsten (Liu et al., 2023), phase transitions (Fransson, Wiktor, et al., 2023) and dynamics of halide perovskites (Fransson, Rosander, et al., 2023) as well as thermal transport in two-dimensional materials (Sha et al., 2023). Here, we present `calorine`, a Python package that simplifies the construction, analysis and use of NEP models via `GPUMD`.

Statement of need

`GPUMD` is a package written in C++/CUDA that enables MD simulations as well as the construction of NEP models, with all computations running on a discrete GPU. For efficiency reasons this package uses a set of text based input and output files. `calorine` provides a Python interface that makes it easy to access the functionality of `GPUMD` and integrate it in Python based workflows. This includes but is not limited to managing the construction of NEP models as well as setting up and analyzing MD simulations.

`calorine` also exposes two `ASE Calculator` objects (Larsen et al., 2017), one using the CPU and one using the GPU. This has the expressed purpose of making NEP models transferable for use outside of `GPUMD`, since the calculators can be used by other codes, as well as on machines without discrete GPUs. Examples of such use cases include calculating force constants using `hiphive` (Eriksson et al., 2019) and phonon dispersions using phonopy (Togo, 2023; Togo et al., 2023).

The full documentation for `calorine` in addition to examples and tutorials can be found at https://calorine.materialsmodeling.org/.

Related software and recent work

Two other software packages that serve as companion software for GPUMD are PyNEP (Wang, 2023) and GPYUMD (Gabourie, 2023), focusing on NEP construction and MD simulations within GPUMD respectively. calorine differs from these two by having a broader scope, encompassing both NEP construction and sampling with MD simulations. Additionally, calorine exposes an interface for modifying potential files, further improving the transferability of NEP.

Examples of recently published work supported by calorine include a study of the through-plane lattice thermal conductivity in van-der-Waals structures (Eriksson et al., 2023), and a study of dynamic modes in halide perovskites under a continous-order phase transition (Fransson, Rosander, et al., 2023).

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