

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

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DOI: [10.xxxxxx/draft](https://doi.org/10.xxxxxx/draft)

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Submitted: 21 October 2023

Published: unpublished

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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.

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 continuous-order phase transition (Fransson, Rosander, et al., 2023).

Acknowledgements

We acknowledge and greatly appreciate contributions made by Petter Rosander. This work was funded by the Swedish Research Council (Grant Nos. 2018-06482, 2020-04935, and 2021-05072) as well as the Swedish Foundation for Strategic Research (SSF) via the SwedNess program (Grant No. GSn15-0008), and enabled by computational resources provided by the National Academic Infrastructure for Supercomputing in Sweden (NAISS) and the Swedish National Infrastructure for Computing (SNIC) at C3SE, UPPMAX, and HPC2N partially funded by the Swedish Research Council (Grant Nos. 2018-05973 and 2022-06725).

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