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Quantum-accurate large-scale atomistic simulation of fusion materials with LAMMPS and FitSNAP

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Molecular dynamics (MD) is a powerful materials simulation approach whose accuracy is limited by the interatomic potential (IAP). The quest for improved accuracy has resulted in a decades-long growth in the complexity of IAPs, many of which are implemented in the LAMMPS MD code.[1] Traditional physics-based IAPs are now being rapidly supplanted by machine-learning potentials (MLIAPs). The SNAP (Spectral Neighbor Analysis Potential) [2] approach is an early example of this, but new improved MLIAP approaches continue to emerge each year. The FitSNAP software[3], tightly integrated with LAMMPS, provides an automated methodology for generating accurate and robust application-specific MLIAPs, including support for Atomic Cluster Expansion (ACE) descriptors, and the PyTorch and JAX neural network libraries. Each MLIAP is trained on a large set of quantum electronic structure calculations of energy, force, and stress for many small configurations of atoms. The resultant potentials enable high-fidelity large-scale MD simulations of diverse materials, yielding insight into their behavior on lengthscales and timescales unreachable by other methods. The relatively large computational cost of using MLIAPs is offset by combining LAMMPS' spatial parallel algorithms with Kokkos-based hierarchical multithreading, enabling the efficient use of Exa-scale CPU and GPU platforms, allowing large-scale production simulations at speeds approaching 30 ns/day with millions to billions of atoms. These capabilities have been used by myself and collaborators to study diverse materials systems including shock compression of diamond, free expansion of molten aluminum, the magnetic/structural phase transition in shocked iron, and plasma-exposed materials for fusion energy.

[1] Thompson et al., Comp. Phys. Comm., 271:108171, 2022. DOI 10.1016/j.cpc.2021.108171
[2] Thompson et al., J. Comp. Phys., 285:316, 2015. DOI 10.1016/j.jcp.2014.12.018
[3] Rohskopf et al., Journal of Open Source Software, 8: 5118, 2023. DOI 10.21105/joss.05118

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