

Abstract Submitted
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Implementation of EAM and FS potentials in HOOMD-blue¹ LIN YANG, Ames Lab, Iowa State University, FENG ZHANG, Ames Lab, ALEX TRAVESSET, Iowa State University, Ames Lab, CAIZHUANG WANG, KAIMING HO, Ames Lab, Iowa State University — HOOMD-blue^[1] is a general-purpose software to perform classical molecular dynamics simulations entirely on GPUs. We provide full support for EAM and FS type potentials in HOOMD-blue, and report accuracy and efficiency benchmarks, including comparisons with the LAMMPS^[2] GPU^[3] package. Two problems were selected to test the accuracy: the determination of the glass transition temperature of $\text{Cu}_{64.5}\text{Zr}_{35.5}$ alloy using an FS potential and the calculation of pair distribution functions of Ni_3Al using an EAM potential. In both cases, the results using HOOMD-blue are indistinguishable from those obtained by the GPU package in LAMMPS within statistical uncertainties. As tests for time efficiency, we benchmark time-steps per second using LAMMPS GPU and HOOMD-blue on one NVIDIA Tesla GPU. Compared to our typical LAMMPS simulations on one CPU cluster node which has 16 CPUs, LAMMPS GPU can be 3-3.5 times faster, and HOOMD-blue can be 4-5.5 times faster. [1] Anderson, J. A., Lorenz, C. D., Travasset, A. J Comp Phys, 227(10), 5342–5359, (2008). [2] S. Plimpton, J Comp Phys, 117, 1-19 (1995). [3] W. M. Brown, P. Wang, S. J. Plimpton, A. N. Tharrington, Comp Phys Comm, 182, 898-911, (2011).

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