Abstract Submitted
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A New Look at the Evaluation of Embedded Atom Potential Models.[1] JAMES N. GLOSLI, KYLE J. CASPERSEN, DAVID F. RICHARDS, ROBERT E. RUDD, FRED H. STREITZ, Lawrence Livermore National Laboratory — The embedded atom method (EAM) potentials have been used extensively since introduced by Daw and Baskes in the mid 1980's due to their simple incorporation of many-body effects that are missed by simple pair potentials. The computational cost of the inclusion of this additional physics has traditionally been a second pass over the pair data. We will report on an implementation of the EAM model within a molecular dynamics algorithm (MD) that does not require this second pass, substantially reducing the computer time and memory required for evaluation of the potential. The second pass is avoided by using a forward extrapolation in time of the density derivative of the embedding function $dF(\rho(t))/d\rho$. The error in this approximation is controllable and consistent with the error introduced by the finite time step numerical integrators used in the MD.

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