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Characteristic curves of shockless compression from atomistic molecular dynamics[1] J. MATTHEW D. LANE, JONATHAN A. ZIMMERMAN, AIDAN P. THOMPSON, Sandia National Labs — Ramp loading experiments, such as those on Sandia's Z-machine, are increasingly used to produce shockless (quasi-isentropic) compression, enabling high-pressure off-Hugoniot states to be studied. One approach used to interpret data from such experiments is the method of characteristics. For arbitrary loading trajectories characteristic curves can be used to predict the steepening of the propagating ramp wave into a shock. Here, we present a method to extract characteristic curves from molecular dynamics simulations used to model a ramp loading response. This requires calculating the adiabatic sound speed within the material as a function of position and time. This was accomplished using extensions of the Hardy method for converting the instantaneous atom properties into continuum mechanics field variables. The method has been implemented in LAMMPS using the ATC package, and has been demonstrated using Lennard-Jones argon and EAM aluminum.

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