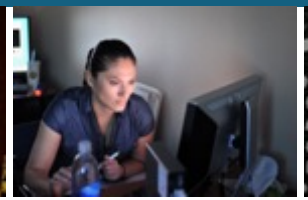
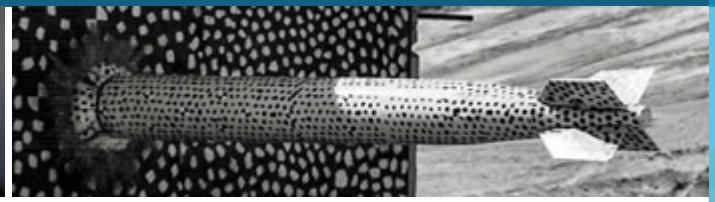
SAND2022-12647R

Sandia National Laboratories

Large-Scale Atomistic Simulations





PRESENTED BY

Principal Investigator/Lab: Stan Moore (SNL)

Platform/Campaign ID: Sierra/ATCC13-335
Code Name: LAMMPS
Program: ASC LSCI

SNL R&A #:

UNLIMITED RELEASE

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Large-Scale Atomistic Simulations: Investigating Free Expansion of Aluminum

Background Description:

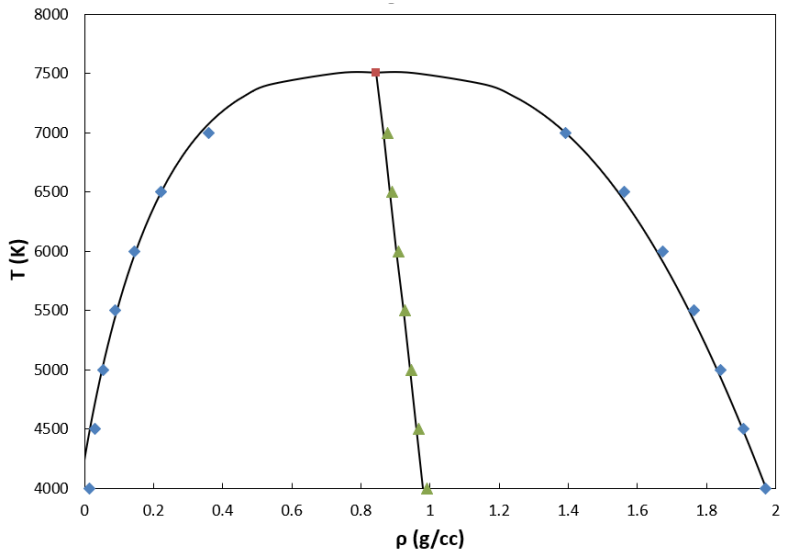
- Investigating free expansion of a supercritical fluid into two-phase liquid-vapor coexistence region
- We have transitioned from the simple Lennard-Jones model to a realistic SNAP machine learning potential for aluminum, trained using DFT quantum chemistry calculations

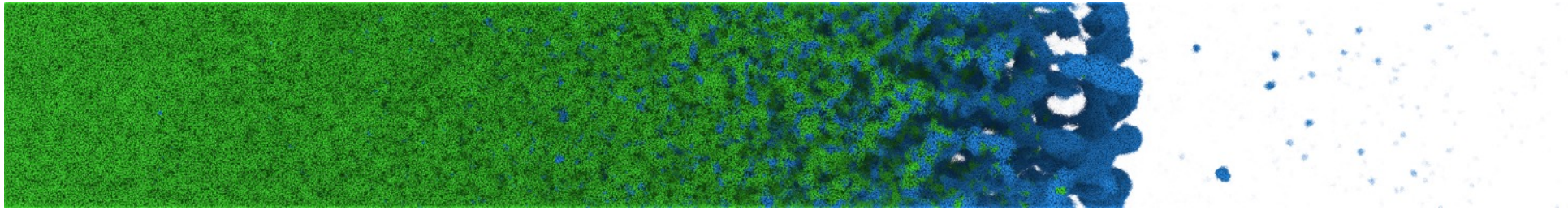
Potential Consequences/Issues:

- Hydrocodes generally cannot model this deep spinodal region accurately

Resolution/Impact:

- We ran an extreme-scale (~1.5 billion atom) free expansion simulation of aluminum on 8192 GPUs on LLNL Sierra (47% of the full machine)
- This information will provide a basis for two-phase equations-of-state models in hydrocode simulations of free expansion (e.g. exploding wires)





Take Home Message: The physically realistic SNAP machine-learning potential captures liquid-vapor coexistence behavior for free expansion of aluminum at a level not generally accessible to hydrocodes.