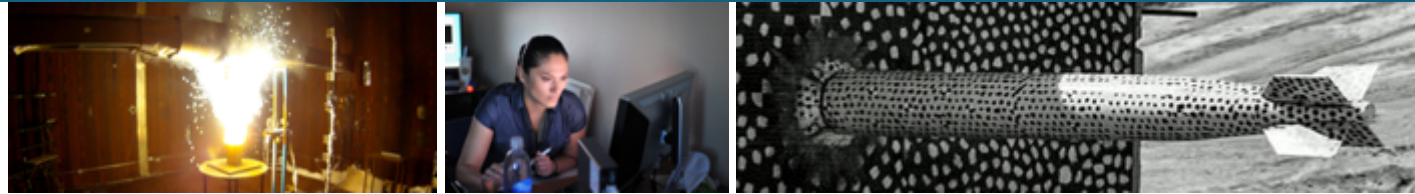




# Large-Scale Atomistic Simulations



PRESENTED BY

Principal Investigator/Lab: Stan Moore (SNL)

Platform/Campaign ID: Sierra/ATCC11-343

Code Name: LAMMPS

Program: ASC LSCI

Usage: 1.4 days

SNL R&A # (SAND, PR):

UNLIMITED RELEASE



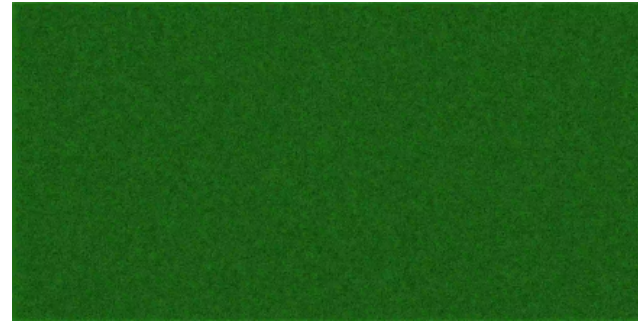


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# Large-Scale Atomistic Simulations: Investigating Free Expansion

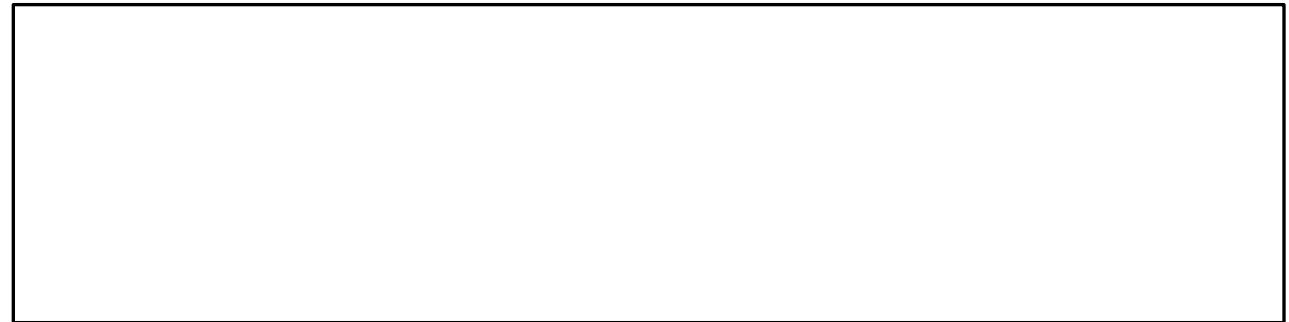
## Background Description:

- Investigating free expansion of a supercritical fluid into two-phase liquid-vapor coexistence region
- Ran a huge molecular dynamics simulation (24 billion Lennard-Jones atoms) on 8192 GPUs (47% of LLNL Sierra) using LAMMPS/Kokkos software, currently visualizing the results



## Potential Consequences/Issues:

- Hydrocodes generally cannot model this deep spinodal region accurately



## Resolution/Impact:

- 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: Atomistic simulations of free expansion through the liquid-vapor region unlock unprecedented insight into phase change kinetics and fluid microstructure evolution**