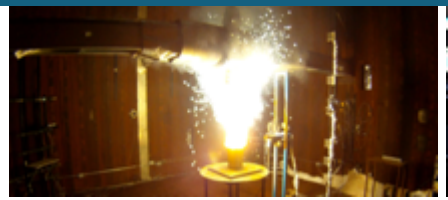
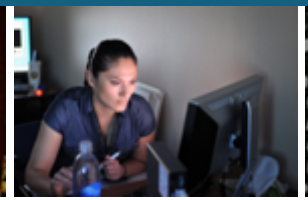
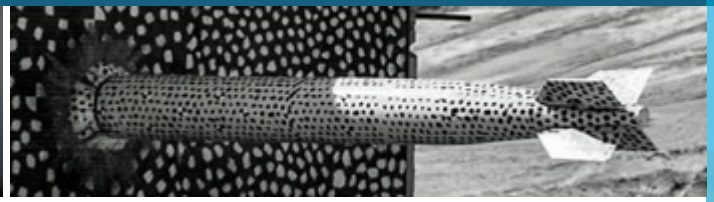
SAND2022-3439R

Sandia National Laboratories

# Large-Scale Atomistic Simulations







*PRESENTED BY*

Principal Investigator/Lab: Stan Moore (SNL)

Platform/Campaign ID: Sierra/ATCC12-336
Code Name: LAMMPS
Program: ASC LSCI

*SNL R&A #:*

UNLIMITED RELEASE

U.S. DEPARTMENT OF ENERGY | NNSA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

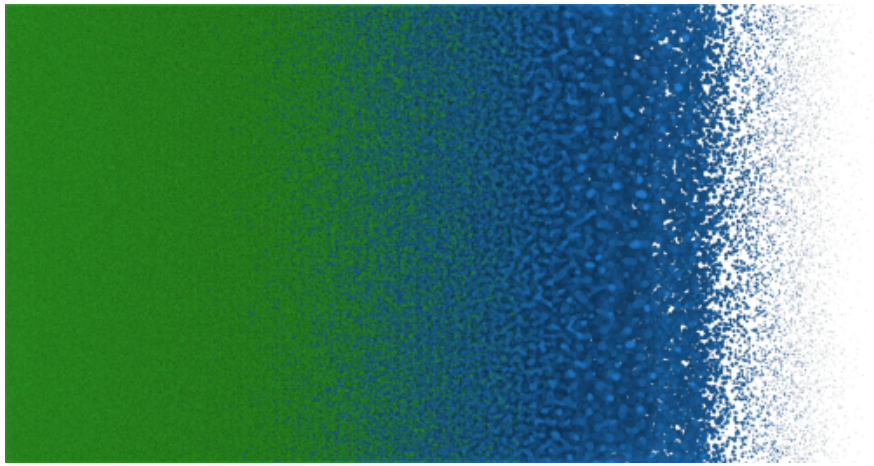
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

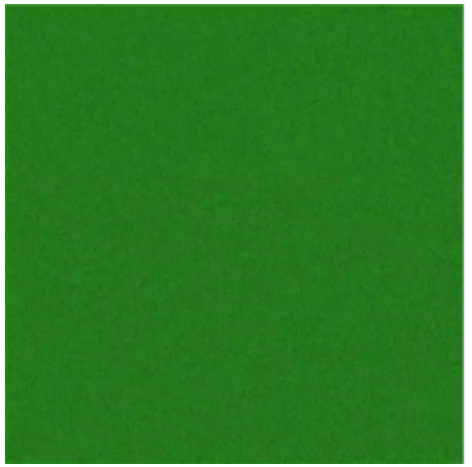
UNCLASSIFIED

# 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 (6 billion Lennard-Jones atoms) on 5760 GPUs (33% of LLNL Sierra) using LAMMPS/Kokkos software
- Improved visualization workflow, started preliminary simulations of aluminum using SNAP machine learning potential





## 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*