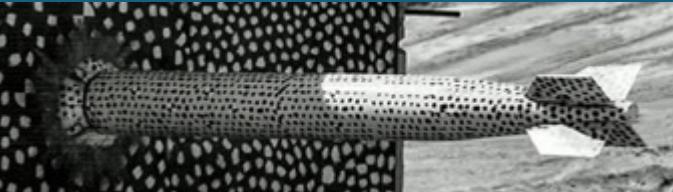
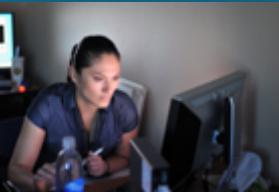




Sandia  
National  
Laboratories

SAND2021-3565R

# Large-Scale Atomistic Simulations



## PRESENTED BY

Principal Investigator/Lab: Stan Moore (SNL)

Platform/Campaign ID: Sierra/ATCC10-339

Code Name: LAMMPS

Program: ASC LSCI

Usage: 0.6 days

SNL R&A # (SAND, PR):



UNLIMITED RELEASE

UNCLASSIFIED

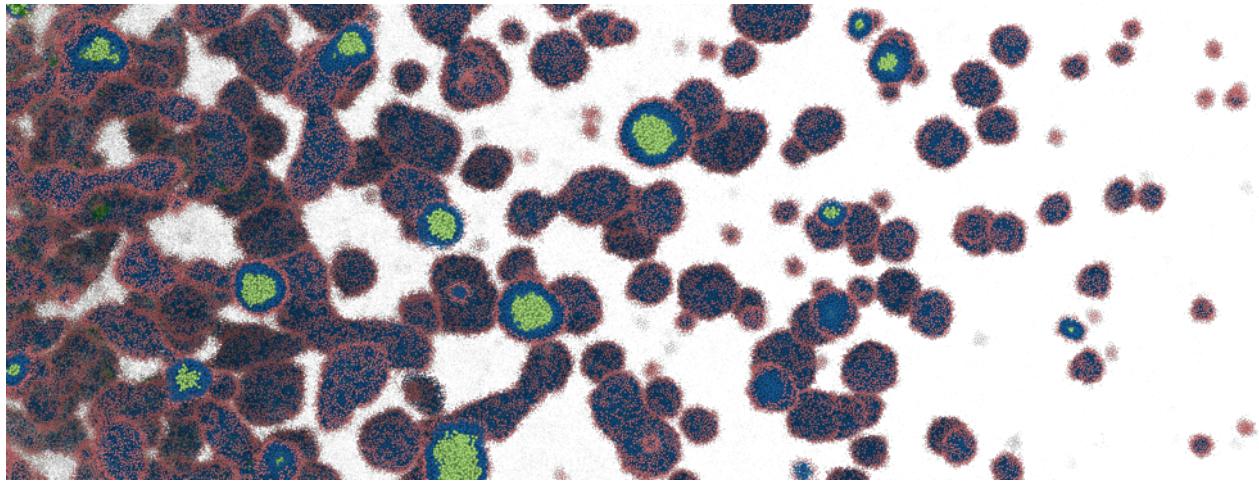
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# Large-Scale Atomistic Simulations: Investigating Free Expansion



## Background Description:

- Investigating free expansion of a supercritical fluid into two-phase liquid-vapor coexistence region
- Running 24 billion Lennard-Jones atoms in the LAMMPS/Kokkos software on 5760 GPUs (33% of LLNL Sierra)

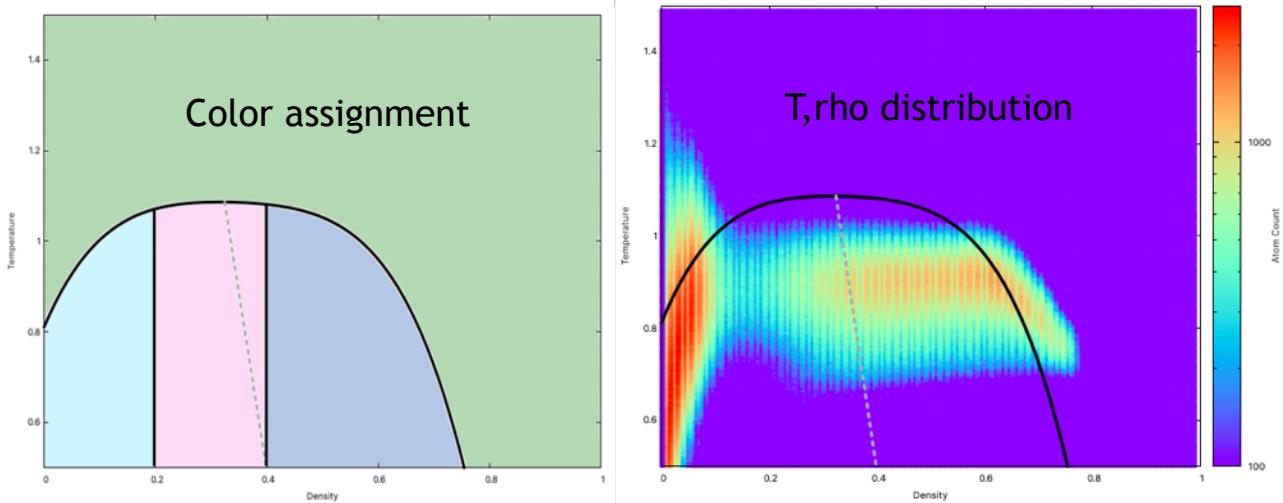


## Potential Consequences/Issues:

- Hydrocodes generally cannot model the 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



**Take Home Message:** Atomistic simulations can capture physics of free expansion into two-phase region