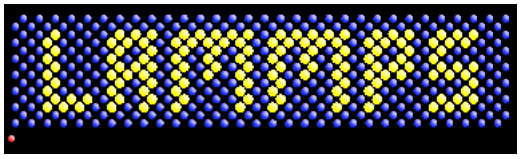
SCC22 LAMMPS Application Challenge

Changes allowed:



Changes that speed up the simulation without changing the numerical results output to the screen and/or log file. Allowed changes include:

- Number of MPI ranks
- MPI and thread affinity (binding tasks and threads to physical resources)
- Number of OpenMP threads per MPI rank
- Compiler optimization flags
- MPI library
- Version of compiler
- Version of CUDA and other TPLs
- GPU-aware flags
- CUDA MPS on/off
- Use of any LAMMPS accelerator package
- Any package option (see https://lammps.sandia.gov/doc/package.html), **with the condition that you must use double precision** (FP64)
- Atom sorting on/off
- Newton flag on/off
- Use of half or full neighbor list
- Can add load balancing
- LAMMPS “processors” command
- Multiple Kokkos backends (e.g. CUDA + OpenMP)
- Use of “kk/device” or “kk/host” suffix for any kernel to run on CPU or GPU

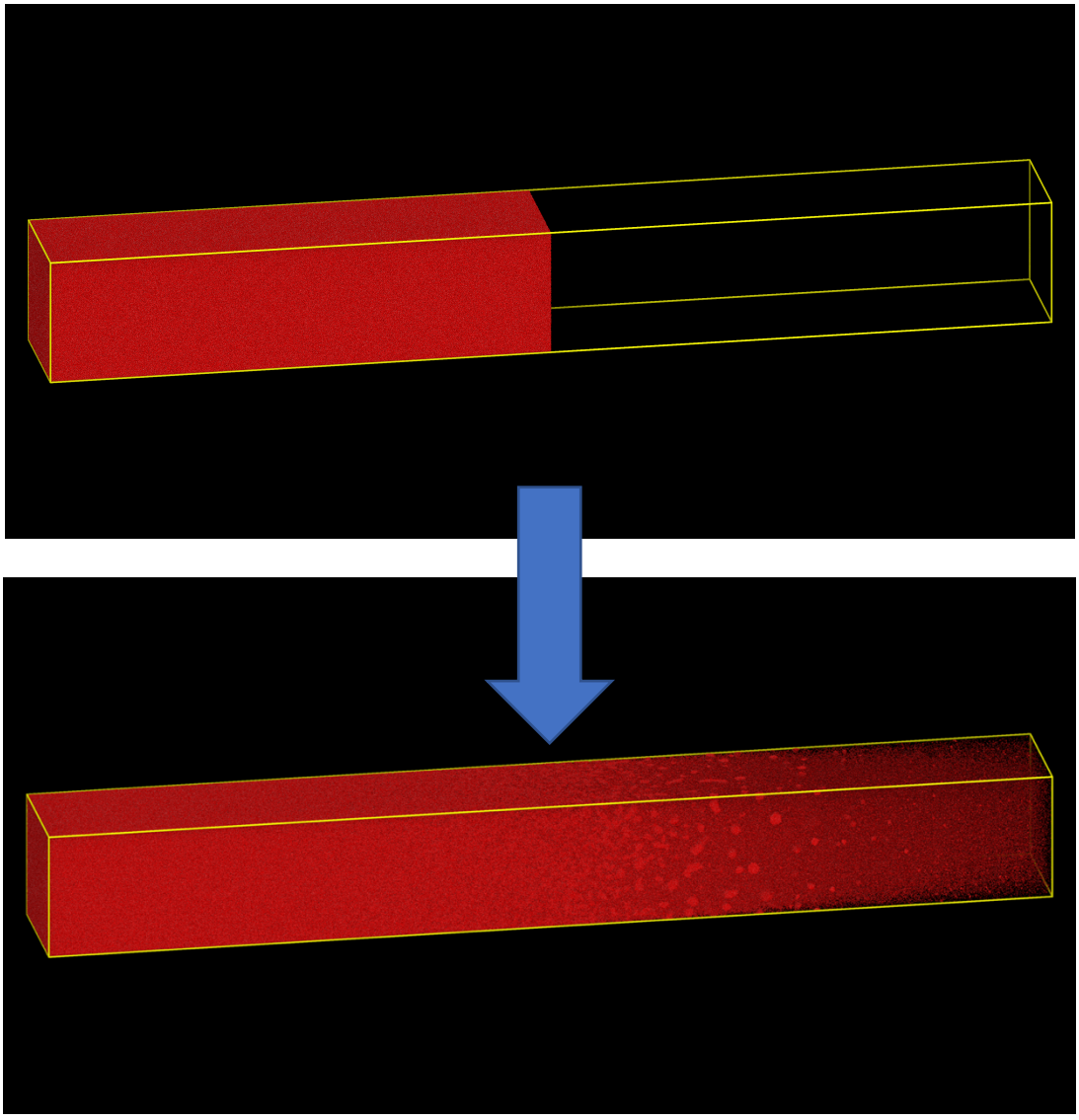
LAMMPS Changes NOT allowed

Anything that changes the numerical results output to the screen and/or log file is **not allowed**. Things not allowed include:

- **Do NOT use single or mixed precision: MUST use double precision (FP64)**
- Do NOT remove or modify any existing style in the input: pair, fix, etc.
- Timestep value
- Neighborlist parameters with neigh_modify command, except binsize
- Force cutoff distance

Task 1: Free expansion of supercritical fluid

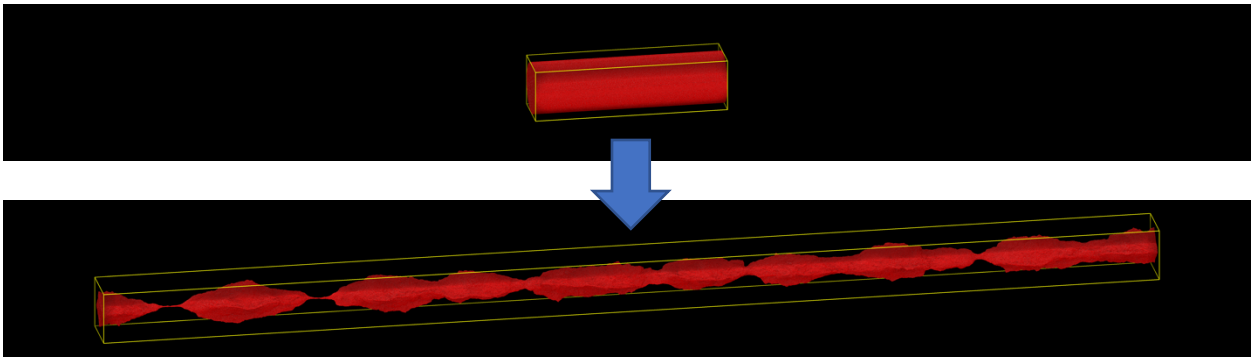
The Lennard-Jones (LJ) interatomic potential is a simple empirical model that still captures many relevant physics phenomena of materials. One can think of LJ as modeling a noble gas such as argon. In this simulation, supercritical LJ fluid is expanded into vacuum. Supercritical means the material is so hot that there is no longer a clear distinction between the liquid and vapor phases. However, when the supercritical fluid expands, the temperature drops below the critical temperature, and the fluid rapidly phase-separates into liquid droplets and vapor bubbles.



HINT: This problem has large density variations in the x-direction, so adding load balancing to the input may give significant speedup.

Task 2: Tensile test of copper nanowire

The embedded-atom-model (EAM) interatomic potential is more complex than the LJ potential and can model the behavior of metals such as copper. In this simulation, a copper nanowire is stretched to its breaking point.



Task 3: Visualization

Create a visualization image of both simulations, preferably at an interesting point in the simulation. This can be accomplished using the LAMMPS in-situ "dump_image" command (as shown above), OVITO, VMD, or other visualization software.

Summary of Scoring Breakdown:

100 total points:

- Interview: 50 points
- Free expansion simulation: 20 points
- Tensile test simulation: 20 points
- Visualizations: 10 points (5 points each)

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