16200 atoms

env OMP\_NUM\_THREADS=8 /usr/local/Cellar/lammps/20220623/bin/lmp\_mpi -sf omp -in \*.in

Loop time of 137.909 on 8 procs for 10000 steps with 16200 atoms

Performance: 6.265 ns/day, 3.831 hours/ns, 72.511 timesteps/s

648.1% CPU use with 1 MPI tasks x 8 OpenMP threads

mpirun -np 8 /usr/local/Cellar/lammps/20220623/bin/lmp\_mpi -in \*.in

Loop time of 144.099 on 8 procs for 10000 steps with 16200 atoms

Performance: 5.996 ns/day, 4.003 hours/ns, 69.397 timesteps/s

93.5% CPU use with 8 MPI tasks x 1 OpenMP threads