

LAMMPS

1. Running screenshot

```
perf stat numactl --interleave=all mpirun -x LD_LIBRARY_PATH
-np 16 --host head:8,work1:8 --map-by core --bind-to-core lmp
_mpi -in in.lj
LAMMPS (2 Aug 2023 - Update 3)
OMP_NUM_THREADS environment is not set. Defaulting to 1 thread. (src/comm.cpp:98)
  using 1 OpenMP thread(s) per MPI task
Lattice spacing in x,y,z = 1.6795962 1.6795962 1.6795962
Created orthogonal box = (0 0 0) to (33.591924 33.591924 33.591924)
  2 by 2 by 4 MPI processor grid
Created 32000 atoms
  using lattice units in orthogonal box = (0 0 0) to (33.591924 33.591924 33.591924)
  create_atoms CPU = 0.002 seconds
Generated 0 of 0 mixed pair_coeff terms from geometric mixing rule
Neighbor list info ...
  update: every = 20 steps, delay = 0 steps, check = no
  max neighbors/atom: 2000, page size: 100000
  master list distance cutoff = 2.6
  ghost atom cutoff = 2.6
  binsize = 1.3, bins = 26 26 26
  1 neighbor lists, perpetual/occasional/extra = 1 0 0
  (1) pair lj/cut, perpetual
    attributes: half, newton on
    pair build: half/bin/atomonly/newton
    stencil: half/bin/3d
    bin: standard
Setting up Verlet run ...
  Unit style      : lj
  Current step    : 0
  Time step       : 0.005
Per MPI rank memory allocation (min/avg/max) = 2.66 | 2.672 | 2.685 Mbytes

```

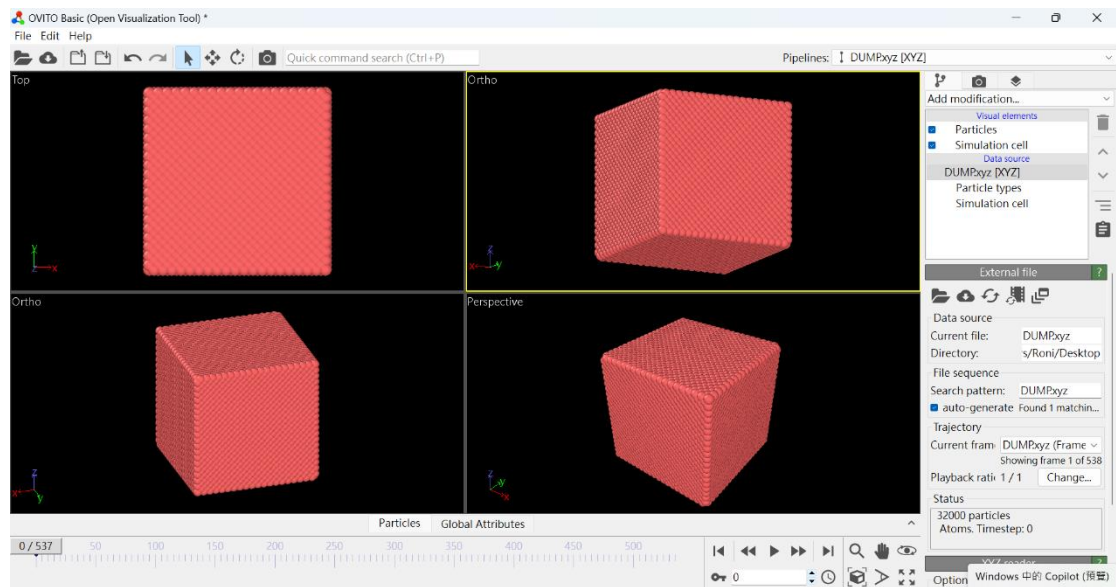
Step	Temp	E_pair	E_mol
TotEng	Press		
0	1.44	-6.7733681	0
134356	-5.0197073		-4.6
10000	0.60118887	-5.7726319	0
708768	0.1493339		-4.8

```
Loop time of 15.0218 on 16 procs for 10000 steps with 32000 atoms

Performance: 287581.752 tau/day, 665.699 timesteps/s, 21.302
Matom-step/s
80.3% CPU use with 16 MPI tasks x 1 OpenMP threads
```

2. Visualization screenshot of Lennard Jones Simulation

By OVITO :



Video link:

<https://youtu.be/OSYqPKcTKw0>

3. Additional notes for grading

Visualization of in.chain (polymer)

