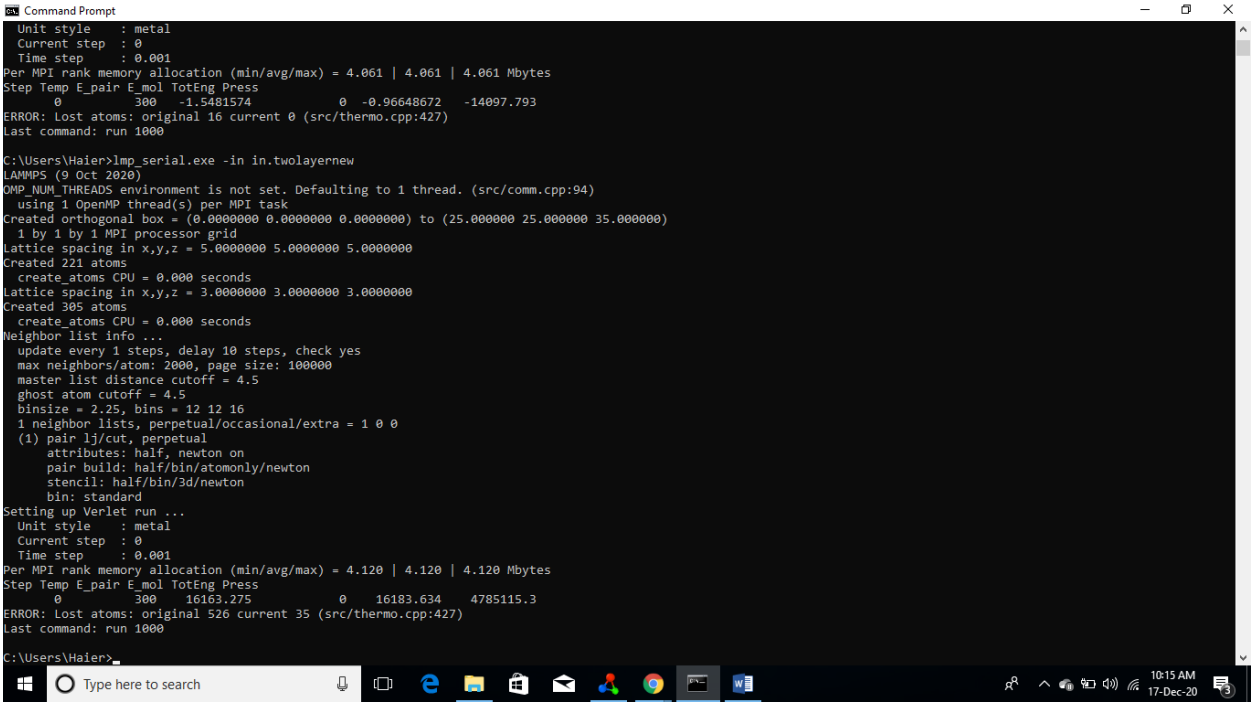
Command Prompt
Unit style : metal
Current step : 0
Time step : 0.001
Per MPI rank memory allocation (min/avg/max) = 4.061 | 4.061 | 4.061 Mbytes
Step Temp E_pair E_mol TotEng Press
0 300 -1.5481574 0 -0.96648672 -14097.793
ERROR: Lost atoms: original 16 current 0 (src/thermo.cpp:427)
Last command: run 1000
C:\Users\Haier>lmp_serial.exe -in in.twolayernew
LAMMPS (9 Oct 2020)
OMP_NUM_THREADS environment is not set. Defaulting to 1 thread. (src/comm.cpp:94)
using 1 OpenMP thread(s) per MPI task
Created orthogonal box = (0.0000000 0.0000000 0.0000000) to (25.000000 25.000000 35.000000)
1 by 1 by 1 MPI processor grid
Lattice spacing in x,y,z = 5.0000000 5.0000000 5.0000000
Created 221 atoms
create_atoms CPU = 0.000 seconds
Lattice spacing in x,y,z = 3.0000000 3.0000000 3.0000000
Created 305 atoms
create_atoms CPU = 0.000 seconds
Neighbor list info ...
update every 1 steps, delay 10 steps, check yes
max neighbors/atom: 2000, page size: 100000
master list distance cutoff = 4.5
ghost atom cutoff = 4.5
binsize = 2.25, bins = 12 12 16
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/newton
bin: standard
Setting up Verlet run ...
Unit style : metal
Current step : 0
Time step : 0.001
Per MPI rank memory allocation (min/avg/max) = 4.120 | 4.120 | 4.120 Mbytes
Step Temp E_pair E_mol TotEng Press
0 300 16163.275 0 16183.634 4785115.3
ERROR: Lost atoms: original 526 current 35 (src/thermo.cpp:427)
Last command: run 1000
C:\Users\Haier>
Type here to search
10:15 AM
17-Dec-20