

--- UNCLASSIFIED --- Fri Jan 12 15:17:51 PST 2018 --- UNCLASSIFIED ---

LAMMPS (23 Oct 2017)

using 8 OpenMP thread(s) per MPI task
using multi-threaded neighbor list subroutines
using multi-threaded neighbor list subroutines

Reading data file ...

triclinic box = (0 0 0) to (22.326 11.1412 13.779) with tilt (0 -5.02603 0)

128 by 64 by 96 MPI processor grid

reading atoms ...

304 atoms

reading velocities ...

304 velocities

Replicating atoms ...

triclinic box = (0 0 0) to (5715.46 2852.15 7936.68) with tilt (0 -2894.99 0)

WARNING: Triclinic box skew is large (./domain.cpp:197)

96 by 64 by 128 MPI processor grid

bounding box image = (0 -1 -1) to (0 1 1)

bounding box extra memory = 0.03 MB

average # of replicas added to proc = 140.68 out of 37748736 (0.00 %)

11475615744 atoms

Time spent = 48.1101 secs

Info-Info-Info-Info-Info-Info-Info-Info-Info-Info

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Total time information (MPI rank 0):

CPU time: 0:00:51

Wall time: 0:00:50

Info-Info-Info-Info-Info-Info-Info-Info-Info-Info

Last active /omp style is pair_style reax/c/omp

Neighbor list info ...

update every 10 steps, delay 0 steps, check no

max neighbors/atom: 2000, page size: 100000

master list distance cutoff = 11

ghost atom cutoff = 11

binsize = 5.5, bins = 1566 519 1444

2 neighbor lists, perpetual/occasional/extra = 2 0 0

(1) pair reax/c/omp, perpetual

attributes: half, newton off, ghost, omp

pair build: half/bin/newtoff/ghost/omp

stencil: half/ghost/bin/3d/newtoff

bin: standard

(2) fix qeq/reax/omp, perpetual, copy from (1)

attributes: half, newton off, ghost

pair build: copy

stencil: none

bin: none

Setting up Verlet run ...

Unit style : real

Current step : 0

Time step : 0.1

Per MPI rank memory allocation (min/avg/max) = 852.5 | 862.9 | 870.6 Mbytes

Step Temp PotEng Press E_vdwl E_coul Volume

0 300 -113.27833 439.0204 -111.57687 -1.7014647 1.2937845e+11

100 302.57604 -113.28529 10375.05 -111.58659 -1.6986952 1.2937845e+11

Loop time of 338.746 on 6291456 procs for 100 steps with 11475615744 atoms

Performance: 0.003 ns/day, 9409.622 hours/ns, 0.295 timesteps/s

100.0% CPU use with 786432 MPI tasks x 8 OpenMP threads

MPI task timing breakdown:

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Section	min time	avg time	max time	%varavg	%total
Pair	198.79	208.58	219.83	17.5	61.57
Neigh	9.8382	10.839	11.708	11.4	3.20
Comm	0.45483	6.8664	21.038	107.3	2.03
Output	0.00061423	0.065955	0.093445	4.9	0.02
Modify	106.84	112.39	114.96	12.3	33.18
Other		0.003563			0.00

Nlocal: 14592 ave 14742 max 14359 min
Histogram: 105391 88064 68689 0 0 0 148 167874 222249 134017
Nghost: 26299.6 ave 26590 max 25930 min
Histogram: 125120 11493 125516 15 0 29046 106306 200351 74474 114111
Neighs: 4.35631e+06 ave 4.39759e+06 max 4.28991e+06 min
Histogram: 98843 87027 76274 0 0 0 1 152879 192559 178849

Total # of neighbors = 3.42594e+12
Ave neighs/atom = 298.541
Neighbor list builds = 10
Dangerous builds not checked

Info-Info-Info-Info-Info-Info-Info-Info-Info-Info-Info-Info
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Total time information (MPI rank 0):
CPU time: 0:06:39
Wall time: 0:06:38

Info-Info-Info-Info-Info-Info-Info-Info-Info-Info-Info-Info

Info-Info-Info-Info-Info-Info-Info-Info-Info-Info-Info-Info
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Total time information (MPI rank 0):
CPU time: 0:06:39
Wall time: 0:06:38

Info-Info-Info-Info-Info-Info-Info-Info-Info-Info-Info-Info

Total wall time: 0:06:39
2018-01-12 12:14:30.478 (WARN) [0x400033b0250] 9108867:ibm.runjob.client.Job: 1195 INF
O RAS events
2018-01-12 12:14:30.480 (WARN) [0x400033b0250] 9108867:ibm.runjob.client.Job: 182 WARN
RAS events
2018-01-12 12:14:30.480 (WARN) [0x400033b0250] 9108867:ibm.runjob.client.Job: most rec
ent RAS event text: A BQL lane was spared.
2018-01-12 12:14:30.481 (WARN) [0x400033b0250] 9108867:ibm.runjob.client.Job: with sev
erity INFO

real 7m16.815s
user 0m0.250s
sys 0m0.098s

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#!/bin/bash

```
#MSUB -l partition=seq
#MSUB -l nodes=98304:ppn=16
#MSUB -q pall
#MSUB -l walltime=00:30:00
#MSUB -l advres=jan12-dat
#MSUB -l qos=exempt
#MSUB -o jobout.%j
#MSUB -N bench96K
#MSUB -A snlexec
#MSUB -j oe
```

```
export OMP_PLACES=threads
export OMP_PROC_BIND=true
export OMP_NUM_THREADS=8
```

NODES=98304

```
cd reax_benchmark
time srun -N ${NODES} --reservation=jan12-dat --tasks-per-node 8 ../src/lmp_bgq -sf omp
-pk omp 8 -v x 256 -v y 256 -v z 576 -v t 100 -in in.reaxc.hns -nocite -log log.reax.s
eq.96K
```

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