

## LAMPIRAN

```

File Edit Search View Format Encoding Syntax Special Tools
out.dat out.dat out.dat out.dat out.dat out.dat out.dat
15033 1499800 1314.4293 -55163.138 -57511.711 0.27490515 3.054909e-05 0.21298443 2.3668093e-05
15034 1499900 1320.5109 -55163.208 -57522.648 0.28853895 3.2062021e-05 0.20537059 2.2820476e-05
15035 1500000 1323.9291 -55163.275 -57528.822 0.30467005 3.3852228e-05 0.19849999 2.2055554e-05
15036 Loop time of 110392 on 5 procs for 1500000 steps with 13824 atoms
15037
15038 Performance: 1.174 ns/day, 20.443 hours/ns, 13.588 timesteps/s
15039 96.3% CPU use with 5 MPI tasks x no OpenMP threads
15040
15041 MPI task timing breakdown:
15042 Section | min time | avg time | max time |%varavg| %total
15043 -----|-----|-----|-----|-----|-----
15044 Pair | 81270 | 93161 | 1.0552e+05 | 3179.8 | 84.39
15045 Neigh | 147.56 | 222.03 | 279.81 | 402.8 | 0.20
15046 Comm | 4187.9 | 15330 | 26048 | 6779.7 | 13.89
15047 Output | 14.908 | 15.07 | 15.277 | 3.1 | 0.01
15048 Modify | 247.2 | 1528.7 | 5875.8 | 5597.7 | 1.38
15049 Other | | 135.7 | | | 0.12
15050
15051 Nlocal: 2764.80 ave 3404 max 1970 min
15052 Histogram: 2 0 0 0 0 0 0 1 2
15053 Nghost: 4328.80 ave 5862 max 2775 min
15054 Histogram: 2 0 0 0 0 0 2 0 1
15055 Neighs: 101431.0 ave 129796 max 62750 min
15056 Histogram: 1 1 0 0 0 0 1 0 2
15057 FullNghs: 202863.0 ave 256934 max 133930 min
15058 Histogram: 2 0 0 0 0 0 1 0 2
15059
15060 Total # of neighbors = 1014314
15061 Ave neighs/atom = 73.373409
15062 Neighbor list builds = 24900
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 30:39:52
15066

```

Lampiran 1 Data Log Temperatur 1223 K

```

File Edit Search View Format Encoding Syntax Special Tools
out.dat out.dat out.dat out.dat out.dat out.dat out.dat
15033 1499800 1314.4293 -55163.138 -57511.711 0.27490515 3.054909e-05 0.21298443 2.3668093e-05
15034 1499900 1320.5109 -55163.208 -57522.648 0.28853895 3.2062021e-05 0.20537059 2.2820476e-05
15035 1500000 1323.9291 -55163.275 -57528.822 0.30467005 3.3852228e-05 0.19849999 2.2055554e-05
15036 Loop time of 110392 on 5 procs for 1500000 steps with 13824 atoms
15037
15038 Performance: 1.174 ns/day, 20.443 hours/ns, 13.588 timesteps/s
15039 96.3% CPU use with 5 MPI tasks x no OpenMP threads
15040
15041 MPI task timing breakdown:
15042 Section | min time | avg time | max time |%varavg| %total
15043 -----|-----|-----|-----|-----|-----
15044 Pair | 81270 | 93161 | 1.0552e+05 | 3179.8 | 84.39
15045 Neigh | 147.56 | 222.03 | 279.81 | 402.8 | 0.20
15046 Comm | 4187.9 | 15330 | 26048 | 6779.7 | 13.89
15047 Output | 14.908 | 15.07 | 15.277 | 3.1 | 0.01
15048 Modify | 247.2 | 1528.7 | 5875.8 | 5597.7 | 1.38
15049 Other | | 135.7 | | | 0.12
15050
15051 Nlocal: 2764.80 ave 3404 max 1970 min
15052 Histogram: 2 0 0 0 0 0 0 1 2
15053 Nghost: 4328.80 ave 5862 max 2775 min
15054 Histogram: 2 0 0 0 0 0 2 0 1
15055 Neighs: 101431.0 ave 129796 max 62750 min
15056 Histogram: 1 1 0 0 0 0 1 0 2
15057 FullNghs: 202863.0 ave 256934 max 133930 min
15058 Histogram: 2 0 0 0 0 0 1 0 2
15059
15060 Total # of neighbors = 1014314
15061 Ave neighs/atom = 73.373409
15062 Neighbor list builds = 24900
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 30:39:52
15066

```

Lampiran 2 Data Log Temperatur 1323 K

```

File Edit Search View Format Encoding Syntax Special Tools
out.dat out.dat out.dat out.dat out.dat out.dat out
15033 1499800 1418.3799 -54801.703 -57336.012 0.09369042 1.0411435e-05 0.1722691 1.9143564e-05
15034 1499900 1422.5629 -54801.774 -57343.557 0.096696062 1.0744723e-05 0.17859537 1.9845253e-05
15035 1500000 1412.6494 -54801.818 -57325.887 0.10123243 1.1248048e-05 0.17934092 1.9926769e-05
15036 Loop time of 108891 on 5 procs for 1500000 steps with 13824 atoms
15037
15038 Performance: 1.190 ns/day, 20.165 hours/ns, 13.775 timesteps/s
15039 96.8% CPU use with 5 MPI tasks x no OpenMP threads
15040
15041 MPI task timing breakdown:
15042 Section | min time | avg time | max time |%varavg| %total
15043 -----|-----|-----|-----|-----|-----
15044 Pair | 80217 | 92095 | 1.0395e+05 | 3120.0 | 84.58
15045 Neigh | 157.98 | 233.6 | 292.94 | 400.7 | 0.21
15046 Comm | 4285.3 | 14956 | 24989 | 6692.1 | 13.73
15047 Output | 14.081 | 14.19 | 14.39 | 2.8 | 0.01
15048 Modify | 227 | 1469.5 | 5628.9 | 5460.3 | 1.35
15049 Other | | 122.2 | | | 0.11
15050
15051 Nlocal: 2764.80 ave 3444 max 1889 min
15052 Histogram: 2 0 0 0 0 0 0 1 2
15053 Nghost: 4341.20 ave 5820 max 2774 min
15054 Histogram: 2 0 0 0 0 0 2 0 1
15055 Neighs: 101801.0 ave 131771 max 59198 min
15056 Histogram: 1 1 0 0 0 0 0 1 0 2
15057 FullNghs: 203603.0 ave 261789 max 132818 min
15058 Histogram: 2 0 0 0 0 0 0 1 0 2
15059
15060 Total # of neighbors = 1018014
15061 Ave neighs/atom = 73.641059
15062 Neighbor list builds = 26386
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 30:14:51

```

### Lampiran 3 Data Log Temperatur 1423 K

```

File Edit Search View Format Encoding Syntax Special Tools
out.dat out.dat out.dat out.dat out.dat out.dat out
15033 1499800 1532.1563 -54400.215 -57137.815 0.10481162 1.1647289e-05 0.21037694 2.3378333e-05
15034 1499900 1520.1128 -54400.164 -57116.245 0.10096222 1.1218773e-05 0.19811364 2.2014094e-05
15035 1500000 1511.9418 -54400.101 -57101.583 0.099637275 1.1070808e-05 0.20292608 2.2547342e-05
15036 Loop time of 108950 on 5 procs for 1500000 steps with 13824 atoms
15037
15038 Performance: 1.190 ns/day, 20.176 hours/ns, 13.768 timesteps/s
15039 96.0% CPU use with 5 MPI tasks x no OpenMP threads
15040
15041 MPI task timing breakdown:
15042 Section | min time | avg time | max time |%varavg| %total
15043 -----|-----|-----|-----|-----|-----
15044 Pair | 80134 | 92032 | 1.0336e+05 | 3031.6 | 84.47
15045 Neigh | 169.75 | 247.37 | 310.78 | 402.9 | 0.23
15046 Comm | 4829.8 | 15055 | 24160 | 6468.1 | 13.82
15047 Output | 16.793 | 17.06 | 17.499 | 6.0 | 0.02
15048 Modify | 265.67 | 1448.3 | 5187.9 | 4975.1 | 1.33
15049 Other | | 150.1 | | | 0.14
15050
15051 Nlocal: 2764.80 ave 3435 max 1998 min
15052 Histogram: 2 0 0 0 0 0 0 2 1
15053 Nghost: 4335.00 ave 5912 max 2761 min
15054 Histogram: 2 0 0 0 0 0 2 0 1
15055 Neighs: 101002.0 ave 131051 max 63339 min
15056 Histogram: 1 1 0 0 0 0 0 1 0 2
15057 FullNghs: 202004.0 ave 259909 max 131531 min
15058 Histogram: 2 0 0 0 0 0 0 1 0 2
15059
15060 Total # of neighbors = 1010018
15061 Ave neighs/atom = 73.062645
15062 Neighbor list builds = 27836
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 30:15:49

```

### Lampiran 4 Data Log Temperatur 1523 K



```

MobaTextEditor
File Edit Search View Format Encoding Syntax Special Tools
out.dat
15033 1499800 1664.2362 -53491.071 -56429.817 356.81409 0.039651297 395.90623 0.043995448
15034 1499900 1666.0701 -53491.276 -56433.26 356.63335 0.03962857 396.2311 0.044028613
15035 1500000 1665.5285 -53491.456 -56432.484 356.70537 0.03963393 396.38528 0.044042809
15036 Loop time of 112041 on 5 procs for 1500000 steps with 13662 atoms
15037
15038 Performance: 1.157 ns/day, 20.748 hours/ns, 13.388 timesteps/s
15039 96.4% CPU use with 5 MPI tasks x no OpenMP threads
15040
15041 MPI task timing breakdown:
15042 Section | min time | avg time | max time | %varavg | %total
15043 -----|-----|-----|-----|-----|-----
15044 Pair | 78668 | 92853 | 1.0769e+05 | 3654.0 | 82.87
15045 Neigh | 147.83 | 266.33 | 355.64 | 569.1 | 0.24
15046 Comm | 3597.5 | 16835 | 29007 | 7224.9 | 15.03
15047 Output | 14.195 | 14.284 | 14.491 | 2.8 | 0.01
15048 Modify | 237.99 | 1933 | 7872.8 | 6786.7 | 1.73
15049 Other | | 139.3 | | | 0.12
15050
15051 Nlocal: 2732.40 ave 3517 max 1691 min
15052 Histogram: 2 0 0 0 0 0 0 1 2
15053 Nghost: 4096.60 ave 5190 max 2544 min
15054 Histogram: 2 0 0 0 0 0 0 0 3
15055 Neighs: 95184.2 ave 132834 max 50982 min
15056 Histogram: 2 0 0 0 0 0 0 1 1
15057 FullNghs: 190368.0 ave 265947 max 101499 min
15058 Histogram: 2 0 0 0 0 0 0 1 1
15059
15060 Total # of neighbors = 951842
15061 Ave neighs/atom = 69.670766
15062 Neighbor list builds = 30270
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 31:07:21
15066

```

### Lampiran 5 Data Log Temperatur 1670 K

```

File Edit Search View Format Encoding Syntax Special Tools
out.dat out.dat
15033 1499800 1722.6351 -53387.239 -56429.107 514.84612 0.057212753 564.23875 0.062701554
15034 1499900 1713.1122 -53387.105 -56412.157 514.93806 0.057219154 564.09316 0.062681197
15035 1500000 1719.5318 -53386.98 -56423.369 515.2205 0.057246722 563.79933 0.06264437
15036 Loop time of 108782 on 5 procs for 1500000 steps with 13662 atoms
15037
15038 Performance: 1.191 ns/day, 20.145 hours/ns, 13.789 timesteps/s
15039 96.5% CPU use with 5 MPI tasks x no OpenMP threads
15040
15041 MPI task timing breakdown:
15042 Section | min time | avg time | max time | %varavg | %total
15043 -----|-----|-----|-----|-----|-----
15044 Pair | 76898 | 90522 | 1.0415e+05 | 3529.8 | 83.21
15045 Neigh | 151.77 | 269.39 | 357.63 | 567.1 | 0.25
15046 Comm | 3886.9 | 16084 | 27649 | 7103.8 | 14.79
15047 Output | 14.75 | 14.886 | 15.213 | 4.4 | 0.01
15048 Modify | 239.65 | 1757.3 | 6915.9 | 6199.6 | 1.62
15049 Other | | 134.2 | | | 0.12
15050
15051 Nlocal: 2732.40 ave 3497 max 1694 min
15052 Histogram: 2 0 0 0 0 0 0 1 2
15053 Nghost: 4198.60 ave 5351 max 2484 min
15054 Histogram: 1 1 0 0 0 0 0 0 3
15055 Neighs: 94968.4 ave 130695 max 50610 min
15056 Histogram: 2 0 0 0 0 0 0 1 0 2
15057 FullNghs: 189937.0 ave 261227 max 101492 min
15058 Histogram: 2 0 0 0 0 0 0 1 0 2
15059
15060 Total # of neighbors = 949684
15061 Ave neighs/atom = 69.512809
15062 Neighbor list builds = 30857
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 30:13:02
15066

```

### Lampiran 6 Data Log Temperatur 1710 K

```

File Edit Search View Format Encoding Syntax Special Tools
out.dat out.dat out.dat
15033 1499800 1749.4195 -53400.017 -56489.182 681.57753 0.075740936 800.24528 0.088928
15034 1499900 1756.0367 -53400.119 -56500.969 681.36603 0.075712384 799.1036 0.088795208
15035 1500000 1752.9971 -53400.191 -56495.673 680.50721 0.075611913 799.56089 0.088840099
15036 Loop time of 111488 on 5 procs for 1500000 steps with 13662 atoms
15037
15038 Performance: 1.162 ns/day, 20.646 hours/ns, 13.454 timesteps/s
15039 95.5% CPU use with 5 MPI tasks x no OpenMP threads
15040
15041 MPI task timing breakdown:
15042 Section | min time | avg time | max time |%varavg| %total
15043 -----|-----|-----|-----|-----|-----
15044 Pair | 78233 | 92421 | 1.0666e+05 | 3622.7 | 82.90
15045 Neigh | 156.18 | 279.34 | 368.72 | 581.9 | 0.25
15046 Comm | 3991.3 | 16688 | 28740 | 7191.4 | 14.97
15047 Output | 17.396 | 17.653 | 18.004 | 5.5 | 0.02
15048 Modify | 286.15 | 1910.8 | 7423.4 | 6351.8 | 1.71
15049 Other | | 171.5 | | | 0.15
15050
15051 Nlocal: 2732.40 ave 3537 max 1676 min
15052 Histogram: 2 0 0 0 0 0 0 1 2
15053 Nghost: 4167.80 ave 5202 max 2563 min
15054 Histogram: 1 1 0 0 0 0 0 0 3
15055 Neighs: 94957.4 ave 131224 max 50553 min
15056 Histogram: 2 0 0 0 0 0 0 2 1
15057 FullNghs: 189915.0 ave 262190 max 99947 min
15058 Histogram: 2 0 0 0 0 0 0 2 1
15059
15060 Total # of neighbors = 949574
15061 Ave neighs/atom = 69.504758
15062 Neighbor list builds = 31398
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 30:58:08
15066

```

### Lampiran 7 Data Log Temperatur 1750 K

```

File Edit Search View Format Encoding Syntax Special Tools
out.dat out.dat out.dat out.dat
15033 1499800 1788.3425 -53271.882 -56429.779 847.0715 0.094131607 982.21809 0.1091499
15034 1499900 1775.6322 -53271.306 -56406.758 846.5445 0.094066771 982.68121 0.10919408
15035 1500000 1779.8636 -53270.749 -56413.672 847.18501 0.094131667 982.73996 0.10919333
15036 Loop time of 110830 on 5 procs for 1500000 steps with 13662 atoms
15037
15038 Performance: 1.169 ns/day, 20.524 hours/ns, 13.534 timesteps/s
15039 95.6% CPU use with 5 MPI tasks x no OpenMP threads
15040
15041 MPI task timing breakdown:
15042 Section | min time | avg time | max time |%varavg| %total
15043 -----|-----|-----|-----|-----|-----
15044 Pair | 77705 | 91917 | 1.0601e+05 | 3623.2 | 82.94
15045 Neigh | 159.41 | 284.07 | 376.13 | 584.3 | 0.26
15046 Comm | 3982.6 | 16563 | 28545 | 7205.1 | 14.94
15047 Output | 16.643 | 16.785 | 16.894 | 2.8 | 0.02
15048 Modify | 280.88 | 1885.6 | 7281.4 | 6265.3 | 1.70
15049 Other | | 162.9 | | | 0.15
15050
15051 Nlocal: 2732.40 ave 3543 max 1677 min
15052 Histogram: 2 0 0 0 0 0 0 1 2
15053 Nghost: 4214.40 ave 5256 max 2565 min
15054 Histogram: 1 1 0 0 0 0 0 0 3
15055 Neighs: 94632.4 ave 130348 max 50197 min
15056 Histogram: 2 0 0 0 0 0 0 2 1
15057 FullNghs: 189265.0 ave 260498 max 99481 min
15058 Histogram: 2 0 0 0 0 0 0 2 1
15059
15060 Total # of neighbors = 946324
15061 Ave neighs/atom = 69.266872
15062 Neighbor list builds = 31884
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 30:47:10
15066

```

### Lampiran 8 Data Log Temperatur 1790 K



```

File Edit Search View Format Encoding Syntax Special Tools
out.dat out.dat out.dat out.dat out.dat
15033 1499800 1815.7741 -53157.625 -56363.961 983.69504 0.10931402 1161.8423 0.12911081
15034 1499900 1805.1301 -53157.786 -56345.326 984.17967 0.10936059 1160.7979 0.12898614
15035 1500000 1809.4802 -53158.019 -56353.241 983.58011 0.10928668 1160.3971 0.12893301
15036 Loop time of 107968 on 5 procs for 1500000 steps with 13662 atoms
15037
15038 Performance: 1.200 ns/day, 19.994 hours/ns, 13.893 timesteps/s
15039 96.3% CPU use with 5 MPI tasks x no OpenMP threads
15040
15041 MPI task timing breakdown:
15042 Section | min time | avg time | max time |%varavg| %total
15043 -----|-----|-----|-----|-----|-----
15044 Pair | 76035 | 89928 | 1.037e+05 | 3585.6 | 83.29
15045 Neigh | 157.05 | 283.11 | 378.01 | 585.5 | 0.26
15046 Comm | 3467.1 | 15828 | 27682 | 7263.6 | 14.66
15047 Output | 16.05 | 16.458 | 16.935 | 8.0 | 0.02
15048 Modify | 257.69 | 1768.6 | 6961 | 6214.0 | 1.64
15049 Other | | 144 | | | 0.13
15050
15051 Nlocal: 2732.40 ave 3515 max 1687 min
15052 Histogram: 2 0 0 0 0 0 0 1 2
15053 Nghost: 4152.00 ave 5175 max 2522 min
15054 Histogram: 1 1 0 0 0 0 0 0 3
15055 Neighs: 94414.8 ave 128699 max 51157 min
15056 Histogram: 2 0 0 0 0 0 0 2 1
15057 FullNghs: 188830.0 ave 256911 max 100820 min
15058 Histogram: 2 0 0 0 0 0 0 1 2
15059
15060 Total # of neighbors = 944148
15061 Ave neighs/atom = 69.107598
15062 Neighbor list builds = 32166
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 29:59:28
15066

```

### Lampiran 9 Data Log Temperatur 1811 K

```

File Edit Search View Format Encoding Syntax Special Tools
out.dat out.dat out.dat out.dat out.dat out.dat out.dat
15034 1499900 1847.6535 -53201.67 -56464.299 1132.4373 0.12583476 1376.8918 0.15299818
15035 1500000 1856.1244 -53202.094 -56479.681 1132.3674 0.1258186 1378.5977 0.15317752
15036 Loop time of 108712 on 5 procs for 1500000 steps with 13662 atoms
15037
15038 Performance: 1.192 ns/day, 20.132 hours/ns, 13.798 timesteps/s
15039 95.8% CPU use with 5 MPI tasks x no OpenMP threads
15040
15041 MPI task timing breakdown:
15042 Section | min time | avg time | max time |%varavg| %total
15043 -----|-----|-----|-----|-----|-----
15044 Pair | 76675 | 90449 | 1.0384e+05 | 3491.7 | 83.20
15045 Neigh | 164.1 | 291.86 | 387.06 | 582.4 | 0.27
15046 Comm | 4041.1 | 15951 | 27192 | 6961.5 | 14.67
15047 Output | 17.983 | 18.156 | 18.44 | 3.9 | 0.02
15048 Modify | 270.24 | 1847.8 | 7034.1 | 6100.6 | 1.70
15049 Other | | 153.6 | | | 0.14
15050
15051 Nlocal: 2732.40 ave 3438 max 1690 min
15052 Histogram: 2 0 0 0 0 0 0 0 3
15053 Nghost: 4161.00 ave 5289 max 2489 min
15054 Histogram: 1 1 0 0 0 0 0 0 3
15055 Neighs: 94351.8 ave 124537 max 53072 min
15056 Histogram: 2 0 0 0 0 0 0 1 2
15057 FullNghs: 188704.0 ave 248188 max 103439 min
15058 Histogram: 1 1 0 0 0 0 0 0 1 2
15059
15060 Total # of neighbors = 943518
15061 Ave neighs/atom = 69.061484
15062 Neighbor list builds = 32709
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 30:11:51

```

### Lampiran 10 Data Log Temperatur 1851 K

```

File Edit Search View Format Encoding Syntax Special Tools
out.dat out.dat out.dat out.dat out.dat out.dat out.dat
15033 1499800 1900.2379 -53207.876 -56563.359 1472.1097 0.16358956 1810.0625 0.20114488
15034 1499900 1884.8594 -53208.215 -56536.543 1472.9563 0.16367272 1810.2689 0.2011544
15035 1500000 1893.1809 -53208.591 -56551.613 1472.9298 0.16365886 1808.9918 0.20099909
15036 Loop time of 107014 on 5 procs for 1500000 steps with 13662 atoms
15037
15038 Performance: 1.211 ns/day, 19.817 hours/ns, 14.017 timesteps/s
15039 96.4% CPU use with 5 MPI tasks x no OpenMP threads
15040
15041 MPI task timing breakdown:
15042 Section | min time | avg time | max time |%varavg| %total
15043 -----|-----|-----|-----|-----|-----
15044 Pair | 75856 | 89372 | 1.0193e+05 | 3393.0 | 83.51
15045 Neigh | 168.84 | 296.38 | 384.52 | 565.6 | 0.28
15046 Comm | 4270.8 | 15466 | 26026 | 6856.4 | 14.45
15047 Output | 15.764 | 15.843 | 15.928 | 1.7 | 0.01
15048 Modify | 262.76 | 1719.9 | 6375.8 | 5702.5 | 1.61
15049 Other | | 144.5 | | | 0.14
15050
15051 Nlocal: 2732.40 ave 3404 max 1655 min
15052 Histogram: 1 1 0 0 0 0 0 0 3
15053 Nghost: 4146.60 ave 5204 max 2509 min
15054 Histogram: 2 0 0 0 0 0 0 0 3
15055 Neighs: 94291.4 ave 121686 max 53654 min
15056 Histogram: 2 0 0 0 0 0 0 0 3
15057 FullNghs: 188583.0 ave 243268 max 103019 min
15058 Histogram: 1 1 0 0 0 0 0 0 3
15059
15060 Total # of neighbors = 942914
15061 Ave neighs/atom = 69.017274
15062 Neighbor list builds = 33250
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 29:43:34

```

### Lampiran 11 Data Log Temperatur 1891 K

```

File Edit Search View Format Encoding Syntax Special Tools
out.dat out.dat out.dat out.dat out.dat out.dat out.dat
15033 1499800 1939.8409 -53096.506 -56521.921 1859.2393 0.20660969 2003.3386 0.22262286
15034 1499900 1943.2266 -53096.825 -56528.219 1856.7843 0.20632312 2004.3249 0.22271762
15035 1500000 1933.8685 -53097.131 -56512 1857.5971 0.20639968 2003.5557 0.2226173
15036 Loop time of 104375 on 5 procs for 1500000 steps with 13662 atoms
15037
15038 Performance: 1.242 ns/day, 19.329 hours/ns, 14.371 timesteps/s
15039 96.6% CPU use with 5 MPI tasks x no OpenMP threads
15040
15041 MPI task timing breakdown:
15042 Section | min time | avg time | max time |%varavg| %total
15043 -----|-----|-----|-----|-----|-----
15044 Pair | 74533 | 87601 | 98935 | 3253.3 | 83.93
15045 Neigh | 170.79 | 297.08 | 381.73 | 548.1 | 0.28
15046 Comm | 4678.1 | 14771 | 24483 | 6687.2 | 14.15
15047 Output | 16.498 | 16.722 | 17.04 | 4.4 | 0.02
15048 Modify | 236.24 | 1563.8 | 5545.2 | 5170.5 | 1.50
15049 Other | | 125.3 | | | 0.12
15050
15051 Nlocal: 2732.40 ave 3398 max 1675 min
15052 Histogram: 1 1 0 0 0 0 0 0 3
15053 Nghost: 4122.40 ave 5173 max 2499 min
15054 Histogram: 2 0 0 0 0 0 0 0 3
15055 Neighs: 94018.8 ave 121214 max 54349 min
15056 Histogram: 2 0 0 0 0 0 0 0 3
15057 FullNghs: 188038.0 ave 242534 max 103817 min
15058 Histogram: 1 1 0 0 0 0 0 0 3
15059
15060 Total # of neighbors = 940188
15061 Ave neighs/atom = 68.817743
15062 Neighbor list builds = 33760
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 28:59:35

```

### Lampiran 12 Data Log Temperatur 1931 K