

## LAMPIRAN

```
MobaTextEditor
File Edit Search View Format Encoding Syntax Special Tools
out.dat
15032 1499700 1664.1217 -53823.373 -56727.07 1.6686792 0.00018544588 1.6141314 0.00017938382
15033 1499800 1656.6487 -53823.595 -56714.253 1.7236166 0.0001915385 1.5718494 0.00017467322
15034 1499900 1670.6624 -53823.833 -56738.943 1.7828162 0.00018921441 1.6388201 0.00018210326
15035 1500000 1663.8876 -53824.065 -56727.354 1.6704333 0.0001856037 1.6088794 0.00018676437
15036 Loop time of 52350 on 14 procs for 1500000 steps with 13500 atoms
15037
15038 Performance: 2.476 ns/day, 0.694 hours/ns, 28.653 timesteps/s
15039 95.3% CPU use with 14 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 | 32617 | 43521 | 47726 | 2973.2 | 83.14
15045 Neigh | 49.767 | 100.02 | 222.5 | 536.9 | 0.31
15046 Comm | 2795.0 | 6594.3 | 16287 | 6724.7 | 12.60
15047 Output | 14.597 | 14.834 | 15.857 | 7.6 | 0.03
15048 Modify | 1026 | 1905.9 | 3225.7 | 2009.4 | 3.64
15049 Other | | 153.8 | | | 0.29
15050
15051 Mlocal: 964.286 ave 1222 max 387 min
15052 Histogram: 4 0 0 0 0 0 0 10
15053 Nghost: 2447.00 ave 2981 max 1259 min
15054 Histogram: 4 0 0 0 0 0 0 10
15055 Neighs: 31398.7 ave 40956 max 7167 min
15056 Histogram: 2 1 1 0 0 0 0 10
15057 FullNghs: 62797.4 ave 81093 max 19979 min
15058 Histogram: 4 0 0 0 0 0 0 10
15059
15060 Total # of neighbors = 879164
15061 Ave neighs/atom = 65.123259
15062 Neighbor list builds = 30481
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 14:32:30
15066
```

### Lampiran 1 Data Log Temperatur 1670K Fe (001) - Fe (001)

```
MobaTextEditor
File Edit Search View Format Encoding Syntax Special Tools
out.dat
1 LAMMPS (29 Sep 2021 - Update 1)
2 Reading data file .. (0.000000 0.000000 -10.000000) to (44.100000 44.100000 98.200000)
3 orthogonal box = (0.000000 0.000000 -10.000000) to (44.100000 44.100000 98.200000)
4 1 by 2 by 7 MPI processor grid
5 reading atoms ...
6 13500 atoms
7 read_data CPU = 0.017 seconds
8 900 atoms in group Fe1diff
9 5850 atoms in group Fe1base
10 900 atoms in group Fe2diff
11 5850 atoms in group Fe2base
12 Neighbor list info ...
13 update every 1 steps, delay 10 steps, check yes
14 max neighbors/atom: 2000, page size: 100000
15 master list distance cutoff = 6
16 ghost atom cutoff = 6
17 binsize = 3, bins = 15 15 37
18 2 neighbor lists, perpetual/occasional/extra = 2 0 0
19 (1) pair: meam/c, perpetual
20 attributes: full, newton on
21 pair build: full/bin/atomonly
22 stencil: full/bin/3d
23 bin: standard
24 (2) pair: meam/c, perpetual, half/full from (1)
25 attributes: half, newton on
26 pair build: half/full/newton
27 stencil: none
28 bin: none
29 Setting up Verlet run ...
30 Unit style : metal
31 Current step : 0
32 Time step : 0.001
33 Per MPI rank memory allocation (min/avg/max) = 11.71 | 12.25 | 12.55 Mbytes
34 Step Temp TotEng PotEng c_msd_Fe1[4] v_twopoint_Fe1 c_msd_Fe2[4] v_twopoint_Fe2
35 0 1973 -55380.628 -58823.281 8.6964026e-27 1.4494004e-21 3.6603146e-28 6.1005243e-23
36 100 058.25355 -55379.787 -56877.339 0.14979947 0.24966329 0.16006516 0.2667726
```

### Lampiran 2 Data Log Temperatur 1973K Fe (001) - Fe (001)

```

MobaTextEditor
File Edit Search View Format Encoding Syntax Special Tools
out.dat
15032 1499700 2282.5541 -49445.584 -53288.782 1504.5636 0.16720718 1459.9912 0.16225369
15033 1499800 2179.2826 -49445.808 -53248.261 1504.8736 0.16723048 1459.2427 0.1621597
15034 1499900 2198.6491 -49446.059 -53282.444 1504.5771 0.16718637 1461.4356 0.16239256
15035 1500000 2211.8829 -49446.299 -53305.775 1504.8166 0.16720185 1461.314 0.16236822
15036 Loop time of 22199.2 on 14 procs for 1500000 steps with 13500 atoms
15037
15038 Performance: 5.840 ns/day, 4.109 hours/ns, 67.597 timesteps/s
15039 99.2% CPU use with 14 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 | 15853 | 19517 | 20911 | 1449.5 | 87.95
15045 Neigh | 52.566 | 104.58 | 126 | 311.9 | 0.47
15046 Comm | 797.91 | 2005.7 | 5310.6 | 4817.0 | 9.04
15047 Output | 4.719 | 4.7475 | 5.0189 | 3.5 | 0.02
15048 Modify | 255.1 | 539.14 | 949.21 | 1211.1 | 2.43
15049 Other | | 19.16 | | | 0.09
15050
15051 Nlocal: 964.286 ave 1121 max 568 min
15052 Histogram: 3 1 0 0 0 0 0 0 10
15053 Nghost: 2385.57 ave 2798 max 1392 min
15054 Histogram: 4 0 0 0 0 0 0 0 10
15055 Neighs: 30186.5 ave 36119 max 12908 min
15056 Histogram: 2 0 1 1 0 0 0 0 10
15057 FullNghs: 60373.0 ave 72275 max 31083 min
15058 Histogram: 4 0 0 0 0 0 0 0 10
15059
15060 Total # of neighbors = 845222
15061 Ave neighs/atom = 62.609037
15062 Neighbor list builds = 36593
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 6:09:50
15066

```

### Lampiran 3 Data Log Temperatur 2173K Fe (001) - Fe (001)

```

MobaTextEditor
File Edit Search View Format Encoding Syntax Special Tools
out.dat
15032 1499700 2368.1853 -48465.799 -52598.004 2347.7684 0.26091534 2424.87 0.2694839
15033 1499800 2381.2262 -48465.48 -52620.441 2347.2285 0.26083706 2424.6853 0.26944541
15034 1499900 2354.4935 -48465.147 -52573.462 2348.2659 0.26093582 2424.4724 0.26940378
15035 1500000 2359.3767 -48464.801 -52581.637 2347.3109 0.26081232 2426.8006 0.26964451
15036 Loop time of 21397.1 on 14 procs for 1500000 steps with 13500 atoms
15037
15038 Performance: 6.057 ns/day, 3.962 hours/ns, 70.103 timesteps/s
15039 99.2% CPU use with 14 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 | 15751 | 19053 | 20236 | 1312.0 | 89.04
15045 Neigh | 60.097 | 110.41 | 130.9 | 291.1 | 0.52
15046 Comm | 664.36 | 1772 | 4826.4 | 3914.7 | 8.28
15047 Output | 4.8024 | 4.8251 | 5.0724 | 3.1 | 0.02
15048 Modify | 225.06 | 439.24 | 765.16 | 1013.2 | 2.95
15049 Other | | 18.09 | | | 0.08
15050
15051 Nlocal: 964.286 ave 1113 max 611 min
15052 Histogram: 3 1 0 0 0 0 0 0 10
15053 Nghost: 2372.43 ave 2767 max 1435 min
15054 Histogram: 4 0 0 0 0 0 0 0 10
15055 Neighs: 29949.9 ave 35730 max 14264 min
15056 Histogram: 2 0 1 1 0 0 0 0 10
15057 FullNghs: 59899.7 ave 71357 max 33666 min
15058 Histogram: 4 0 0 0 0 0 0 0 10
15059
15060 Total # of neighbors = 838596
15061 Ave neighs/atom = 62.118222
15062 Neighbor list builds = 38586
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 5:56:37
15066

```

### Lampiran 4 Data Log Temperatur 2373K Fe (001) - Fe (001)

```

MobaTextEditor
File Edit Search View Format Encoding Syntax Special Tools
out.dat
15032 1499700 2591.2192 -47305.33 -51826.688 3318.6787 0.36881584 3293.4795 0.36601537
15033 1499800 2571.6496 -47305.119 -51792.346 3317.4535 0.3686551 3296.1876 0.3662919
15034 1499900 2575.412 -47304.937 -51798.729 3318.2284 0.36871662 3293.954 0.36601929
15035 1500000 2588.8 -47304.746 -51821.898 3317.9616 0.3686624 3293.8798 0.36598664
15036 Loop time of 20799.5 on 14 procs for 150000 steps with 13500 atoms
15037
15038 Performance: 6.231 ns/day, 3.852 hours/ns, 72.117 timesteps/s
15039 99.3% CPU use with 14 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 | 15589 | 18598 | 19718 | 1193.0 | 89.42
15045 Neigh | 67.36 | 114.44 | 133.41 | 266.6 | 0.55
15046 Comm | 629.56 | 1643.4 | 4386.9 | 3601.7 | 7.90
15047 Output | 4.9251 | 4.9505 | 5.2 | 3.1 | 0.02
15048 Modify | 205.19 | 421.61 | 734.46 | 1836.0 | 2.03
15049 Other | | 16.79 | | | 0.08
15050
15051 Nlocal: 964.286 ave 1094 max 655 min
15052 Histogram: 3 1 0 0 0 0 0 0 10
15053 Nghost: 2361.29 ave 2782 max 1557 min
15054 Histogram: 4 0 0 0 0 0 0 10
15055 Neighs: 29504.3 ave 34342 max 15468 min
15056 Histogram: 2 0 2 0 0 0 0 10
15057 FullNghs: 59008.6 ave 68677 max 35935 min
15058 Histogram: 4 0 0 0 0 0 0 10
15059
15060 Total # of neighbors = 826120
15061 Ave neighs/atom = 61.194074
15062 Neighbor list builds = 40411
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 5:46:39
15066

```

### Lampiran 5 Data Log Temperatur 2573K Fe (001) - Fe (001)

```

MobaTextEditor
File Edit Search View Format Encoding Syntax Special Tools
out.dat
15032 1499700 1651.4556 -53955.921 -56833.675 2.7017374 0.0003002531 4.7873746 0.00053203692
15033 1499800 1672.2175 -53956.539 -56870.472 2.6529039 0.00029480641 4.8272071 0.00053642787
15034 1499900 1666.9512 -53957.151 -56861.907 2.7268663 0.00030300535 4.7524325 0.00052808326
15035 1500000 1672.8473 -53957.772 -56872.802 2.7264023 0.00030293359 4.9637248 0.00055152497
15036 Loop time of 29982.7 on 14 procs for 150000 steps with 13482 atoms
15037
15038 Performance: 4.322 ns/day, 5.552 hours/ns, 50.029 timesteps/s
15039 98.7% CPU use with 14 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 | 18554 | 25319 | 28063 | 2506.2 | 84.45
15045 Neigh | 21.753 | 92.478 | 121.84 | 459.1 | 0.31
15046 Comm | 1178 | 3707.1 | 9887.5 | 5964.9 | 12.36
15047 Output | 5.1657 | 5.202 | 5.5641 | 4.4 | 0.02
15048 Modify | 390.13 | 830.65 | 1481.1 | 1512.7 | 2.77
15049 Other | | 28.04 | | | 0.09
15050
15051 Nlocal: 963.000 ave 1235 max 293 min
15052 Histogram: 4 0 0 0 0 0 0 10
15053 Nghost: 2391.09 ave 3013 max 1196 min
15054 Histogram: 4 0 0 0 0 2 2 6
15055 Neighs: 31419.4 ave 41525 max 4938 min
15056 Histogram: 2 2 0 0 0 0 0 10
15057 FullNghs: 62838.7 ave 82619 max 13993 min
15058 Histogram: 4 0 0 0 0 0 0 10
15059
15060 Total # of neighbors = 879742
15061 Ave neighs/atom = 65.253078
15062 Neighbor list builds = 30553
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 8:19:43
15066

```

### Lampiran 6 Data Log Temperatur 1670K Fe (001) - Fe (111)

```

MobaTextEditor
File Edit Search View Format Encoding Syntax Special Tools
out.dat
15032 1499700 1968.6454 -52762.773 -56193.248 10.380065 0.0011535713 30.309815 0.0033684309
15033 1499800 1977.097 -52763.017 -56208.22 10.455796 0.00116101 30.336966 0.0033712235
15034 1499900 1959.26 -52763.25 -56177.37 10.422798 0.0011581659 30.204678 0.0033562991
15035 1500000 1968.8061 -52763.5 -56194.255 10.358165 0.0011580073 30.244974 0.0033605527
15036 Loop time of 27636.2 on 14 procs for 1500000 steps with 13482 atoms
15037
15038 Performance: 4.689 ns/day, 5.118 hours/ns, 54.277 timesteps/s
15039 98.9% CPU use with 14 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 | 17106 | 23265 | 25620 | 2324.5 | 84.18
15045 Neigh | 25.319 | 98.295 | 127.5 | 457.2 | 0.36
15046 Comm | 1229.4 | 3411.1 | 8954.2 | 5474.8 | 12.34
15047 Output | 4.8935 | 4.9335 | 5.2643 | 4.1 | 0.02
15048 Modify | 402.89 | 831.89 | 1518.1 | 1467.9 | 3.01
15049 Other | 24.9 | | | | 0.09
15050
15051 Nlocal: 963.000 ave 1226 max 301 min
15052 Histogram: 4 0 0 0 0 0 0 0 10
15053 Nghost: 2411.57 ave 3015 max 1232 min
15054 Histogram: 4 0 0 0 0 0 0 4 6
15055 Neighs: 31480.3 ave 41317 max 4779 min
15056 Histogram: 2 2 0 0 0 0 0 0 10
15057 FullNghs: 62960.6 ave 82357 max 14462 min
15058 Histogram: 4 0 0 0 0 0 0 0 10
15059
15060 Total # of neighbors = 801448
15061 Ave neighs/atom = 65.379617
15062 Neighbor list builds = 34095
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 7:40:36
15066

```

### Lampiran 7 Data Log Temperatur 1973K Fe (001) - Fe (111)

```

MobaTextEditor
File Edit Search View Format Encoding Syntax Special Tools
out.dat
15032 1499700 2161.2515 -51981.3 -55747.402 3.8907193 0.00043238862 7.0375799 0.00078210975
15033 1499800 2166.1207 -51981.739 -55756.325 3.8533711 0.00042820944 7.0924679 0.00078815707
15034 1499900 2167.5871 -51982.132 -55759.274 3.863378 0.00042929285 6.9948262 0.00077725473
15035 1500000 2161.8614 -51982.523 -55749.687 3.946139 0.00043845989 7.0974417 0.00078860464
15036 Loop time of 25658.9 on 14 procs for 1500000 steps with 13482 atoms
15037
15038 Performance: 5.051 ns/day, 4.752 hours/ns, 58.459 timesteps/s
15039 99.1% CPU use with 14 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 | 16458 | 22097 | 24352 | 2230.6 | 86.12
15045 Neigh | 27.159 | 101.34 | 132.28 | 456.1 | 0.39
15046 Comm | 869.93 | 2074.6 | 8077.9 | 5716.7 | 11.20
15047 Output | 4.6357 | 4.6735 | 4.9499 | 3.6 | 0.02
15048 Modify | 233.35 | 560.83 | 1065.4 | 1339.2 | 2.19
15049 Other | 19.99 | | | | 0.08
15050
15051 Nlocal: 963.000 ave 1220 max 317 min
15052 Histogram: 4 0 0 0 0 0 0 0 10
15053 Nghost: 2405.64 ave 2996 max 1206 min
15054 Histogram: 4 0 0 0 0 0 0 4 6
15055 Neighs: 31141.6 ave 40728 max 4956 min
15056 Histogram: 2 2 0 0 0 0 0 0 10
15057 FullNghs: 62283.3 ave 81318 max 15291 min
15058 Histogram: 4 0 0 0 0 0 0 0 10
15059
15060 Total # of neighbors = 871966
15061 Ave neighs/atom = 64.676309
15062 Neighbor list builds = 36171
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 7:07:38
15066

```

### Lampiran 8 Data Log Temperatur 2173K Fe (001) - Fe (111)

```

MobaTextEditor
File Edit Search View Format Encoding Syntax Special Tools
out.dat out.dat out.dat
15032 1499700 2377.4498 -48371.928 -52514.767 2226.4532 0.24743318 2423.958 0.26938254
15033 1499800 2358.0838 -48372.344 -52481.437 2224.5184 0.24720167 2423.8149 0.26934868
15034 1499900 2366.9132 -48372.768 -52497.247 2226.4803 0.24740319 2426.2203 0.26959801
15035 1500000 2360.2295 -48373.244 -52486.076 2226.3739 0.24737488 2426.5326 0.26961473
15036 Loop time of 21697.2 on 14 procs for 1500000 steps with 13482 atoms
15037
15038 Performance: 5.973 ns/day, 4.018 hours/ns, 69.134 timesteps/s
15039 99.2% CPU use with 14 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 | 15444 | 19162 | 20599 | 1555.3 | 88.31
15045 Neigh | 50.341 | 107.93 | 131.04 | 343.0 | 0.50
15046 Comm | 616.31 | 1974.1 | 5405.5 | 4505.3 | 9.10
15047 Output | 4.6365 | 4.6828 | 4.923 | 3.1 | 0.02
15048 Modify | 215.59 | 431.23 | 771.53 | 992.3 | 1.99
15049 Other | | 17.62 | | | 0.08
15050
15051 Nlocal: 963.000 ave 1133 max 547 min
15052 Histogram: 4 0 0 0 0 0 0 0 10
15053 Nghost: 2363.50 ave 2774 max 1374 min
15054 Histogram: 4 0 0 0 0 0 0 10
15055 Neighs: 29714.2 ave 36027 max 12345 min
15056 Histogram: 2 0 2 0 0 0 0 10
15057 FullNghs: 59428.4 ave 71941 max 29234 min
15058 Histogram: 4 0 0 0 0 0 0 10
15059
15060 Total # of neighbors = 831998
15061 Ave neighs/atom = 61.711764
15062 Neighbor list builds = 38707
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 6:01:37
15066
C:\Users\Sholeh\AppData\Roaming\Moba\term\slash\RemoteFiles\UNIX Plain text 15066 lines Row #1 Col #1

```

### Lampiran 9 Data Log Temperatur 2373K Fe (001) - Fe (111)

```

MobaTextEditor
File Edit Search View Format Encoding Syntax Special Tools
out.dat out.dat out.dat
15032 1499700 2570.7909 -47298.795 -51778.452 3694.9187 0.41062864 3323.5146 0.36935327
15033 1499800 2575.5291 -47299.424 -51787.428 3695.5557 0.41067205 3326.5427 0.36966515
15034 1499900 2570.3541 -47300.118 -51779.104 3695.0939 0.41059336 3326.0154 0.36958191
15035 1500000 2566.785 -47300.835 -51773.601 3695.4348 0.41060387 3328.1673 0.36979636
15036 Loop time of 22659.8 on 14 procs for 1500000 steps with 13482 atoms
15037
15038 Performance: 5.719 ns/day, 4.196 hours/ns, 66.197 timesteps/s
15039 99.2% CPU use with 14 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 | 16475 | 20096 | 21457 | 1471.7 | 88.69
15045 Neigh | 61.451 | 120.42 | 143.92 | 331.8 | 0.53
15046 Comm | 659.52 | 1983.5 | 5344.2 | 4337.7 | 8.75
15047 Output | 4.7803 | 4.8146 | 5.0651 | 3.2 | 0.02
15048 Modify | 225.84 | 436.57 | 751.99 | 986.1 | 1.93
15049 Other | | 10.3 | | | 0.08
15050
15051 Nlocal: 963.000 ave 1125 max 579 min
15052 Histogram: 4 0 0 0 0 0 0 10
15053 Nghost: 2353.57 ave 2754 max 1398 min
15054 Histogram: 4 0 0 0 0 0 0 10
15055 Neighs: 29496.4 ave 35766 max 13013 min
15056 Histogram: 2 0 2 0 0 0 0 10
15057 FullNghs: 58992.9 ave 71445 max 30649 min
15058 Histogram: 4 0 0 0 0 0 0 10
15059
15060 Total # of neighbors = 825900
15061 Ave neighs/atom = 61.259457
15062 Neighbor list builds = 40517
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 6:17:39
15066
C:\Users\Sholeh\AppData\Roaming\Moba\term\slash\RemoteFiles\UNIX Plain text 15066 lines Row #1 Col #1

```

### Lampiran 10 Data Log Temperatur 2573K Fe (001) - Fe (111)

```

MobaTextEditor
File Edit Search View Format Encoding Syntax Special Tools
out.dat
15032 1499700 2771.4577 -46225.112 -51054.532 4497.7667 0.49985182 4265.6775 0.47405897
15033 1499800 2789.9165 -46226.145 -51087.731 4502.4328 0.50033702 4269.3102 0.47443186
15034 1499900 2783.1541 -46227.142 -51076.944 4502.2511 0.50028347 4271.9073 0.47468801
15035 1500000 2791.4155 -46228.231 -51092.429 4501.3767 0.50015296 4272.0303 0.47467003
15036 Loop time of 23599.4 on 14 procs for 1500000 steps with 13482 atoms
15037
15038 Performance: 5.492 ns/day, 4.370 hours/ns, 63.561 timesteps/s
15039 98.8% CPU use with 14 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 | 16929 | 20332 | 21610 | 1342.7 | 86.15
15045 Neigh | 68.943 | 124.02 | 146.11 | 304.7 | 0.53
15046 Comm | 1134.1 | 2323.9 | 5241.8 | 3348.4 | 9.85
15047 Output | 5.1583 | 5.2017 | 5.5578 | 4.3 | 0.02
15048 Modify | 424.6 | 788.96 | 1326.8 | 1298.1 | 3.34
15049 Other | | 25.76 | | | 0.11
15050
15051 Nlocal: 963.000 ave 1103 max 609 min
15052 Histogram: 3 1 0 0 0 0 0 0 10
15053 Nghost: 2330.50 ave 2788 max 1450 min
15054 Histogram: 4 0 0 0 0 0 0 10
15055 Neighs: 29892.4 ave 34398 max 14545 min
15056 Histogram: 2 0 2 0 0 0 0 10
15057 FullNghs: 58184.9 ave 68923 max 32530 min
15058 Histogram: 3 1 0 0 0 0 0 10
15059
15060 Total # of neighbors = 814588
15061 Ave neighs/atom = 60.420412
15062 Neighbor list builds = 42302
15063 Dangerous builds = 0
15064 All done!
15065 Total wall time: 6:33:19
15066

```

Lampiran 11 Data Log Temperatur 2573K Fe (001) - Fe (111)

