

## LAMPIRAN

### 1.1 Proses menjalankan Simulasi dengan Aplikasi Moba Exterm

```
• MobaXterm 20.3 •
(SSH client, X-server and networking tools)

> SSH session to mahasiswa@metal.mdsim.xyz
• SSH compression : ✓
• SSH-browser      : ✓
• X11-forwarding  : x (disabled or not supported by server)
• DISPLAY         : 192.168.100.8:0.0
> For more info, ctrl+click on help or visit our website

Welcome to Ubuntu 18.04.5 LTS (GNU/Linux 3.10.0-1160.21.1.vz7.174.13 x86_64)

• Documentation: https://help.ubuntu.com
• Management:   https://landscape.canonical.com
• Support:      https://ubuntu.com/advantage
Last login: Thu Jul 8 19:55:26 2021 from 102.1.111.103
mahasiswa@metal:~$ cd kerja/
mahasiswa@metal:~/kerja$ ls
andy  dodang  dait  diam  Khoirudin  rizal  septian  taufan  tmp
mahasiswa@metal:~/kerja$ cd andy/
mahasiswa@metal:~/kerja/andy$ ls
TiN.meam  coba.dat  config  latihan  ni10ti50a140  ni20ti50a130  ni30ti50a120
mahasiswa@metal:~/kerja/andy$ cd ni10ti50a140/
mahasiswa@metal:~/kerja/andy/ni10ti50a140$ ls
#02 NiAlli.meam  coba.lampstrj  coba.lmp  input.nitial  library.meam  log.lammps  myjob.slurm  ni10ti50a140.lmp  out.dat  parallel_226.log
mahasiswa@metal:~/kerja/andy/ni10ti50a140$ sbatch myjob.slurm
Submitted batch job 98
mahasiswa@metal:~/kerja/andy/ni10ti50a140$
```

### 1.2 Log Lammps Optimasi Ni10Ti50A140

```
D:\AFS\UMPO\SKRIPSI\Hasil Moba Exterm\ni10ti50a140\optimasi\log.lammps - Notepad++
File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?
log.lammps x
366 3080 0 -147088.5 -147088.5 0.00014774779 509777.71 78.952441 79.014027 81.71675
367 3090 0 -147088.5 -147088.5 0.07773128 509777.71 78.952455 79.014033 81.71673
368 3100 0 -147088.5 -147088.5 0.71900042 509777.42 78.952403 79.014007 81.716762
369 3110 0 -147088.5 -147088.5 0.06992937 509777.81 78.952486 79.014079 81.716666
370 3120 0 -147088.5 -147088.5 0.013913853 509777.71 78.952447 79.014024 81.716746
371 3130 0 -147088.5 -147088.5 -0.36408488 509777.75 78.952404 79.014007 81.716816
372 3140 0 -147088.5 -147088.5 -0.2335877 509777.83 78.952468 79.014033 81.716734
373 3150 0 -147088.5 -147088.5 -0.10545472 509777.73 78.952435 79.01402 81.716767
374 3160 0 -147088.5 -147088.5 -0.62826298 509777.74 78.952391 79.013943 81.716893
375 3170 0 -147088.5 -147088.5 -0.17010707 509777.79 78.95244 79.014044 81.716745
376 3180 0 -147088.5 -147088.5 -0.031882674 509777.71 78.952433 79.014029 81.716757
377 3190 0 -147088.5 -147088.5 0.24477031 509777.61 78.952418 79.014029 81.716756
378 3200 0 -147088.5 -147088.5 1.0619921 509777.46 78.952533 79.0142 81.716645
379 3210 0 -147088.5 -147088.5 2.737796 509776.45 78.952119 79.014019 81.716889
380 3220 0 -147088.5 -147088.5 0.5216997 509777.63 78.95246 79.01407 81.716672
381 3230 0 -147088.5 -147088.5 0.088510124 509777.67 78.952435 79.01402 81.716756
382 3240 0 -147088.5 -147088.5 0.037203324 509777.7 78.952442 79.01403 81.716745
383 3250 0 -147088.5 -147088.5 0.0082974268 509777.71 78.952441 79.014029 81.716748
384 3260 0 -147088.5 -147088.5 0.64427244 509777.48 78.952417 79.014024 81.71674
385 3270 0 -147088.5 -147088.5 -0.031502114 509777.75 78.952456 79.014035 81.716732
386 3279 0 -147088.5 -147088.5 0.024337699 509777.71 78.952439 79.014032 81.716746
387 Loop time of 930.218 on 8 procs for 3279 steps with 32000 atoms
388
389 97.9% CPU use with 8 MPI tasks x no OpenMP threads
390
391 Minimization stats:
392 Stopping criterion = energy tolerance
393 Energy initial, next-to-last, final =
394 -146508.284172992 -147088.498875228 -147088.498875228
395 Force two-norm initial, final = 8940.0308 0.020088498
396 Force max component initial, final = 8930.6774 0.015280106
397 Final line search alpha, max atom move = 0.37160152 0.0056781106
398 Iterations, force evaluations = 3279 6398
399
400 MPI task timing breakdown:
401 Section | min time | avg time | max time | |%varavg| |%total
402 -----|-----|-----|-----|-----|-----|-----
403 Pair | 842.86 | 848.82 | 853.58 | | 13.2 | 91.25
404 Neigh | 0.036479 | 0.041543 | 0.053039 | | 2.5 | 0.00
405 Comm | 70.952 | 75.664 | 81.771 | | 45.1 | 8.13
406 Output | 0.024026 | 0.025722 | 0.03634 | | 2.5 | 0.00
407 Modify | 0 | 0 | 0 | | 0.0 | 0.00
408 Other | | 5.668 | | | | 0.61
409
```

### 1.3 Log Lammmps Optimasi Ni20Ti50Al30

```
D:\AFS\UMPO\SKRIPSI(Hasil Moba Extern)\ni20ti50al30\optimasi\log.lammps - Notepad++
File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?
log.lammps x
551 4940 0 -149870.07 -149870.07 -25.284665 490177 78.060122 78.268587 80.229893
552 4950 0 -149870.11 -149870.11 5.7422451 490165.84 78.064905 78.262256 80.229639
553 4960 0 -149870.14 -149870.14 7.787325 490165.32 78.058768 78.268636 80.229322
554 4970 0 -149870.17 -149870.17 -42.052012 490181.73 78.067106 78.261401 80.230855
555 4980 0 -149870.2 -149870.2 103.78625 490131.76 78.056093 78.267448 80.227795
556 4990 0 -149870.23 -149870.23 -158.69872 490221.67 78.065397 78.267321 80.233308
557 5000 0 -149870.26 -149870.26 120.72376 490126.57 78.063959 78.259821 80.226681
558 5010 0 -149870.29 -149870.29 -59.779664 490188.94 78.05914 78.271576 80.229792
559 5020 0 -149870.32 -149870.32 13.179505 490162.84 78.065891 78.261171 80.229248
560 5030 0 -149870.35 -149870.35 4.1848365 490165.59 78.058897 78.26822 80.229661
561 5040 0 -149870.38 -149870.38 -20.556861 490173.24 78.064684 78.262467 80.230861
562 5050 0 -149870.41 -149870.41 44.969762 490150.6 78.05827 78.266493 80.229621
563 5060 0 -149870.44 -149870.44 -84.371858 490194.66 78.064257 78.264798 80.232418
564 5070 0 -149870.47 -149870.47 98.143962 490132.69 78.061437 78.261949 80.228092
565 5080 0 -149870.5 -149870.5 -78.342595 490194.08 78.059652 78.270941 80.230758
566 5090 0 -149870.53 -149870.53 34.532767 490154.93 78.067216 78.258999 80.228819
567 5100 0 -149870.55 -149870.55 -1.8675016 490167.34 78.056029 78.271458 80.229574
568 5110 0 -149870.58 -149870.58 -31.351297 490176.05 78.066868 78.260191 80.231411
569 5120 0 -149870.61 -149870.61 57.869382 490145.33 78.05694 78.266928 80.229679
570 5130 0 -149870.63 -149870.63 -79.001217 490192.05 78.063766 78.264729 80.232565
571 5140 0 -149870.66 -149870.66 70.164655 490141.34 78.061246 78.262568 80.22907
572 5150 0 -149870.69 -149870.69 -43.552808 490180.56 78.060271 78.267839 80.231088
573 5160 0 -149870.72 -149870.72 19.478806 490158.47 78.063663 78.261789 80.230189
574 5170 0 -149870.75 -149870.75 -5.3275034 490166.82 78.058169 78.26807 80.230764
575 5174 0 -149870.75 -149870.75 7.6084178 490160.86 78.056913 78.267246 80.231925
576 Loop time of 1478.45 on 9 procs for 5174 steps with 32000 atoms
577
578 96.6% CPU use with 9 MPI tasks x no OpenMP threads
579
580 Minimization stats:
581 Stopping criterion = max force evaluations
582 Energy initial, next-to-last, final =
583 | -148488.22268085 -149870.752809903 -149870.754136865
584 Force two-norm initial, final = 22681.102 26.987844
585 Force max component initial, final = 15314.571 22.393484
586 Final line search alpha, max atom move = 2.6495530e-05 0.00059332723
587 Iterations, force evaluations = 5174 10000
588
589 MPI task timing breakdown:
590 Section | min time | avg time | max time | %varavg| %total
591 -----|-----|-----|-----|-----|-----
592 Pair | 1289.5 | 1318.3 | 1338.5 | 37.3 | 89.17
593 Neigh | 0.060602 | 0.075947 | 0.092976 | 3.3 | 0.01
594 Comm | 126.4 | 146.67 | 175.6 | 112.6 | 9.92
595 Output | 0.038144 | 0.041449 | 0.065829 | 4.2 | 0.00
596 Modify | 0 | 0 | 0 | 0.0 | 0.00
```



## 1.4 Log Lammps Optimasi Ni30Ti50Al20

```
D:\AFS\UMPO\SKRIPSI\Hasil Moba Extern\ni30ti50al20\optimasi\log.lammps - Notepad++
File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window Z
log.lammps
572 5150 0 -152673.97 -152673.97 -1.5488506 469252.53 75.981054 79.261254 77.918462
573 5160 0 -152673.98 -152673.98 -5.5897715 469253.6 75.979075 79.263065 77.918888
574 5170 0 -152673.98 -152673.98 23.153305 469244.14 75.981615 79.259468 77.918248
575 5180 0 -152673.98 -152673.98 -15.742502 469256.96 75.980345 79.262251 77.918945
576 5190 0 -152673.98 -152673.98 8.5111894 469248.97 75.98032 79.261566 77.918317
577 5200 0 -152673.98 -152673.98 -11.09548 469255.42 75.98082 79.261828 77.918618
578 5210 0 -152673.99 -152673.99 17.642336 469245.76 75.979092 79.262406 77.918217
579 5220 0 -152673.99 -152673.99 -9.7682831 469254.79 75.982436 79.259862 77.918788
580 5230 0 -152673.99 -152673.99 -2.3297393 469252.25 75.979561 79.262575 77.918649
581 5240 0 -152673.99 -152673.99 2.8441352 469250.66 75.980662 79.261574 77.918238
582 5250 0 -152673.99 -152673.99 -5.8564597 469253.41 75.980136 79.26231 77.91851
583 5260 0 -152674 -152674 25.38777 469243.01 75.980374 79.260905 77.917922
584 5270 0 -152674 -152674 -49.525452 469267.66 75.981652 79.262127 77.919503
585 5280 0 -152674 -152674 20.725248 469244.37 75.978776 79.26255 77.918169
586 5290 0 -152674 -152674 -2.7813511 469252.34 75.980914 79.261646 77.918189
587 5300 0 -152674 -152674 0.19354483 469251.22 75.980062 79.26226 77.918272
588 5310 0 -152674.01 -152674.01 2.4634848 469250.42 75.980804 79.261386 77.918238
589 5320 0 -152674.01 -152674.01 -20.234794 469257.71 75.979222 79.263541 77.918952
590 5330 0 -152674.01 -152674.01 39.058115 469238.46 75.980473 79.260804 77.917164
591 5340 0 -152674.01 -152674.01 -20.899485 469258.16 75.980965 79.262294 77.918466
592 5350 0 -152674.01 -152674.01 5.7381734 469249.25 75.979946 79.26259 77.918066
593 5360 0 -152674.01 -152674.01 -3.1472622 469252.15 75.98059 79.261897 77.918243
594 5369 0 -152674.02 -152674.02 28.40995 469241.85 75.980342 79.261306 77.917367
595 Loop time of 1615.95 on 8 procs for 5369 steps with 32000 atoms
596
597 96.4% CPU use with 8 MPI tasks x no OpenMP threads
598
599 Minimization stats:
600 Stopping criterion = max force evaluations
601 Energy initial, next-to-last, final =
602 -149927.589877026 -152674.016139835 -152674.016358026
603 Force two-norm initial, final = 47046.143 15.337973
604 Force max component initial, final = 28509.101 10.274599
605 Final line search alpha, max atom move = 0.00011099295 0.0011404081
606 Iterations, force evaluations = 5369 10000
607
608 MPI task timing breakdown:
609 Section | min time | avg time | max time | %varavg| %total
610 -----|-----|-----|-----|-----|-----
611 Pair | 1465.1 | 1471.3 | 1477.8 | 10.9 | 91.05
612 Neigh | 0.16568 | 0.17607 | 0.201 | 2.6 | 0.01
613 Comm | 125.18 | 131.64 | 137.73 | 36.2 | 8.15
614 Output | 0.072529 | 0.087712 | 0.13203 | 6.2 | 0.01
615 Modify | 0 | 0 | 0 | 0.0 | 0.00
616 Other | 12.77 | 12.77 | 12.77 | 0.0 | 0.79
```

## 1.5 Log Lammps Uji Tarik Ni10Ti50Al40

```
log.lammps
1122 # Use cfg for AtomEye
1123 #dump 1 all cfg 250 dump.tensile_*.cfg mass type xs ys zs c_csym c_peratom fx fy fz
1124 #dump_modify 1 element Ni Al Ti
1125 #dump 2 all custom 250 dump.lammpstrj id type x y z
1126 #dump_modify 2 sort id
1127
1128 # Display thermo
1129 thermo 100
1130 thermo_style custom step v_strain temp v_p2 v_p3 v_p4 ke pe press
1131
1132 run 100000
1133 Per MPI rank memory allocation (min/avg/max) = 16.76 | 16.88 | 17.04 Mbytes
1134 Step v_strain Temp v_p2 v_p3 v_p4 KinEng PotEng Press
1135 0 -3.5880341e-16 299.00803 -0.20368834 -0.20576167 0.45453718 1236.7556 -145838.22 -150.29059
1136 100 0.001 302.21788 -0.24366843 -0.069317285 -0.10987109 1250.0322 -145855.02 1409.5227
1137 200 0.002 297.90234 -0.081560324 0.15193782 -0.050197805 1232.1823 -145836.39 -67.26564
1138 300 0.003 298.83974 0.018744475 -0.030822884 0.023964424 1236.0596 -145839.74 -39.620049
1139 400 0.004 298.98927 0.10859337 -0.07528197 -0.0023596134 1236.678 -145839.16 -103.17262
1140 500 0.005 296.94712 0.23359927 0.061452233 0.011543397 1228.2313 -145829.22 -1021.983
1141 600 0.006 298.62478 0.29758403 -0.0045938365 -0.049948219 1235.1704 -145834.3 -810.13991
1142 700 0.007 299.23116 0.4316098 0.00024978158 0.069548031 1237.6785 -145834.57 -1671.3587
1143 800 0.008 301.90479 0.48275527 0.021842736 -0.0038877867 1249.1094 -145843.47 -1669.8374
1144 900 0.009 297.08085 0.56871253 -0.018128075 -0.03555013 1228.0258 -145820.31 -1716.7478
1145 1000 0.01 300.26813 0.70380731 0.027957896 0.056407527 1241.9676 -145830.19 -2624.8758
1146 1100 0.011 299.28933 0.7596021 -0.013950275 -0.019105049 1237.5883 -145822.26 -2421.8226
1147 1200 0.012 297.73242 0.87791091 0.044914787 0.0093807374 1231.4795 -145812.23 -3107.0881
1148 1300 0.013 299.47167 0.95080249 -0.012903516 0.0043905494 1238.6734 -145815.17 -3140.9917
1149 1400 0.014 297.41832 1.0366916 -0.01903893 0.0029785681 1230.1803 -145802.12 -3402.1042
1150 1500 0.015 299.8597 1.142937 0.015874926 0.0069323997 1240.2783 -145807.37 -3885.8144
1151 1600 0.016 298.6852 1.2495306 0.01542361 -0.0055332927 1235.4203 -145797.3 -4198.0699
1152 1700 0.017 298.34081 1.2910484 0.035266547 -0.025057497 1233.9959 -145790.39 -4102.4146
1153 1800 0.018 298.70288 1.4454856 0.015792689 0.031129539 1235.4935 -145786.07 -4975.3593
1154 1900 0.019 298.83596 1.5065048 -0.0032127922 -0.027019706 1236.0439 -145780.46 -4920.9076
1155 2000 0.02 298.27385 1.5874385 0.034698817 0.0084453826 1233.7189 -145771.75 -5435.2757
1156 2100 0.021 299.16168 1.6977434 -0.016012417 0.0071137705 1237.3911 -145768.74 -5629.4793
1157 2200 0.022 298.84214 1.7765884 -0.015852997 -0.0080431168 1236.0695 -145760.39 -5842.3075
1158 2300 0.023 298.84642 1.8646649 0.02393052 0.012391656 1236.0872 -145753.14 -6336.6235
1159 2400 0.024 298.83006 1.9668108 -0.0018335049 -0.011360161 1236.0195 -145745.51 -6505.3904
1160 2500 0.025 298.56089 2.055917 0.021876536 0.0089909345 1234.9062 -145736.49 -6955.9482
1161 2600 0.026 298.91974 2.1462029 -0.0042730067 0.0035080891 1236.3904 -145729.81 -7151.4598
1162 2700 0.027 297.52215 2.2570952 0.0011063876 0.016733584 1230.6097 -145715.57 -7583.1172
```

## 1.6 Log Lammmps Uji Tarik Ni20Ti50Al30

```

log.lammps
1118 # Output strain and stress info to file
1119 # for units metal, pressure is in [bars] = 100 [kPa] = 1/10000 [GPa]
1120 # p2, p3, p4 are in GPa
1121 variable strain equal "(lx - v_l0)/v_l0"
1122 variable p1 equal "v_strain"
1123 variable p2 equal "-pxx/10000"
1124 variable p3 equal "-pyy/10000"
1125 variable p4 equal "-pzz/10000"
1126 fix def1 all print 100 "${p1} ${p2} ${p3} ${p4}" file ni20ti50al30_100.def1.dat screen no
1127
1128 # Use cfg for AtomEye
1129 #dump      1 all cfg 250 dump.tensile_*.cfg mass type xs ys zs c_csym c_peratom fx fy fz
1130 #dump_modify 1 element Ni Al Ti
1131 dump      2 all custom 250 dump.lammpstrj id type x y z
1132 dump_modify 2 sort id
1133
1134 # Display thermo
1135 thermo 100
1136 thermo_style custom step v_strain temp v_p2 v_p3 v_p4 ke pe press
1137
1138 run      100000
1139 Per MPI rank memory allocation (min/avg/max) = 16.85 | 16.92 | 17.02 Mbytes
1140 Step v_strain Temp v_p2 v_p3 v_p4 KinEng PotEng Press
1141   0 3.6301943e-16 298.94868 -0.28146008 -0.23583548 0.33545428 1236.5102 -148624.83 606.13762
1142 100 0.001 300.50141 -0.32193202 -0.031570064 -0.098414424 1242.9325 -148633.73 1506.3883
1143 200 0.002 296.5103 -0.13608592 0.10699635 -0.031547185 1226.4245 -148616.58 202.1225
1144 300 0.003 300.96916 -0.073213665 -0.046953719 0.0017827702 1244.8673 -148634.75 394.61538
1145 400 0.004 300.52496 0.049516534 0.0020598325 0.057853124 1243.0299 -148632.03 -364.76497
1146 500 0.005 300.37593 0.14440369 0.00882546246 -0.023351276 1242.4136 -148630.29 -406.2596
1147 600 0.006 298.11584 0.23615626 0.045375897 -0.00054885745 1233.0653 -148610.34 -936.61098
1148 700 0.007 300.15299 0.30878374 -0.01035231 -0.02669082 1241.4914 -148626.01 -905.80203
1149 800 0.008 299.40971 0.41935482 0.014832806 0.043448734 1238.4171 -148620.75 -1592.1212
1150 900 0.009 298.06097 0.4793496 -0.0060547688 -0.0094842813 1232.8384 -148612.73 -1546.0352
1151 1000 0.01 298.70648 0.59442388 0.022038186 0.0044199231 1235.5083 -148612.68 -2069.6066
1152 1100 0.011 300.21238 0.71621951 -0.0039924727 0.030428984 1241.7371 -148615.77 -2475.5201
1153 1200 0.012 300.25157 0.76375635 -0.005282997 0.030834605 1241.8991 -148612.54 -2631.0265
1154 1300 0.013 297.57391 0.87987918 0.0021361588 -0.00012549516 1230.8238 -148597.76 -2939.6328
1155 1400 0.014 297.02958 0.89946709 -0.021855678 -0.016636613 1228.5724 -148591.57 -2869.916
1156 1500 0.015 297.68115 1.011091 0.0056957188 0.026358739 1231.2674 -148590.05 -3477.1517
1157 1600 0.016 298.0619 1.0795752 -0.049081452 -0.059285303 1232.8423 -148587.12 -3237.3615
1158 1700 0.017 298.644 1.2217722 0.051295776 0.04461598 1235.2499 -148584.66 -4392.28

```

## 1.7 Log Lammmps Uji Tarik Ni30Ti50Al20

```

log.lammps
1112 # Output strain and stress info to file
1113 # for units metal, pressure is in [bars] = 100 [kPa] = 1/10000 [GPa]
1114 # p2, p3, p4 are in GPa
1115 variable strain equal "(lx - v_l0)/v_l0"
1116 variable p1 equal "v_strain"
1117 variable p2 equal "-pxx/10000"
1118 variable p3 equal "-pyy/10000"
1119 variable p4 equal "-pzz/10000"
1120 fix def1 all print 100 "${p1} ${p2} ${p3} ${p4}" file Al_sc_100.def1.dat screen no
1121
1122 # Use cfg for AtomEye
1123 #dump      1 all cfg 250 dump.tensile_*.cfg mass type xs ys zs c_csym c_peratom fx fy fz
1124 #dump_modify 1 element Ni Al Ti
1125 dump      2 all custom 250 dump.lammpstrj id type x y z
1126 dump_modify 2 sort id
1127
1128 # Display thermo
1129 thermo 100
1130 thermo_style custom step v_strain temp v_p2 v_p3 v_p4 ke pe press
1131
1132 run      100000
1133 Per MPI rank memory allocation (min/avg/max) = 17.02 | 17.08 | 17.13 Mbytes
1134 Step v_strain Temp v_p2 v_p3 v_p4 KinEng PotEng Press
1135   0 0 300.58824 -0.86761338 0.65857714 0.25401733 1243.2917 -151470.47 -149.93694
1136 100 0.001 302.76001 -1.2808155 -0.29737691 -0.27898461 1252.2746 -151484.03 6190.59
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