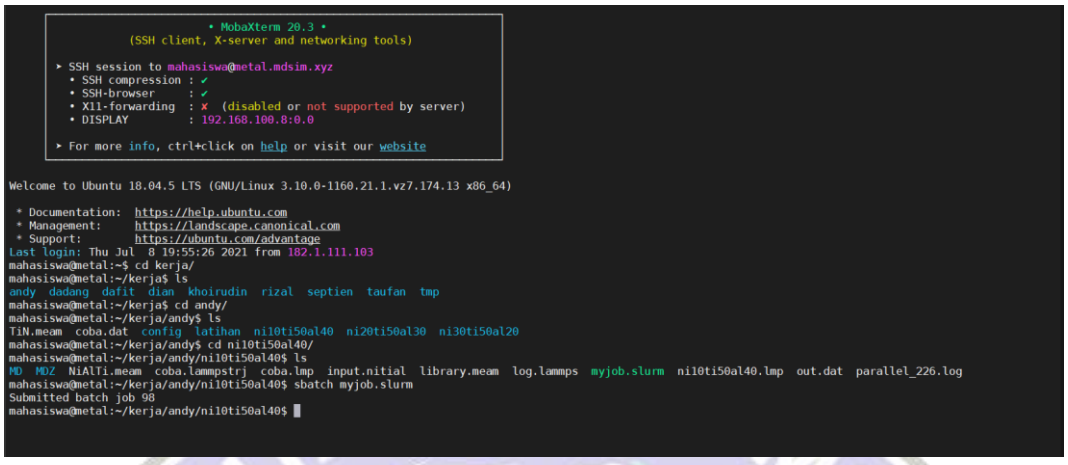
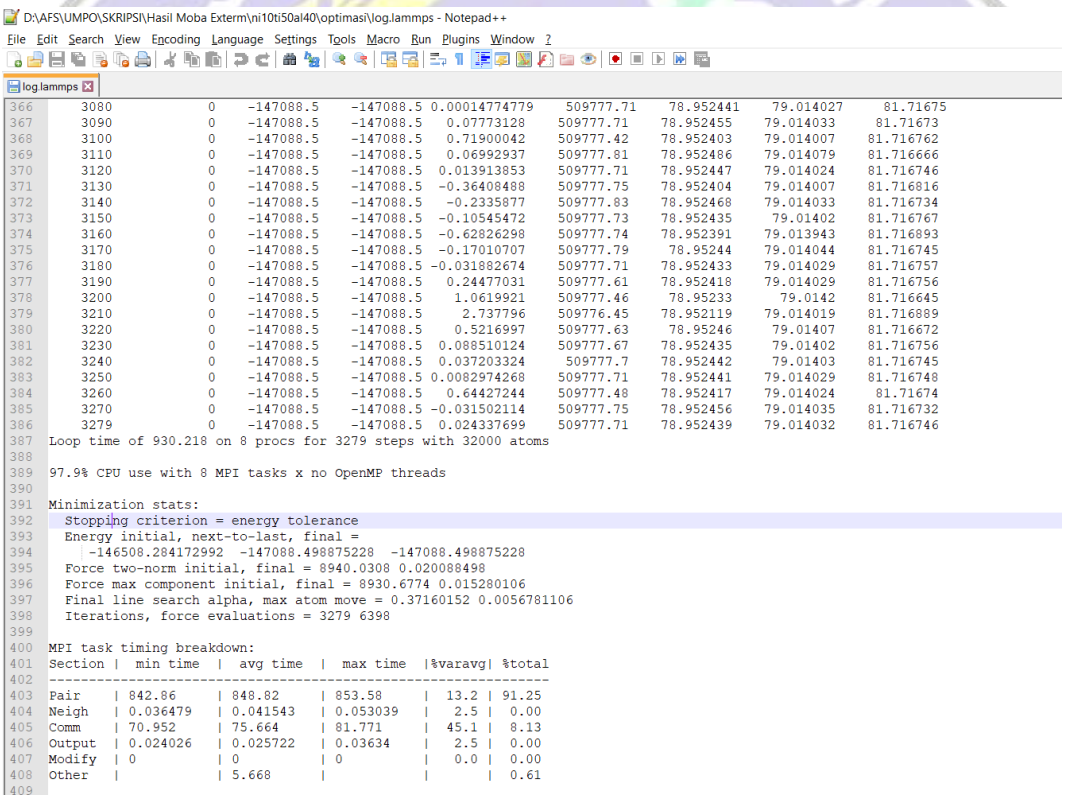
LAMPIRAN

1.1 Proses menjalankan Simulasi dengan Aplikasi Moba Exterm



1.2 Log Lammps Optimasi Ni10Ti50Al40



1.3 Log Lammps Optimasi Ni20Ti50Al30

D:\AFS\UMPO\SKRIPSI\Hasil Moba Exterm\ni20ti50al30\optimasi\log.lammps - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

log.lammps

```
    4940            0   -149870.07   -149870.07   -25.284665       490177    78.060122    78.268587    80.229893
    4950            0   -149870.11   -149870.11    5.7422451    490165.84    78.064905    78.262256    80.229639
    4960            0   -149870.14   -149870.14     7.787325    490165.32    78.058768    78.268636    80.229322
    4970            0   -149870.17   -149870.17   -42.052012    490181.73    78.067106    78.261401    80.230855
    4980            0    -149870.2    -149870.2    103.78625    490131.76    78.056093    78.267448    80.227795
    4990            0   -149870.23   -149870.23   -158.69872    490221.67    78.065397    78.267321     80.23308
    5000            0   -149870.26   -149870.26    120.72376    490126.57    78.063959    78.259821    80.226681
    5010            0   -149870.29   -149870.29   -59.779064    490188.94     78.05914    78.271576    80.229792
    5020            0   -149870.32   -149870.32    13.179505    490162.84    78.065891    78.261171    80.229248
    5030            0   -149870.35   -149870.35    4.1848365    490165.59    78.058897     78.26822    80.229661
    5040            0   -149870.38   -149870.38   -20.556861    490173.24    78.064684    78.262467    80.230861
    5050            0   -149870.41   -149870.41    44.969762     490150.6     78.05827    78.266493    80.229621
    5060            0   -149870.44   -149870.44   -84.371858    490194.66    78.064257    78.264798    80.232418
    5070            0   -149870.47   -149870.47    98.143962    490132.69    78.061437    78.261949    80.228092
    5080            0    -149870.5    -149870.5   -78.342595    490194.08    78.059652    78.270941    80.230758
    5090            0   -149870.53   -149870.53    34.532767    490154.93    78.067216    78.258999    80.228819
    5100            0   -149870.55   -149870.55   -1.8675016    490167.34    78.056029    78.271458    80.229574
    5110            0   -149870.58   -149870.58   -31.351297    490176.05    78.066868    78.260191    80.231411
    5120            0   -149870.61   -149870.61    57.869382    490145.33     78.05694    78.266928    80.229679
    5130            0   -149870.63   -149870.63   -79.001217    490192.05    78.063766    78.264729    80.232565
    5140            0   -149870.66   -149870.66    70.164655    490141.34    78.061246    78.262568     80.22907
    5150            0   -149870.69   -149870.69   -43.552808    490180.56    78.060271    78.267839    80.231088
    5160            0   -149870.72   -149870.72    19.478806    490158.47    78.063663    78.261789    80.230189
    5170            0   -149870.75   -149870.75   -5.3275034    490166.82    78.058169     78.26807    80.230764
    5174            0   -149870.75   -149870.75    7.6084178    490160.86    78.056913    78.267246    80.231925
Loop time of 1478.45 on 9 procs for 5174 steps with 32000 atoms

96.6% CPU use with 9 MPI tasks x no OpenMP threads

Minimization stats:
  Stopping criterion = max force evaluations
  Energy initial, next-to-last, final =
      -148488.22268085  -149870.752809903  -149870.754136865
  Force two-norm initial, final = 22681.102 26.987844
  Force max component initial, final = 15314.571 22.393484
  Final line search alpha, max atom move = 2.6495530e-05 0.00059332723
  Iterations, force evaluations = 5174 10000

MPI task timing breakdown:
Section |  min time  |  avg time  |  max time  |%varavg| %total
---------------------------------------------------------------
Pair    | 1289.5     | 1318.3     | 1338.5     |  37.3 | 89.17
Neigh   | 0.060602   | 0.075947   | 0.092976   |   3.3 |  0.01
Comm    | 126.4      | 146.67     | 175.6      | 112.6 |  9.92
Output  | 0.038144   | 0.041449   | 0.065829   |   4.2 |  0.00
Modify  | 0          | 0          | 0          |   0.0 |  0.00
```

1.4 Log Lammps Optimasi Ni30Ti50Al20

D:\AFS\UMPO\SKRIPSI\Hasil Moba Exterm\ni30ti50al20\optimasi\log.lammps - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

log.lammps

```
     5150            0   -152673.97   -152673.97   -1.5488506    469252.53    75.981054    79.261254    77.918462
     5160            0   -152673.98   -152673.98   -5.5897715    469253.6     75.979075    79.263065    77.918888
     5170            0   -152673.98   -152673.98    23.153305    469244.14    75.981615    79.259468    77.918248
     5180            0   -152673.98   -152673.98   -15.742502    469256.96    75.980345    79.262251    77.918945
     5190            0   -152673.98   -152673.98    8.5111894    469248.97     75.98032    79.261566    77.918317
     5200            0   -152673.98   -152673.98   -11.09548    469255.42     75.98082    79.261828    77.918618
     5210            0   -152673.99   -152673.99    17.642336    469245.76    75.979092    79.262406    77.918217
     5220            0   -152673.99   -152673.99   -9.7682831    469254.79    75.982436    79.259862    77.918788
     5230            0   -152673.99   -152673.99   -2.3297393    469252.25    75.979561    79.262575    77.918649
     5240            0   -152673.99   -152673.99    2.8441352    469250.66    75.980662    79.261574    77.918238
     5250            0   -152673.99   -152673.99   -5.8564597    469253.41    75.980136     79.26231     77.91851
     5260            0      -152674      -152674     25.38777    469243.01    75.980374    79.260905    77.917922
     5270            0      -152674      -152674   -49.525452    469267.66    75.981652    79.262127    77.919503
     5280            0      -152674      -152674    20.725248    469244.37    75.978776     79.26255    77.918169
     5290            0      -152674      -152674   -2.7813511    469252.34    75.980914    79.261646    77.918189
     5300            0      -152674      -152674   0.19354483    469251.22    75.980062     79.26226    77.918272
     5310            0   -152674.01   -152674.01    2.4634848    469250.42    75.980804    79.261386    77.918238
     5320            0   -152674.01   -152674.01   -20.234794    469257.71    75.979222    79.263541    77.918952
     5330            0   -152674.01   -152674.01    39.058115    469238.46    75.980473    79.260804    77.917164
     5340            0   -152674.01   -152674.01   -20.899485    469258.16    75.980965    79.262294    77.918466
     5350            0   -152674.01   -152674.01    5.7381734    469249.25    75.979946    79.262259    77.918066
     5360            0   -152674.01   -152674.01   -3.1472622    469252.15     75.98059    79.261897    77.918243
     5369            0   -152674.02   -152674.02     28.40995    469241.85    75.980342    79.261306    77.917367
Loop time of 1615.95 on 8 procs for 5369 steps with 32000 atoms

96.4% CPU use with 8 MPI tasks x no OpenMP threads

Minimization stats:
  Stopping criterion = max force evaluations
  Energy initial, next-to-last, final =
     -149927.589877026  -152674.016139835  -152674.016358026
  Force two-norm initial, final = 47046.143 15.337973
  Force max component initial, final = 28509.101 10.274599
  Final line search alpha, max atom move = 0.00011099295 0.0011404081
  Iterations, force evaluations = 5369 10000

MPI task timing breakdown:
Section |  min time  |  avg time  |  max time  |%varavg| %total
---------------------------------------------------------------
Pair    | 1465.1     | 1471.3     | 1477.8     |  10.9 | 91.05
Neigh   | 0.16568    | 0.17607    | 0.201      |   2.6 |  0.01
Comm    | 125.18     | 131.64     | 137.73     |  36.2 |  8.15
Output  | 0.072529   | 0.087712   | 0.13203    |   6.2 |  0.01
Modify  | 0          | 0          | 0          |   0.0 |  0.00
Other   |            | 12.77      |            |       |  0.79
```

1.5 Log Lammps Uji Tarik Ni10Ti50Al40

log.lammps

```
# Use cfg for AtomEye
#dump     1 all cfg 250 dump.tensile_*.cfg mass type xs ys zs c_csym c_peratom fx fy fz
#dump_modify 1 element Ni Al Ti
dump     2 all custom 250 dump.lammpstrj id type x y z
dump_modify 2 sort id

# Display thermo
thermo  100
thermo_style  custom step v_strain temp v_p2 v_p3 v_p4 ke pe press

run   100000
Per MPI rank memory allocation (min/avg/max) = 16.76 | 16.88 | 17.04 Mbytes
Step v_strain Temp v_p2 v_p3 v_p4 KinEng PotEng Press
       0 -3.5880341e-16    299.00803  -0.20368834  -0.20576167   0.45453718    1236.7556   -145838.22   -150.29059
     100        0.001    302.21788  -0.24366843 -0.069317285  -0.10987109    1250.0322   -145855.02    1409.5227
     200        0.002    297.90234 -0.081560324   0.15193782 -0.050197805    1232.1823   -145836.39   -67.26564
     300        0.003    298.83974  0.018744475 -0.030822884  0.023964424    1236.0596   -145839.74   -39.620049
     400        0.004    298.98927   0.10859337  -0.07528197 -0.0023596134    1236.678   -145839.16   -103.17262
     500        0.005    296.94712   0.23359927   0.061452233  0.011543397    1228.2313   -145829.22    -1021.983
     600        0.006    298.62478   0.29758403 -0.0045938365 -0.049948219    1235.1704   -145834.3    -810.13991
     700        0.007    299.23116   0.4316098  0.00024978158  0.069548031    1237.6785   -145834.57   -1671.3587
     800        0.008    301.99479   0.48275627  0.021842736 -0.0038877867    1249.1094   -145843.47   -1669.0374
     900        0.009    297.09085   0.56871253 -0.018129075  -0.03555913    1228.8258   -145820.31   -1716.7478
    1000         0.01    300.26813   0.70309731  0.027957896  0.056407527    1241.9676   -145830.19   -2624.8758
    1100        0.011    299.20933   0.7596021 -0.013950275 -0.019105049    1237.5883   -145822.26   -2421.8226
    1200        0.012    297.73242   0.87791091  0.044914787 0.0093007374    1231.4795   -145812.23   -3107.0881
    1300        0.013    299.47167   0.95080249 -0.012903516 0.0043985494    1238.6734   -145815.17   -3140.9917
    1400        0.014    297.41832    1.0366916  -0.01903893 0.0029785681    1230.1803   -145802.12   -3402.1042
    1500        0.015     299.8597    1.142937  0.015874926 0.0069323997    1240.2783   -145807.37   -3885.8144
    1600        0.016     298.6852    1.2495306   0.01542361 -0.0055332927    1235.4203    -145797.3   -4198.0699
    1700        0.017    298.34081    1.2910484 -0.035266547 -0.025057497    1233.9959   -145790.39   -4102.4146
    1800        0.018    298.70288    1.4454856  0.015792689  0.031329539    1235.4935   -145786.07   -4975.3593
    1900        0.019    298.83596    1.5065048 -0.0032127922 -0.027019706    1236.0439   -145780.46   -4920.9076
    2000         0.02    298.27385    1.5874385  0.034698817 0.0084453826    1233.7189   -145771.75   -5435.2757
    2100        0.021    299.16168    1.6977434 -0.016013417 0.0071137705    1237.3911   -145768.74   -5629.4793
    2200        0.022    298.84214    1.7765884 -0.015852997 -0.0080431168    1236.0695   -145760.39   -5842.3075
    2300        0.023    298.84642    1.8646649   0.02393052  0.012391656    1236.0872   -145753.14   -6336.6235
    2400        0.024    298.83006    1.9668108 -0.0018335049 -0.013360161    1236.0195   -145745.51   -6505.3904
    2500        0.025    298.56089     2.055917  0.021876536 0.0089909345    1234.9062   -145736.49   -6955.9482
    2600        0.026    298.91974    2.1462029 -0.0042730067 0.0035080891    1236.3904   -145729.81   -7151.4598
    2700        0.027    297.52215    2.2570952 0.0011063876  0.016733584    1230.6097   -145715.57   -7583.1172
```

1.6 Log Lammps Uji Tarik Ni20Ti50Al30

log.lammps

```
# Output strain and stress info to file
# for units metal, pressure is in [bars] = 100 [kPa] = 1/10000 [GPa]
# p2, p3, p4 are in GPa
variable strain equal "(lx - v_L0)/v_L0"
variable p1 equal "v_strain"
variable p2 equal "-pxx/10000"
variable p3 equal "-pyy/10000"
variable p4 equal "-pzz/10000"
fix def1 all print 100 "${p1} ${p2} ${p3} ${p4}" file ni20ti50al30_100.def1.dat screen no

# Use cfg for AtomEye
#dump     1 all cfg 250 dump.tensile_*.cfg mass type xs ys zs c_csym c_peratom fx fy fz
#dump_modify 1 element Ni Al Ti
dump     2 all custom 250 dump.lammpstrj id type x y z
dump_modify 2 sort id

# Display thermo
thermo  100
thermo_style  custom step v_strain temp v_p2 v_p3 v_p4 ke pe press

run   100000
Per MPI rank memory allocation (min/avg/max) = 16.85 | 16.92 | 17.02 Mbytes
Step v_strain Temp v_p2 v_p3 v_p4 KinEng PotEng Press
       0 3.6301943e-16    298.94868  -0.28146008  -0.23583548   0.33545428    1236.5102   -148624.83    606.13762
     100        0.001    300.50141  -0.32193202 -0.031570064 -0.098414424    1242.9325   -148633.73    1506.3883
     200        0.002     296.5103  -0.13608592   0.10699635 -0.031547185    1226.4245   -148616.58     202.1225
     300        0.003    300.96916 -0.073213665 -0.046953719 0.0017827702    1244.8673   -148634.75    394.61538
     400        0.004    300.52496  0.049516534 0.0020598325  0.057853124    1243.0299   -148632.03   -364.76497
     500        0.005    300.37593   0.14440369 0.00082546246 -0.023351276    1242.4136   -148630.29    -406.2596
     600        0.006    298.11584   0.23615626  0.045375897 -0.00054885745    1233.0653   -148619.34   -936.61098
     700        0.007    300.15299   0.30878374  -0.01035231  -0.02669082    1241.4914   -148626.01   -905.80203
     800        0.008    299.40971   0.41935482  0.014832806  0.043448734    1238.4171   -148620.75   -1592.1212
     900        0.009    298.06097    0.4793496 -0.0060547688 -0.0094842813    1232.8384   -148612.73   -1546.0352
    1000         0.01    298.70648   0.59442388  0.022038186 0.0044199231    1235.5083   -148612.68   -2069.6066
    1100        0.011    300.21238   0.71621951 -0.0039924727  0.030428984    1241.7371   -148615.77   -2475.5201
    1200        0.012    300.25157   0.76375635 -0.005282997  0.030834605    1241.8991   -148612.54   -2631.0265
    1300        0.013    297.57391   0.87987918 0.0021361588 -0.00012549516    1230.8238   -148597.76   -2939.6328
    1400        0.014    297.02958   0.89946709 -0.021855678 -0.016636613    1228.5724   -148591.57    -2869.916
    1500        0.015    297.68115    1.011091 0.0056957188  0.026358739    1231.2674   -148590.05   -3477.1517
    1600        0.016     298.0619   1.0795752 -0.049081452 -0.059285303    1232.8423   -148587.12   -3237.3615
    1700        0.017      298.644   1.2217722  0.051295776   0.04461598    1235.2499   -148584.66    -4392.28
```

1.7 Log Lammps Uji Tarik Ni30Ti50Al20

log.lammps

```
# Output strain and stress info to file
# for units metal, pressure is in [bars] = 100 [kPa] = 1/10000 [GPa]
# p2, p3, p4 are in GPa
variable strain equal "(lx - v_L0)/v_L0"
variable p1 equal "v_strain"
variable p2 equal "-pxx/10000"
variable p3 equal "-pyy/10000"
variable p4 equal "-pzz/10000"
fix def1 all print 100 "${p1} ${p2} ${p3} ${p4}" file Al_SC_100.def1.dat screen no

# Use cfg for AtomEye
#dump     1 all cfg 250 dump.tensile_*.cfg mass type xs ys zs c_csym c_peratom fx fy fz
#dump_modify 1 element Ni Al Ti
dump     2 all custom 250 dump.lammpstrj id type x y z
dump_modify 2 sort id

# Display thermo
thermo  100
thermo_style  custom step v_strain temp v_p2 v_p3 v_p4 ke pe press

run   100000
Per MPI rank memory allocation (min/avg/max) = 17.02 | 17.08 | 17.13 Mbytes
Step v_strain Temp v_p2 v_p3 v_p4 KinEng PotEng Press
       0           0    300.58824  -0.86761338   0.65857714   0.25401733    1243.2917   -151470.47   -149.93694
     100        0.001    302.76001   -1.2808155  -0.29737691  -0.27898461    1252.2746   -151484.03     6190.59
     200        0.002    301.37608  -0.83995984   0.10799621   0.25075494    1246.5503    -151480.9     1604.029
     300        0.003    302.38295  -0.96399664 -0.054239332  -0.09637784    1250.7149   -151487.43    3715.3794
     400        0.004    301.03363  -0.76778762  0.072401472  0.044905312    1245.1339   -151483.99    2168.2695
     500        0.005    302.46114  -0.78441449 -0.061670647  -0.02837834    1251.0384   -151491.79    2914.8782
     600        0.006    301.05563  -0.64521765  0.066552684   0.04772818    1245.2249   -151487.77    1769.7893
     700        0.007    302.43792  -0.60362073 -0.027190159 -0.021751862    1250.9423   -151495.11    2175.2092
     800        0.008    301.06945  -0.53870327  0.034409539  0.011789701    1245.2821   -151490.87    1641.6801
     900        0.009    301.54406  -0.46770906 -0.023449764 -0.018102672    1247.2451   -151494.12    1697.5383
    1000         0.01    302.57862  -0.43491309  0.045229647 -0.049676389    1251.5243   -151499.58    1464.5328
    1100        0.011    303.16268  -0.26176273  0.044696102  0.069274279    1253.9401   -151502.85    492.64116
    1200        0.012    301.30553  -0.27905576 -0.087883172 -0.045890252    1246.2585   -151495.83    1376.0973
    1300        0.013    300.13415 -0.095577664  0.084038452  0.055443149    1241.4135   -151491.37   -146.34646
    1400        0.014    299.77667  -0.13351664 -0.045701539 -0.036413725    1239.9349   -151490.06    718.77301
    1500        0.015     301.3679  0.066148389  0.018104034  0.022274495    1246.5165    -151496.6   -355.08973
    1600        0.016    300.41474  0.057698789 -0.013966531 -0.010958549    1242.5741   -151492.28    -109.2457
    1700        0.017     300.7555   0.15302002  0.029614604 -0.010171892    1243.9835   -151493.19   -574.87576
```