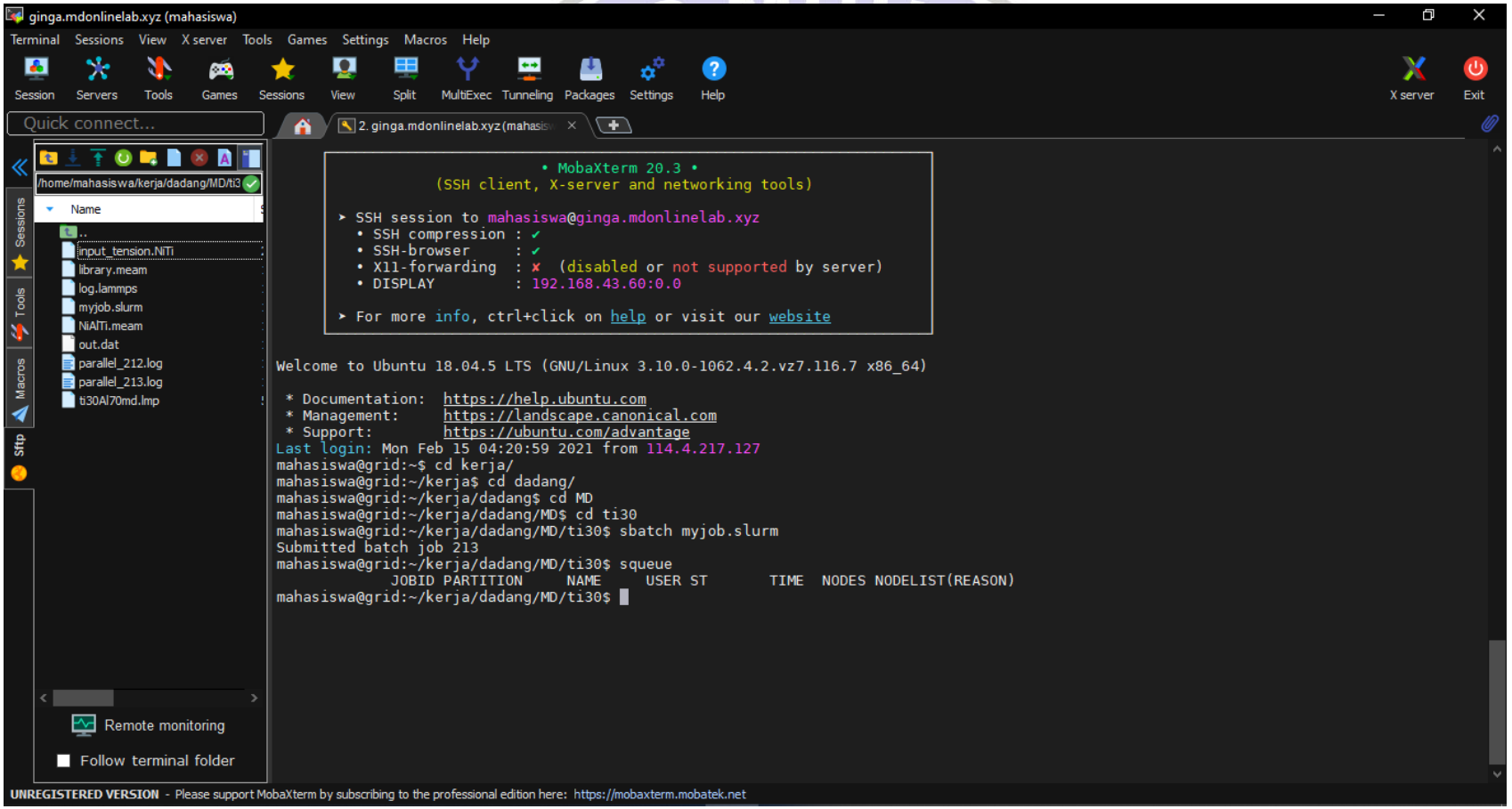
LAMPIRAN

1.1 Proses Menjalankan Simulasi dengan Aplikasi MobaXterm



1.1 Log LAMMPS Optimasi TiAl

log.lammps

```
  update every 1 steps, delay 0 steps, check yes
  max neighbors/atom: 2000, page size: 100000
  master list distance cutoff = 7
  ghost atom cutoff = 7
  binsize = 3.5, bins = 23 23 23
  2 neighbor lists, perpetual/occasional/extra = 2 0 0
  (1) pair meam/c, perpetual
      attributes: full, newton on
      pair build: full/bin/atomonly
      stencil: full/bin/3d
      bin: standard
  (2) pair meam/c, perpetual, half/full from (1)
      attributes: half, newton on
      pair build: halffull/newton
      stencil: none
      bin: none
Per MPI rank memory allocation (min/avg/max) = 86.95 | 86.95 | 86.95 Mbytes
Step Temp TotEng PotEng Press Volume Lx Ly Lz
       0            0   -143648.46   -143648.46    61896.437    510848.86        79.94        79.94        79.94
      10            0      -143975      -143975    23645.203    522647.24    80.456581    80.456581       80.7394
      20            0   -144046.08   -144046.08   -324.92928    530494.41    80.660005    80.660005       81.5388
      30            0   -144051.04   -144051.04   -66.452018    529588.01    80.374914    80.374914      81.97796
      40            0   -144051.04   -144051.04   -5.2076965    529544.34    80.366565    80.366565     81.988232
      50            0   -144051.04   -144051.04  -0.15191111    529540.92    80.365938    80.365938      81.98898
      54            0   -144051.04   -144051.04   0.13525269    529540.74    80.365908    80.365908     81.989015
Loop time of 68.6037 on 1 procs for 54 steps with 32000 atoms

99.4% CPU use with 1 MPI tasks x no OpenMP threads

Minimization stats:
  Stopping criterion = linesearch alpha is zero
  Energy initial, next-to-last, final =
     -143648.462973826  -144051.040400435  -144051.040400435
  Force two-norm initial, final = 34811.819 0.089191496
  Force max component initial, final = 25114.145 0.081947056
  Final line search alpha, max atom move = 1.4896241e-06 1.2207031e-07
  Iterations, force evaluations = 54 119
```

1.2 Log LAMMPS Uji Tarik TiAl

log.lammps

Step	Lx	Ly	Lz	Press	Pxx	Pyy	Pzz	PotEng	Temp
0	80.365908	80.365908	81.989015	2503.0307	2480.171	2504.8411	2524.0801	-144051.04	300
100	80.562237	80.562237	82.18931	-3602.2379	-2802.8389	-2766.2525	-5237.6223	-143438.8	151.05672
200	80.507846	80.507846	82.13382	-574.77533	615.70666	611.20553	-2951.2382	-143410.58	145.04665
300	80.45971	80.45971	82.084712	1932.0577	2603.4943	2628.5007	564.1782	-143434.03	151.97776
400	80.519097	80.519097	82.145299	-1020.0344	54.046249	53.644359	-3167.7938	-143410.73	147.59517
500	80.500795	80.500795	82.126626	-154.19802	835.46821	866.40612	-2164.4684	-143423.47	152.04783
600	80.486123	80.486123	82.111658	662.02494	1465.3116	1494.0429	-973.27972	-143423.81	153.59539
700	80.50881	80.50881	82.134804	-408.33946	526.173	602.1789	-2353.3703	-143402.99	150.03978
800	80.497883	80.497883	82.123656	161.0446	1129.0737	1143.6487	-1789.5886	-143407.94	152.73228
900	80.496345	80.496345	82.122086	204.38166	1132.1999	1151.5738	-1670.6288	-143413.74	155.65276
1000	80.507577	80.507577	82.133545	-308.64389	664.89799	675.82303	-2266.6527	-143403.59	154.73444
1100	80.498684	80.498684	82.124473	211.54404	1116.8122	1099.7436	-1581.9237	-143398.46	155.02913
1200	80.501653	80.501653	82.127502	-2.4193156	958.07722	945.91332	-1911.2485	-143411.53	159.73506
1300	80.507541	80.507541	82.133509	-164.64175	827.64011	817.54908	-2139.1144	-143388.89	155.82121
1400	80.500713	80.500713	82.126543	175.2431	1120.3016	1084.3846	-1678.9569	-143394.68	158.7765
1500	80.50462	80.50462	82.130529	-41.372935	888.62859	913.70198	-1926.4494	-143397.57	161.03683
1600	80.508875	80.508875	82.13487	-144.89978	877.16621	812.76632	-2124.6319	-143383.74	159.26178
1700	80.503357	80.503357	82.12924	152.94553	1160.1953	1128.9738	-1830.3325	-143384.53	161.02081
1800	80.507227	80.507227	82.133188	-48.913011	943.82556	919.36664	-2009.9312	-143382.81	162.17631
1900	80.50952	80.50952	82.135528	-105.15038	873.80585	881.48839	-2070.7454	-143378.25	162.65097
2000	80.506334	80.506334	82.132278	75.175958	1054.5053	1062.5751	-1891.5526	-143377.97	164.16003
2100	80.511048	80.511048	82.137087	-139.70447	908.14334	864.94503	-2192.2018	-143375.8	165.2133
2200	80.510358	80.510358	82.136383	-28.630108	1023.6495	961.35233	-2070.8921	-143365.56	164.31835
2300	80.508344	80.508344	82.134328	99.534807	1048.9444	1058.1487	-1808.4887	-143366.45	166.11811
2400	80.512725	80.512725	82.138798	-81.333929	930.83782	925.56309	-2100.4027	-143359.62	166.05145
2500	80.51163	80.51163	82.137681	16.481977	1036.5034	1029.1095	-2016.167	-143357.56	167.14061
2600	80.510967	80.510967	82.137004	64.769931	1055.0307	1049.8532	-1910.5742	-143356	168.35026
2700	80.514669	80.514669	82.140781	-74.928734	940.97066	988.90762	-2154.6645	-143349.29	168.31705
2800	80.512529	80.512529	82.138598	77.651825	1077.9056	1093.1652	-1938.1153	-143345.95	169.10125
2900	80.514686	80.514686	82.140798	-64.72918	958.92001	962.81567	-2115.9232	-143352.31	172.2311
3000	80.51683	80.51683	82.142985	-109.11848	904.34292	937.56831	-2169.2667	-143343.62	171.72415
3100	80.513335	80.513335	82.13942	124.80264	1129.5832	1180.1142	-1935.2894	-143338.48	172.07597
3200	80.517784	80.517784	82.143959	-108.32926	952.21893	944.41479	-2221.6215	-143339.48	173.91019
3300	80.51831	80.51831	82.144495	-73.111941	972.08973	956.13608	-2147.5616	-143332.95	173.92967
3400	80.515459	80.515459	82.141587	156.74028	1203.9343	1201.2006	-1934.914	-143321.6	172.78453
3500	80.519192	80.519192	82.145396	1.8573418	1054.3478	1017.4011	-2066.1769	-143320.31	174.07053
3600	80.519981	80.519981	82.1462	-46.534727	1006.4928	1006.5272	-2152.6242	-143324.21	176.61471

Normal text file | length : 247.334 lines : 2.170 | Ln : 1.084 Col : 1 Sel : 0 | 0 | Unix (LF) | UTF-8 | INS

1.4 Log LAMMPS Optimasi $Ti_{60\%}Al_{40\%}$

log.lammps | log.lammps | log.lammps

```
      1600            0   -146645.75   -146645.75    0.2955649    534489.29    80.417572    80.425691    82.640559
      1610            0   -146645.75   -146645.75   0.021290592    534489.36    80.417533    80.425708    82.640593
      1620            0   -146645.75   -146645.75    0.11054077    534489.32     80.41752    80.425724    82.640584
      1630            0   -146645.75   -146645.75     1.4736866       534489    80.417467    80.425931    82.640376
      1640            0   -146645.75   -146645.75     0.2924429    534489.33    80.417574    80.425733     82.64052
      1650            0   -146645.75   -146645.75   0.028880994    534489.38    80.417544    80.425702     82.64059
      1660            0   -146645.75   -146645.75   0.085609543    534489.34    80.417528    80.425696    82.640607
      1670            0   -146645.75   -146645.75     1.5015957    534488.61    80.417275    80.425715    82.640736
      1680            0   -146645.75   -146645.75    0.31797253    534489.23     80.41749    80.425717    82.640608
      1690            0   -146645.75   -146645.75    0.02362223    534489.33    80.417545      80.4257    82.640585
      1700            0   -146645.75   -146645.75    0.19329084    534489.25    80.417576    80.425687    82.640553
      1710            0   -146645.75   -146645.75     1.8665924    534488.65    80.417773     80.42548    82.640472
      1720            0   -146645.75   -146645.75    0.14587089     534489.2    80.417548    80.425671    82.640591
      1730            0   -146645.75   -146645.75   0.025322177    534489.22    80.417529     80.42569    82.640594
      1740            0   -146645.75   -146645.75   0.092781031     534489.2    80.417546    80.425686    82.640577
      1750            0   -146645.75   -146645.75     1.7677015    534488.46    80.417638    80.425433    82.640629
      1760            0   -146645.75   -146645.75     0.2058543    534489.15    80.417553    80.425672    82.640577
      1770            0   -146645.75   -146645.75   0.032622231     534489.2    80.417519    80.425695    82.640596
      1780            0   -146645.75   -146645.75   0.048046969    534489.21    80.417527    80.425691    82.640593
      1790            0   -146645.75   -146645.75     0.8112219    534488.99    80.417645    80.425598    82.640533
      1796            0   -146645.75   -146645.75   0.024533229    534489.25    80.417522    80.425704    82.640591
Loop time of 370.018 on 9 procs for 1796 steps with 32000 atoms

97.3% CPU use with 9 MPI tasks x no OpenMP threads

Minimization stats:
  Stopping criterion = energy tolerance
  Energy initial, next-to-last, final =
     -145965.491966331  -146645.745819488  -146645.745819488
  Force two-norm initial, final = 41049.296 0.024103152
  Force max component initial, final = 28246.424 0.019232799
  Final line search alpha, max atom move = 0.062872693 0.0012092178
  Iterations, force evaluations = 1796 3531

```

1.5 Log LAMMPS Uji Tarik $Ti_{60\%}Al_{40\%}$

log.lammps | log.lammps | log.lammps

	Step	Lx	Ly	Lz	Press	Pxx	Pyy	Pzz	PotEng	Temp
64	0	80.417522	80.425704	82.640591	2479.7597	2457.216	2481.5645	2500.4986	-146645.75	300
65	100	80.616631	80.624834	82.845205	-3909.2218	-3054.7515	-3088.5082	-5584.4058	-146074.44	161.06433
66	200	80.554044	80.562241	82.780888	-360.63552	553.99888	521.74993	-2157.6554	-146007.1	145.62685
67	300	80.516143	80.524336	82.741939	1561.5184	2374.5573	2331.7504	-21.752473	-146031.26	152.70403
68	400	80.570222	80.57842	82.797513	-1118.9421	-243.45826	-96.139849	-3017.228	-146019.46	151.14271
69	500	80.54931	80.557506	82.776023	-63.38306	809.18569	889.83447	-1889.1693	-146023.33	153.45235
70	600	80.537519	80.545714	82.763906	672.73866	1505.0728	1509.0916	-995.94838	-146007.3	151.04374
71	700	80.558724	80.566921	82.785697	-462.58876	490.35509	392.12555	-2270.2469	-146004.21	151.77432
72	800	80.551007	80.559204	82.777767	-26.233152	845.97039	854.11549	-1778.7853	-146011.11	154.93989
73	900	80.546505	80.554701	82.77314	238.3364	1036.0743	1170.0823	-1491.1474	-146008.14	155.741
74	1000	80.559034	80.567231	82.786016	-313.85228	583.60851	593.84782	-2119.0132	-145997.77	154.76504
75	1100	80.548295	80.556492	82.77498	213.44588	1092.0905	1102.9439	-1554.6968	-145996.92	156.0999
76	1200	80.553415	80.561612	82.780242	-14.936075	885.53396	965.55597	-1895.8982	-145994.85	157.14451
77	1300	80.55815	80.566348	82.785108	-237.90298	661.56878	728.70115	-2103.9789	-145995.16	158.77553
78	1400	80.550722	80.558918	82.777474	221.96786	1096.1103	1150.564	-1580.7707	-145989.38	158.93904
79	1500	80.557413	80.56561	82.78435	-108.0423	815.98517	842.8733	-1982.9854	-145987.56	160.05955
80	1600	80.556353	80.56455	82.78326	-15.831195	918.1925	927.43573	-1893.1218	-145980.01	159.80128
81	1700	80.555685	80.563882	82.782574	69.972965	1032.6465	998.70867	-1821.4363	-145978.32	160.96065
82	1800	80.559963	80.56816	82.78697	-133.90362	809.52297	774.03503	-1985.2689	-145976.69	162.14102
83	1900	80.557512	80.56571	82.784452	51.128907	1006.1973	1023.0403	-1875.8509	-145971.06	162.35569
84	2000	80.557415	80.565612	82.784352	19.409592	938.48216	982.28627	-1862.5396	-145968.54	163.32517
85	2100	80.563643	80.571841	82.790752	-174.27243	726.34589	806.61868	-2055.7819	-145965.62	164.20011
86	2200	80.555871	80.564068	82.782765	238.82801	1187.381	1195.8785	-1666.7755	-145960.46	164.53453
87	2300	80.560828	80.569026	82.78786	5.3832929	966.40813	970.65632	-1920.9146	-145956.91	165.25914
88	2400	80.566853	80.575051	82.794051	-238.79393	724.97881	709.12943	-2150.49	-145956.12	166.65133
89	2500	80.556692	80.564889	82.783609	263.33365	1147.9054	1208.3829	-1566.2873	-145952.9	167.4589
90	2600	80.565176	80.573374	82.792327	-64.025854	950.10566	962.44676	-2104.63	-145949.17	168.14484
91	2700	80.565353	80.573551	82.792509	-2.1790984	1013.7771	950.39554	-1970.71	-145944.35	168.57038
92	2800	80.558402	80.566599	82.785366	258.51105	1242.6518	1218.8124	-1685.9311	-145943.16	169.87369
93	2900	80.572483	80.580681	82.799836	-325.76543	702.97581	682.10708	-2362.3792	-145939.96	170.69349
94	3000	80.561189	80.569386	82.78823	236.38902	1194.4441	1244.8384	-1730.1154	-145935.07	171.1018
95	3100	80.566422	80.57462	82.793608	37.662495	971.25984	1061.7138	-1919.9862	-145932.83	172.15404
96	3200	80.570309	80.578507	82.797602	-102.82887	890.9855	906.74218	-2106.2143	-145923.16	171.41381
97	3300	80.563206	80.571403	82.790303	251.38179	1316.1184	1204.3837	-1766.3568	-145927.05	173.95158
98	3400	80.570701	80.5789	82.798006	-84.308234	903.88916	943.29619	-2100.1101	-145919.75	173.78069
99	3500	80.57087	80.579068	82.798179	-89.254316	839.17106	997.00703	-2103.941	-145918.44	175.06415
100	3600	80.565084	80.573282	82.792233	278.90959	1284.2651	1290.9167	-1738.453	-145913.9	175.56788

Normal text file | length : 247.314 lines : 2.170 | Ln : 19 Col : 71 Sel : 0 | 0 | Unix (LF) | UTF-8 | INS

1.6 Log LAMMPS Optimasi $Ti_{70\%}Al_{30\%}$

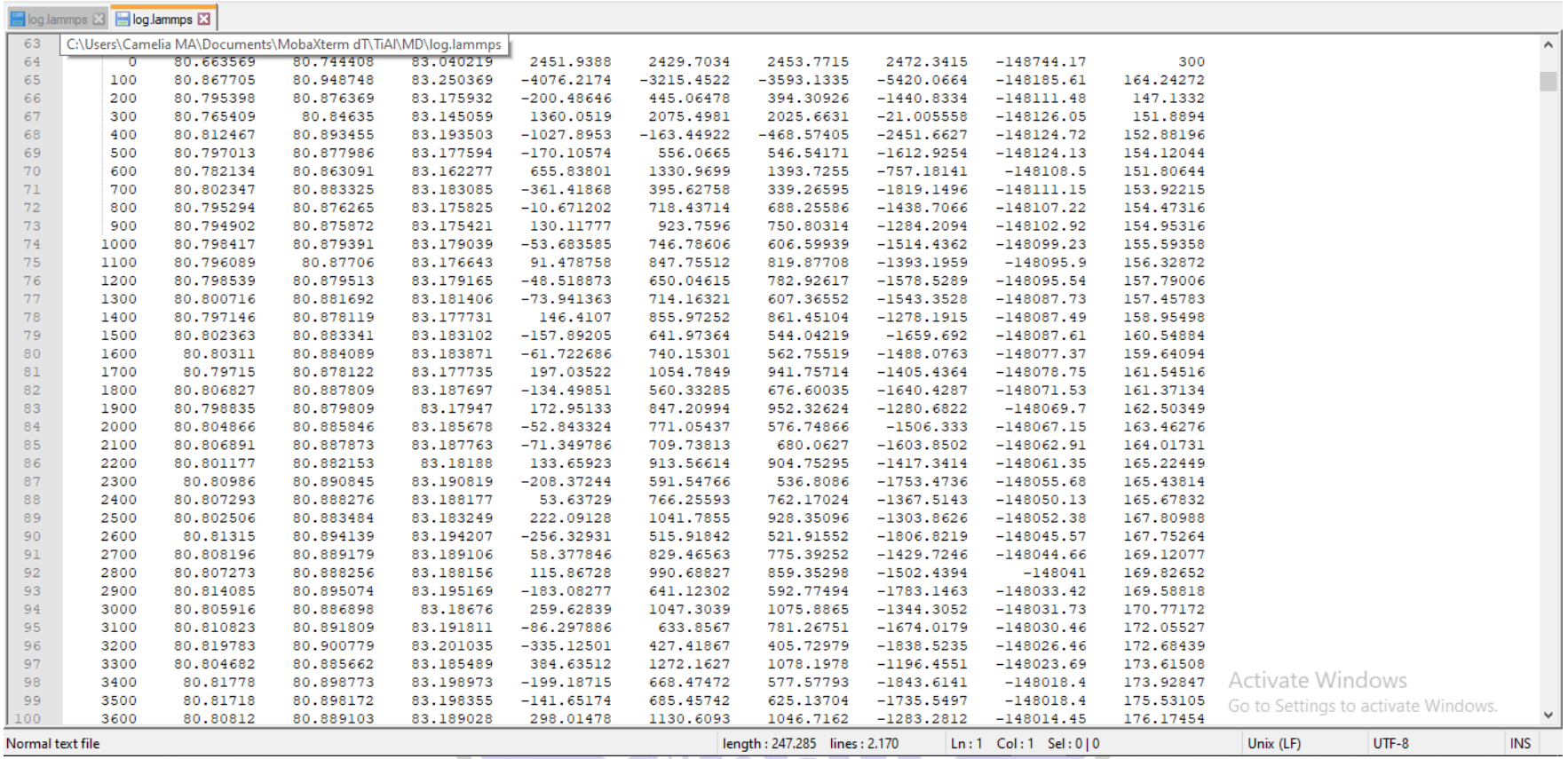
log.lammps log.lammps

```
      4850            0   -148744.16   -148744.16   0.55327221    540852.13    80.663702    80.744191    83.040339
      4860            0   -148744.16   -148744.16    -1.863754    540852.94    80.662463     80.74519    83.040711
      4870            0   -148744.16   -148744.16   0.13861147    540852.34    80.663692    80.744265    83.040305
      4880            0   -148744.17   -148744.17   0.35642114    540851.79    80.661532    80.745539    83.041133
      4890            0   -148744.17   -148744.17  -0.20365238    540852.48    80.663704    80.744234    83.040346
      4900            0   -148744.17   -148744.17    1.2157817    540851.83    80.663042    80.744697    83.040452
      4910            0   -148744.17   -148744.17   -1.3596262    540852.88    80.663831    80.744014    83.040503
      4920            0   -148744.17   -148744.17    0.7076266    540852.15    80.663445    80.744509    83.040278
      4930            0   -148744.17   -148744.17   -4.5709459    540854.13    80.663962    80.743913    83.040663
      4940            0   -148744.17   -148744.17   0.74170313    540852.16    80.663507    80.744477    83.040249
      4950            0   -148744.17   -148744.17   -5.5123905    540854.63    80.663804    80.744302    83.040502
      4960            0   -148744.17   -148744.17    1.6382199     540851.8    80.663511    80.744441    83.040227
      4970            0   -148744.17   -148744.17   -2.5312569    540853.51    80.663612    80.744531    83.040292
      4980            0   -148744.17   -148744.17    3.3321836    540851.13    80.663606    80.744301     83.04017
      4990            0   -148744.17   -148744.17  -0.76788036     540852.8    80.663575    80.744515    83.040238
      5000            0   -148744.17   -148744.17    3.3097941    540851.15    80.663843    80.744091    83.040144
      5010            0   -148744.17   -148744.17  -0.50055296    540852.69    80.663556     80.74452    83.040237
      5020            0   -148744.17   -148744.17   0.85606255    540852.14     80.66379    80.744229    83.040209
      5030            0   -148744.17   -148744.17  -0.63419423    540852.74    80.663436    80.744627    83.040256
      5040            0   -148744.17   -148744.17   0.12105404    540852.44    80.663684    80.744356    83.040234
      5050            0   -148744.17   -148744.17  -0.33838271    540852.59    80.663177    80.744813    83.040309
      5059            0   -148744.17   -148744.17    1.3832407    540851.92    80.663569    80.744408    83.040219
Loop time of 994.396 on 9 procs for 5059 steps with 32000 atoms

97.2% CPU use with 9 MPI tasks x no OpenMP threads

Minimization stats:
  Stopping criterion = max force evaluations
  Energy initial, next-to-last, final =
     -147742.999214559    -148744.1671995  -148744.167200063
  Force two-norm initial, final = 47979.388 0.79761707
  Force max component initial, final = 31158.118 0.49150923
  Final line search alpha, max atom move = 0.0045041968 0.0022138543
  Iterations, force evaluations = 5059 10001
```

1.7 Log LAMMPS Uji Tarik $Ti_{70\%}Al_{30\%}$



log.lammps | log.lammps

C:\Users\Camelia MA\Documents\MobaXterm dT\TiAl\MD\log.lammps

63										
64	0	80.663569	80.744408	83.040219	2451.9388	2429.7034	2453.7715	2472.3415	-148744.17	300
65	100	80.867705	80.948748	83.250369	-4076.2174	-3215.4522	-3593.1335	-5420.0664	-148185.61	164.24272
66	200	80.795398	80.876369	83.175932	-200.48646	445.06478	394.30926	-1440.8334	-148111.48	147.1332
67	300	80.765409	80.84635	83.145059	1360.0519	2075.4981	2025.6631	-21.005558	-148126.05	151.8894
68	400	80.812467	80.893455	83.193503	-1027.8953	-163.44922	-468.57405	-2451.6627	-148124.72	152.88196
69	500	80.797013	80.877986	83.177594	-170.10574	556.0665	546.54171	-1612.9254	-148124.13	154.12044
70	600	80.782134	80.863091	83.162277	655.83801	1330.9699	1393.7255	-757.18141	-148108.5	151.80644
71	700	80.802347	80.883325	83.183085	-361.41868	395.62758	339.26595	-1819.1496	-148111.15	153.92215
72	800	80.795294	80.876265	83.175825	-10.671202	718.43714	688.25586	-1438.7066	-148107.22	154.47316
73	900	80.794902	80.875872	83.175421	130.11777	923.7596	750.80314	-1284.2094	-148102.92	154.95316
74	1000	80.798417	80.879391	83.179039	-53.683585	746.78606	606.59939	-1514.4362	-148099.23	155.59358
75	1100	80.796089	80.87706	83.176643	91.478758	847.75512	819.87708	-1393.1959	-148095.9	156.32872
76	1200	80.798539	80.879513	83.179165	-48.518873	650.04615	782.92617	-1578.5289	-148095.54	157.79006
77	1300	80.800716	80.881692	83.181406	-73.941363	714.16321	607.36552	-1543.3528	-148087.73	157.45783
78	1400	80.797146	80.878119	83.177731	146.4107	855.97252	861.45104	-1278.1915	-148087.49	158.95498
79	1500	80.802363	80.883341	83.183102	-157.89205	641.97364	544.04219	-1659.692	-148087.61	160.54884
80	1600	80.80311	80.884089	83.183871	-61.722686	740.15301	562.75519	-1488.0763	-148077.37	159.64094
81	1700	80.79715	80.878122	83.177735	197.03522	1054.7849	941.75714	-1405.4364	-148078.75	161.54516
82	1800	80.806827	80.887809	83.187697	-134.49851	560.33285	676.60035	-1640.4287	-148071.53	161.37134
83	1900	80.798835	80.879809	83.17947	172.95133	847.20994	952.32624	-1280.6822	-148069.7	162.50349
84	2000	80.804866	80.885846	83.185678	-52.843324	771.05437	576.74866	-1506.333	-148067.15	163.46276
85	2100	80.806891	80.887873	83.187763	-71.349786	709.73813	680.0627	-1603.8502	-148062.91	164.01731
86	2200	80.801177	80.882153	83.18188	133.65923	913.56614	904.75295	-1417.3414	-148061.35	165.22449
87	2300	80.80986	80.890845	83.190819	-208.37244	591.54766	536.8086	-1753.4736	-148055.68	165.43814
88	2400	80.807293	80.888276	83.188177	53.63729	766.25593	762.17024	-1367.5143	-148050.13	165.67832
89	2500	80.802506	80.883484	83.183249	222.09128	1041.7855	928.35096	-1303.8626	-148052.38	167.80988
90	2600	80.81315	80.894139	83.194207	-256.32931	515.91842	521.91552	-1806.8219	-148045.57	167.75264
91	2700	80.808196	80.889179	83.189106	58.377846	829.46563	775.39252	-1429.7246	-148044.66	169.12077
92	2800	80.807273	80.888256	83.188156	115.86728	990.68827	859.35298	-1502.4394	-148041	169.82652
93	2900	80.814085	80.895074	83.195169	-183.08277	641.12302	592.77494	-1783.1463	-148033.42	169.58818
94	3000	80.805916	80.886898	83.18676	259.62839	1047.3039	1075.8865	-1344.3052	-148031.73	170.77172
95	3100	80.810823	80.891809	83.191811	-86.297886	633.8567	781.26751	-1674.0179	-148030.46	172.05527
96	3200	80.819783	80.900779	83.201035	-335.12501	427.41867	405.72979	-1838.5235	-148026.46	172.68439
97	3300	80.804682	80.885662	83.185489	384.63512	1272.1627	1078.1978	-1196.4551	-148023.69	173.61508
98	3400	80.81778	80.898773	83.198973	-199.18715	668.47472	577.57793	-1843.6141	-148018.4	173.92847
99	3500	80.81718	80.898172	83.198355	-141.65174	685.45742	625.13704	-1735.5497	-148018.4	175.53105
100	3600	80.80812	80.889103	83.189028	298.01478	1130.6093	1046.7162	-1283.2812	-148014.45	176.17454

Activate Windows
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Normal text file | length : 247.285 lines : 2.170 | Ln : 1 Col : 1 Sel : 0 | 0 | Unix (LF) | UTF-8 | INS

1.8 Log LAMMPS Optimasi $Ti_{40\%}Al_{60\%}$

log.lammps | log.lammps | log.lammps | log.lammps

```
534      4820            0   -138231.79   -138231.79 -0.091164054    528646.44    80.630373    80.629398    81.315478
535      4830            0   -138231.79   -138231.79  -0.17067093    528646.46    80.630356    80.629408    81.315489
536      4840            0   -138231.79   -138231.79  -0.11292542    528646.44    80.630353    80.629417     81.31548
537      4850            0   -138231.79   -138231.79  0.009536183    528646.36    80.630342    80.629395    81.315502
538      4860            0   -138231.79   -138231.79  0.090868549    528646.34    80.630333    80.629411    81.315491
539      4870            0   -138231.79   -138231.79  0.065602193    528646.36    80.630338    80.629412    81.315487
540      4880            0   -138231.79   -138231.79  0.012339715    528646.37    80.630321    80.629419    81.315499
541      4890            0   -138231.79   -138231.79  -0.11667135    528646.44    80.630338    80.629432    81.315481
542      4900            0   -138231.79   -138231.79  -0.21302714    528646.47    80.630329    80.629433    81.315492
543      4910            0   -138231.79   -138231.79 -0.0042054714     528646.4    80.630337    80.629436    81.315472
544      4920            0   -138231.79   -138231.79  0.080887212    528646.38     80.63035    80.629431     81.31546
545      4930            0   -138231.79   -138231.79  0.056402207     528646.4    80.630348    80.629448    81.315449
546      4940            0   -138231.79   -138231.79 -0.028720357    528646.42    80.630354    80.629428    81.315465
547      4950            0   -138231.79   -138231.79  -0.14802665    528646.46    80.630356    80.629426    81.315472
548      4960            0   -138231.79   -138231.79  -0.17541854     528646.5     80.63038    80.629434    81.315446
549      4970            0   -138231.79   -138231.79   0.11195175    528646.35     80.63035    80.629413    81.315473
550      4980            0   -138231.79   -138231.79 -0.098046843    528646.42    80.630351    80.629412    81.315484
551      4990            0   -138231.79   -138231.79  0.015220055    528646.37    80.630366    80.629383     81.31549
552      5000            0   -138231.79   -138231.79   0.08997503    528646.34    80.630341    80.629407    81.315487
553      5010            0   -138231.79   -138231.79  0.024555833    528646.37    80.630344    80.629414    81.315482
554      5015            0   -138231.79   -138231.79  0.011596308    528646.36     80.63034    80.629399    81.315499
555 Loop time of 1229.88 on 9 procs for 5015 steps with 32000 atoms
556
557 97.5% CPU use with 9 MPI tasks x no OpenMP threads
558
559 Minimization stats:
560   Stopping criterion = max force evaluations
561   Energy initial, next-to-last, final =
562       -137925.764912283   -138231.79063049  -138231.790630513
563   Force two-norm initial, final = 28831.045 0.09540057
564   Force max component initial, final = 19696.541 0.073475149
565   Final line search alpha, max atom move = 0.015504469 0.0011391931
566   Iterations, force evaluations = 5015 10000
567
```

1.9 Log LAMMPS Uji Tarik $Ti_{40\%}Al_{60\%}$

log.lammps | log.lammps | log.lammps | log.lammps

	Step	Lx	Ly	Lz	Press	Pxx	Pyy	Pzz	PotEng	Temp
64	0	80.63034	80.629399	81.315499	2507.1423	2484.265	2509.2251	2527.9368	-138231.79	300
65	100	80.8449	80.843957	81.531883	-3562.8775	-3104.4937	-3048.8367	-4535.3021	-137634.63	154.80451
66	200	80.764112	80.76317	81.450408	34.782246	748.11978	622.05072	-1265.8238	-137604.5	148.4148
67	300	80.753425	80.752483	81.43963	892.93357	1293.8172	1373.1475	11.836008	-137605.84	149.95668
68	400	80.790428	80.789485	81.476947	-762.28145	-196.32934	-127.21337	-1963.3017	-137593.47	148.31107
69	500	80.760187	80.759245	81.44645	590.16929	1173.2869	1125.7797	-528.55866	-137603.91	152.23021
70	600	80.774342	80.773399	81.460724	-27.215198	516.56814	568.41485	-1166.6286	-137597.84	152.19875
71	700	80.780115	80.779173	81.466547	-298.83108	269.80772	193.86538	-1360.1663	-137592.46	152.38357
72	800	80.767455	80.766513	81.453779	322.70823	841.27022	846.98234	-720.12787	-137595.21	154.55078
73	900	80.778971	80.778029	81.465393	-197.33507	355.59802	305.54067	-1253.1439	-137588.63	154.47519
74	1000	80.776047	80.775105	81.462444	43.239601	556.10447	534.79646	-961.18213	-137584.28	154.95422
75	1100	80.772404	80.771462	81.45877	174.90212	753.13891	709.41948	-937.85205	-137581.5	155.82152
76	1200	80.783575	80.782633	81.470037	-221.38442	335.83081	339.73161	-1339.7157	-137578.97	156.75638
77	1300	80.770264	80.769322	81.456613	492.42719	992.97333	1090.2423	-605.9341	-137575.98	157.58718
78	1400	80.778764	80.777822	81.465184	-26.502707	596.12681	449.04173	-1124.6767	-137573.42	158.5179
79	1500	80.785669	80.784727	81.472148	-378.63606	290.11042	131.7023	-1557.7209	-137568.98	159.01242
80	1600	80.776543	80.7756	81.462944	203.58622	675.74257	762.27736	-827.26127	-137562.25	158.95187
81	1700	80.783274	80.782332	81.469733	-119.46404	459.43862	380.66235	-1198.4931	-137563.07	160.71752
82	1800	80.782953	80.782011	81.469409	-70.388724	475.63991	587.81636	-1274.6224	-137559.8	161.49949
83	1900	80.780411	80.779469	81.466845	157.32045	684.26089	717.26486	-929.56438	-137553.5	161.5535
84	2000	80.785225	80.784283	81.4717	-118.5045	425.70509	484.30236	-1265.5209	-137549.42	162.1423
85	2100	80.783382	80.78244	81.469841	87.63038	641.76175	674.46801	-1053.3386	-137548.71	163.5479
86	2200	80.780188	80.779245	81.46662	244.78181	854.12943	705.07201	-824.85601	-137546.33	164.55457
87	2300	80.790809	80.789867	81.477332	-236.62705	351.58872	408.40238	-1469.8723	-137543.99	165.57214
88	2400	80.782914	80.781972	81.46937	223.08756	776.80945	781.36374	-888.91052	-137541.15	166.47002
89	2500	80.785441	80.784498	81.471918	75.524878	630.557	656.38348	-1060.3658	-137537.43	167.15571
90	2600	80.793306	80.792364	81.47985	-306.27338	264.383	326.67595	-1509.8791	-137535.73	168.33238
91	2700	80.784035	80.783092	81.4705	211.85424	763.55012	747.37823	-875.36564	-137527.8	168.00377
92	2800	80.789474	80.788531	81.475985	85.000142	672.94979	628.02345	-1045.9728	-137522.87	168.40501
93	2900	80.78752	80.786577	81.474014	125.04197	659.4871	752.01072	-1036.3719	-137523.64	170.1849
94	3000	80.792863	80.79192	81.479403	-166.12032	485.48787	393.72837	-1377.5772	-137524.58	172.00507
95	3100	80.793531	80.792588	81.480076	-101.24864	500.56082	523.43786	-1327.7446	-137517.55	171.89754
96	3200	80.787485	80.786543	81.473979	208.90478	792.78554	774.04746	-940.11865	-137513.48	172.51039
97	3300	80.797613	80.796671	81.484194	-197.90775	292.10121	491.72165	-1377.5461	-137512.01	173.75157
98	3400	80.78923	80.788288	81.47574	227.02825	756.67976	923.8057	-999.4007	-137501.48	172.80366
99	3500	80.793827	80.792885	81.480376	14.235359	656.44614	551.31973	-1165.0598	-137505.74	175.42695
100	3600	80.800379	80.799436	81.486983	-333.90228	245.96935	280.19423	-1527.8704	-137502.58	176.26662

Normal text file | length : 247.302 lines : 2.170 | Ln : 1 Col : 1 Sel : 0 | 0 | Unix (LF) | UTF-8 | INS

1.10 Log LAMMPS Optimasi $Ti_{30\%}Al_{70\%}$

log.lammps | log.lammps | log.lammps | log.lammps | log.lammps

```
    1080            0   -131540.55   -131540.55    1.1852477    527839.07    80.737747    80.715844    80.996474
    1090            0   -131540.55   -131540.55    1.6769953    527838.59    80.737519    80.715665    80.996809
    1100            0   -131540.55   -131540.55   0.75413599    527839.16    80.737745    80.715763    80.996572
    1110            0   -131540.55   -131540.55    0.2436537    527839.27    80.737729    80.715669    80.996699
    1120            0   -131540.55   -131540.55  0.069339872    527839.35    80.737764    80.715678    80.996667
    1130            0   -131540.55   -131540.55  0.029255504    527839.34    80.737759    80.715668    80.996681
    1140            0   -131540.55   -131540.55  0.024218684    527839.36     80.73776     80.71567    80.996679
    1150            0   -131540.55   -131540.55   0.04865862    527839.37    80.737763     80.71568     80.99667
    1160            0   -131540.55   -131540.55   0.15636811    527839.33    80.737741    80.715673    80.996691
    1170            0   -131540.55   -131540.55   0.38375593    527839.31    80.737767    80.715731    80.996604
    1180            0   -131540.55   -131540.55    1.1535743    527838.81    80.737615    80.715595    80.996817
    1190            0   -131540.55   -131540.55   0.75892539     527839.2    80.737822    80.715729    80.996534
    1200            0   -131540.55   -131540.55    0.2764656    527839.26    80.737746    80.715639    80.996712
    1210            0   -131540.55   -131540.55  0.083379558    527839.37    80.737772    80.715672    80.996668
    1220            0   -131540.55   -131540.55  0.029606524    527839.37    80.737763     80.71567     80.99668
    1230            0   -131540.55   -131540.55   0.01370597    527839.38    80.737763    80.715674    80.996676
    1240            0   -131540.55   -131540.55  0.020340092    527839.38    80.737765    80.715677    80.996671
    1250            0   -131540.55   -131540.55  0.086354189    527839.34    80.737756    80.715665    80.996686
    1260            0   -131540.55   -131540.55    0.2508383    527839.31    80.737795    80.715683    80.996626
    1270            0   -131540.55   -131540.55   0.80491994    527838.97    80.737736    80.715555     80.99676
    1280            0   -131540.55   -131540.55   0.65833571    527839.17    80.737841    80.715654    80.996586
    1287            0   -131540.55   -131540.55 -0.016871284     527839.4    80.737761    80.715674    80.996681
Loop time of 369.951 on 8 procs for 1287 steps with 32000 atoms

98.1% CPU use with 8 MPI tasks x no OpenMP threads

Minimization stats:
  Stopping criterion = energy tolerance
  Energy initial, next-to-last, final =
     -131294.830287726  -131540.550788238  -131540.550788238
  Force two-norm initial, final = 24381.840 0.015227129
  Force max component initial, final = 15762.215 0.011788938
  Final line search alpha, max atom move = 0.12194697 0.0014376252
  Iterations, force evaluations = 1287 2555
```

1.11 Log LAMMPS Uji Tarik $Ti_{30\%}Al_{70\%}$

log.lammps | log.lammps | log.lammps | log.lammps | log.lammps

Step	Lx	Ly	Lz	Press	Pxx	Pyy	Pzz	PotEng	Temp
0	80.737761	80.715674	80.996681	2510.9038	2488.0397	2512.8066	2531.8649	-131540.55	300
100	80.976026	80.953875	81.23571	-3443.3074	-3136.6633	-3226.7347	-3966.5243	-130947.23	155.77521
200	80.863854	80.841733	81.123178	990.37761	1226.7076	1346.7792	397.64601	-130919.18	149.90944
300	80.894973	80.872843	81.154397	30.82751	268.41689	304.81372	-480.74808	-130905	147.6036
400	80.901719	80.879587	81.161165	-339.27222	6.6725342	-184.71341	-839.77578	-130904.59	148.8527
500	80.879758	80.857633	81.139134	544.44578	739.93832	817.55517	75.843855	-130916.11	153.05387
600	80.909211	80.887077	81.168681	-705.88672	-429.67125	-387.53192	-1300.457	-130902.77	151.27404
700	80.889964	80.867835	81.149372	194.03148	518.99354	405.42576	-342.32487	-130903.12	152.82813
800	80.895778	80.873648	81.155205	-48.100962	220.42034	231.41297	-596.13619	-130904.43	154.64488
900	80.903154	80.881022	81.162604	-338.02546	-64.436872	-40.363544	-909.27598	-130899.53	154.97775
1000	80.891999	80.86987	81.151413	265.08691	577.57912	510.37168	-292.69005	-130896.01	155.66274
1100	80.900425	80.878294	81.159867	-12.949112	292.23057	256.42401	-587.50192	-130886.23	154.83445
1200	80.898339	80.876209	81.157774	-2.7247672	222.40543	393.62309	-624.20282	-130890.2	157.33912
1300	80.900849	80.878718	81.160292	26.990204	245.56299	213.73134	-378.32371	-130885.59	157.77978
1400	80.900072	80.877941	81.159513	39.852829	463.66091	287.71051	-631.81293	-130878.09	157.52567
1500	80.902745	80.880613	81.162194	-37.081949	222.13628	271.83208	-605.2142	-130876.64	158.73485
1600	80.899284	80.877153	81.158722	165.15993	422.52156	430.38631	-357.42807	-130876.67	160.30915
1700	80.904882	80.882749	81.164337	-47.713382	256.75607	239.14174	-639.03796	-130873.33	161.06855
1800	80.904728	80.882596	81.164183	4.2904607	259.40569	238.9177	-485.45201	-130866.33	160.94969
1900	80.9014	80.879268	81.160844	133.78225	410.53376	439.54562	-448.73264	-130861.15	161.27116
2000	80.909146	80.887013	81.168616	-134.98155	193.83149	38.204901	-636.98103	-130859.52	162.4539
2100	80.90353	80.881398	81.162981	75.87241	367.28849	383.9406	-523.61186	-130857.41	163.52366
2200	80.910512	80.888378	81.169986	-94.492408	157.34504	131.71938	-572.54164	-130857.86	165.2094
2300	80.906181	80.884049	81.165641	-14.403535	387.77824	192.87713	-623.86597	-130851.59	165.27671
2400	80.913252	80.891118	81.172735	-191.70811	13.964985	142.65817	-731.74748	-130850.13	166.50797
2500	80.903576	80.881444	81.163028	243.16861	454.91907	559.39176	-284.80498	-130844.7	166.78343
2600	80.916899	80.894764	81.176394	-323.53773	-13.875163	-31.139095	-925.59894	-130848.59	169.30944
2700	80.908592	80.886459	81.16806	38.871346	425.56859	255.13545	-564.09001	-130838.85	168.54254
2800	80.914139	80.892004	81.173624	-87.020635	70.981537	319.37093	-651.41437	-130840.23	170.46696
2900	80.911208	80.889074	81.170684	81.945475	472.21389	246.04728	-472.42474	-130832.61	170.21751
3000	80.914453	80.892318	81.17394	-29.626784	236.24876	358.06282	-683.19193	-130832.17	171.70425
3100	80.916009	80.893874	81.1755	-123.15268	141.24923	265.76909	-776.47634	-130826.6	171.95152
3200	80.914045	80.89191	81.17353	92.511737	343.57419	358.44582	-424.4848	-130820.98	172.18492
3300	80.915854	80.893719	81.175345	-60.606956	263.44489	233.07471	-678.34046	-130821.44	173.89431
3400	80.922012	80.899875	81.181523	-278.94634	17.996755	43.986141	-898.82192	-130814.27	173.75698
3500	80.91524	80.893105	81.174729	120.15074	469.46977	414.3829	-523.40045	-130806.99	173.59631
3600	80.920068	80.897931	81.179572	-81.056341	233.97763	205.90147	-683.04812	-130808.28	175.50626

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