



# MD Project on Fortran

## Group members

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# Problems

- Using git is nontrivial
- Start working
- Split the work
- Understand the problem to modify the program
- Unfamiliar with different programming languages

# Solutions to the problems

- Splitting the job according to individual background.
- The work was split as follows
  - Introducing new potential
  - Interface
  - Changing the simulation box geometry
  - Plotting the result
  - Test
  - Modifying the makefile
  - Documentation

4300	51.52583756	16.43399458	-153.89651831	-137.46252373
4400	53.08869594	16.93246307	-154.37591709	-137.44345402
4500	55.28603737	17.63329781	-154.99845634	-137.36515853
4600	50.52525490	16.11486207	-153.47935963	-137.36449756
4700	54.84653681	17.49312057	-154.83400417	-137.34088359
4800	51.57506224	16.44969463	-153.90450914	-137.45481450
4900	44.23946779	14.11003117	-151.44993262	-137.33990145
5000	51.55618628	16.44367421	-153.88370329	-137.44002908
5100	52.12266757	16.62435153	-154.05196408	-137.42761255
5200	52.13002715	16.62669885	-153.96823580	-137.34153696
5300	55.35556133	17.65547225	-155.04035779	-137.38488554
5400	51.28845839	16.35828329	-153.78593865	-137.42765536
5500	49.53566648	15.79923613	-153.13372882	-137.33449269
5600	52.96276129	16.89229663	-154.34734580	-137.45504917
5700	50.09594598	15.97793542	-153.38572872	-137.40779330
5800	51.46571520	16.41481876	-153.74879006	-137.33397130
5900	53.14218747	16.94952401	-154.29467252	-137.34514851
6000	52.92898923	16.88152514	-154.27377338	-137.39224824
6100	58.04377630	18.51286947	-155.82688888	-137.31401940
6200	54.01164128	17.22683342	-154.63489018	-137.40805677
6300	55.52011817	17.70795711	-155.17490943	-137.46695230
6400	50.12992659	15.98877342	-153.32665429	-137.33788087
6500	56.10640541	17.89495147	-155.27205848	-137.37710701
6600	56.34133165	17.96988042	-155.38989872	-137.42001830
6700	48.92908820	15.60577001	-152.93074294	-137.32497293
6800	50.86705783	16.22387898	-153.51852616	-137.29464718
6900	54.29494542	17.31719233	-154.58838121	-137.27118755
7000	54.90145592	17.51063684	-154.87119451	-137.36055555
7100	52.80833130	16.84304170	-154.19187177	-137.34883133
7200	51.52069489	16.43235435	-153.78469258	-137.35233333
7300	48.38021449	15.43070856	-152.78839375	-137.35768133
7400	49.48666251	15.78360648	-153.13325662	-137.34965133
7500	50.58221684	16.13302989	-153.53739404	-137.40436133
7600	56.01190303	17.86481025	-155.36352082	-137.49871133
7700	52.74174994	16.82180580	-154.27725407	-137.45544133
7800	52.39833110	16.71227350	-154.11371283	-137.40143133
7900	56.88454552	18.14313667	-155.54033199	-137.39719133
8000	51.60784846	16.46015169	-153.85738963	-137.39723133
8100	50.75414871	16.18786699	-153.69083733	-137.50297133
8200	51.28855563	16.35831430	-153.70505059	-137.34673133
8300	55.34279672	17.65140102	-155.00202759	-137.35062133
8400	50.99874308	16.26587955	-153.65941491	-137.39353133
8500	56.86547625	18.13705459	-155.55487685	-137.41782133
8600	56.74083956	18.09730213	-155.44463903	-137.34733133
8700	52.09298126	16.61488318	-154.03197990	-137.41709133
8800	50.34814031	16.05837196	-153.40170242	-137.34333133
8900	54.03342233	17.23378041	-154.66360371	-137.42982133
9000	55.30598779	17.63966093	-155.03521370	-137.39555133
9100	53.04007142	16.91695444	-154.38534351	-137.46838133
9200	53.11987387	16.94240716	-154.39128392	-137.44887133
9300	55.12001354	17.58034506	-154.93922146	-137.35887133
9400	53.67118089	17.11824471	-154.59407305	-137.47582133
9500	55.48790169	17.97681777	-155.08043335	-137.38275133
9600	59.67128986	19.03195951	-156.51631981	-137.48436133
9700	53.52121734	17.07041433	-154.54681515	-137.47640133
9800	53.42048111	17.03828485	-154.50307800	-137.46479133
9900	57.65824702	18.38990619	-155.83917640	-137.44927133
10000	54.45012744	17.36668712	-154.78779054	-137.42110133

Simulation Done.

Input Parameters

natoms = 108

mass in AMU = 39.948

epsilon = 0.2379

sigma = 3.405

rcut = 8.5

box length 1 = 17.158

box length 2 = 17.158

box length 3 = 17.158

nr MD steps = 10000

MD time steps = 5.0

output print freq. = 100

Input file = argon\_108.rest

Parameters file = argon\_108.inp

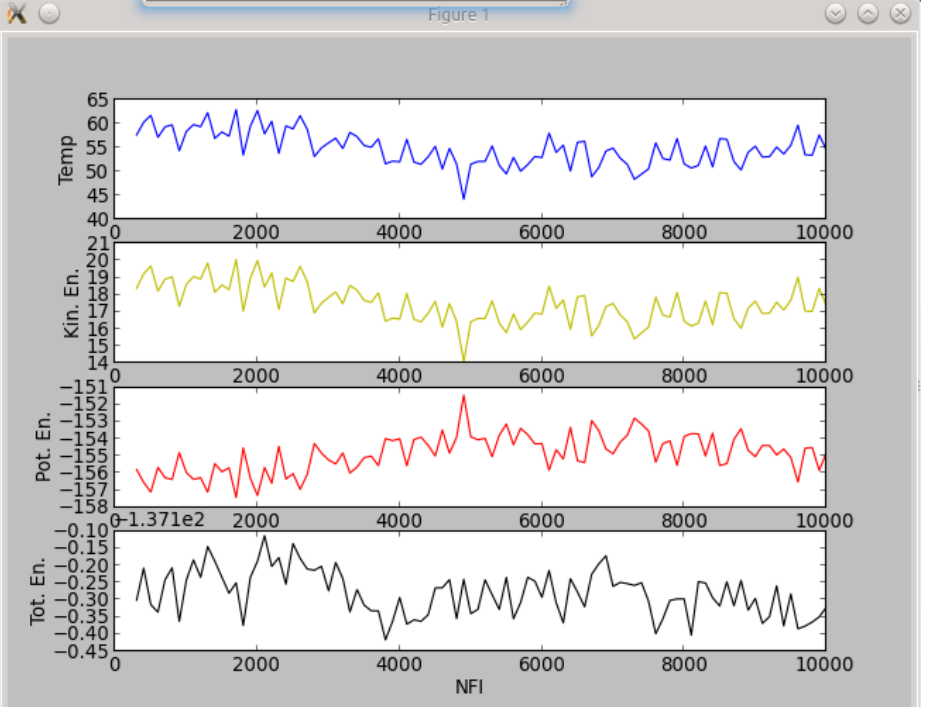
Potential  Lennard-Jones  Morse

Integrator  Verlet  RK4

Input Parameters  Program  User

Method  Serie  Parallel

Calculate Plot



# What we Learn

- How to use git
- Modifying the program
- Working in group
- Using python to integrate your work
- <https://github.com/philippeseil/ljmd-f.git>