CH_ENG 8452: Advanced Chemical Engineering Thermodynamics II
Assignment 5
May 3, 2017
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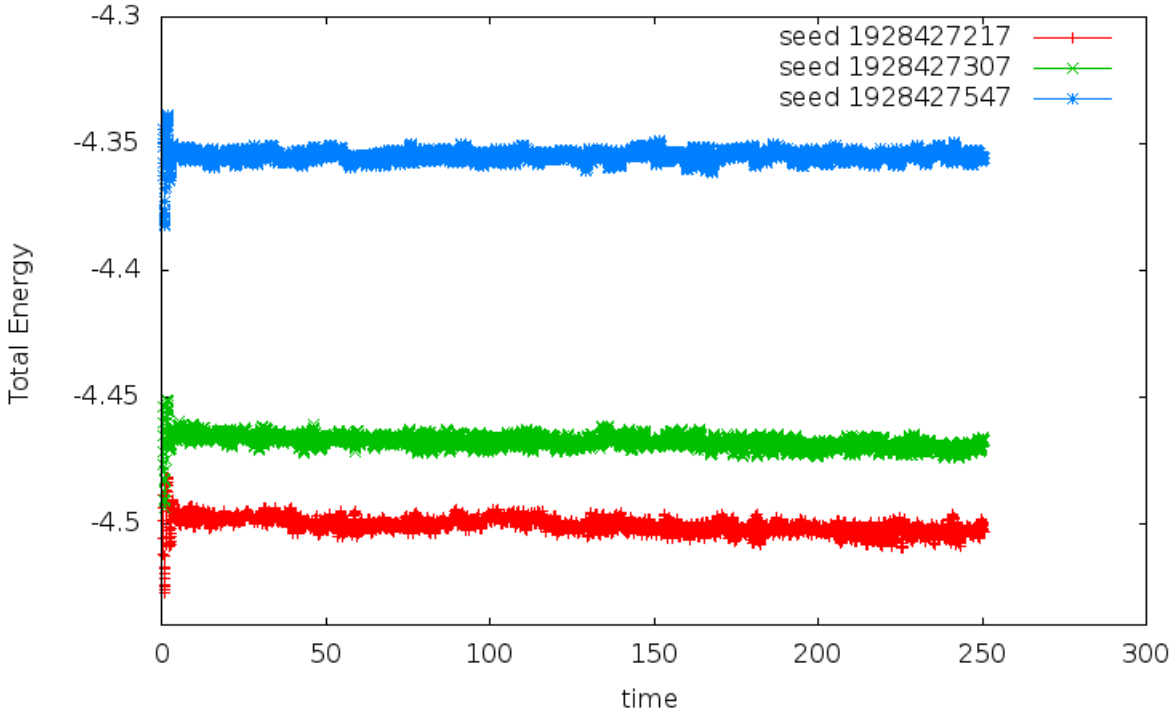

Figure 1: Energy vs time plot for LAMMPS simulation

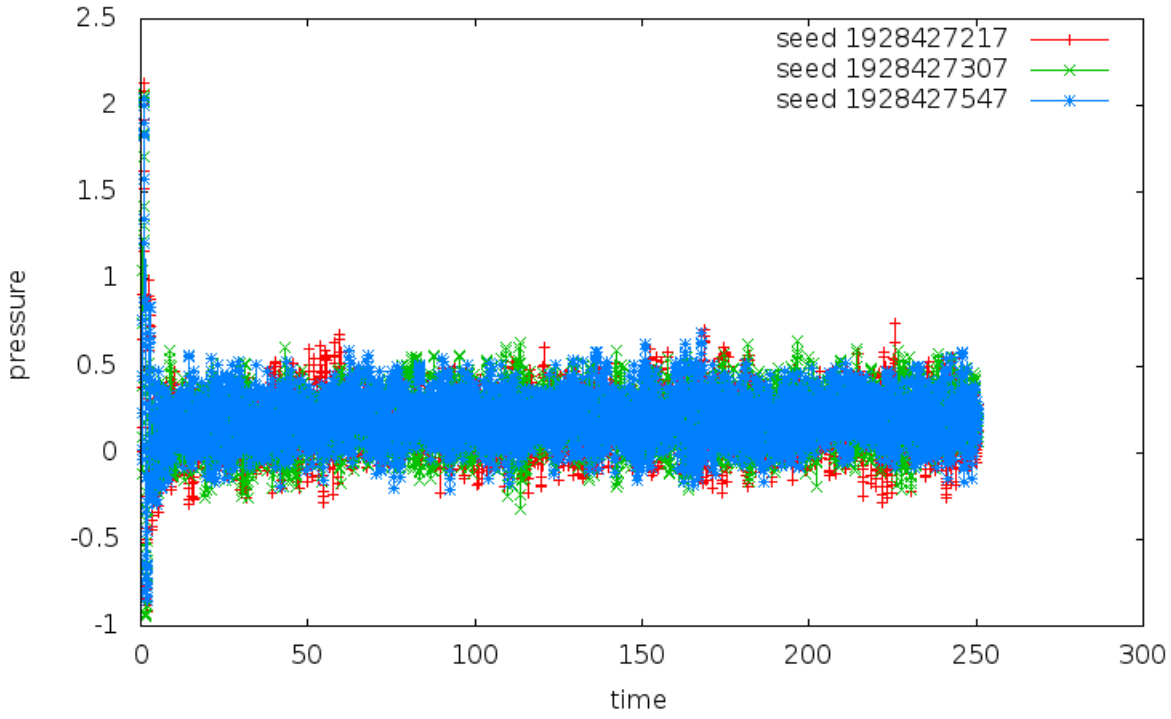

Figure 2: Pressure vs time plot for LAMMPS simulation

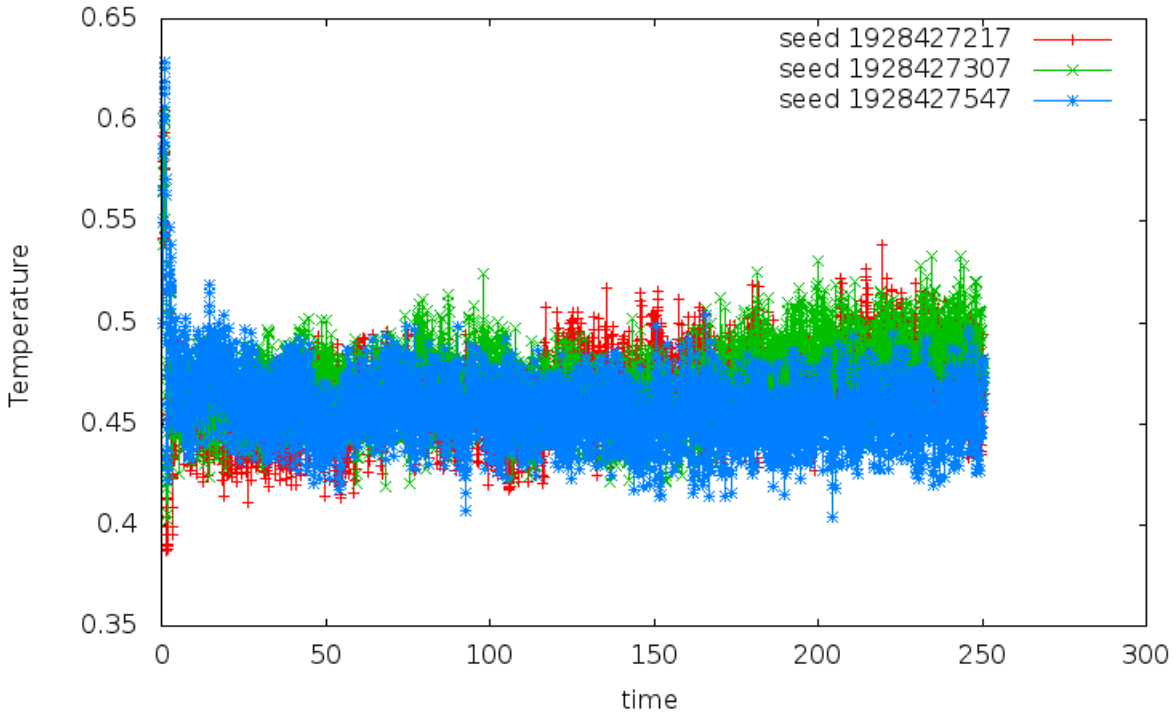

Figure 3: Temperature vs time for LAMMPS simulation

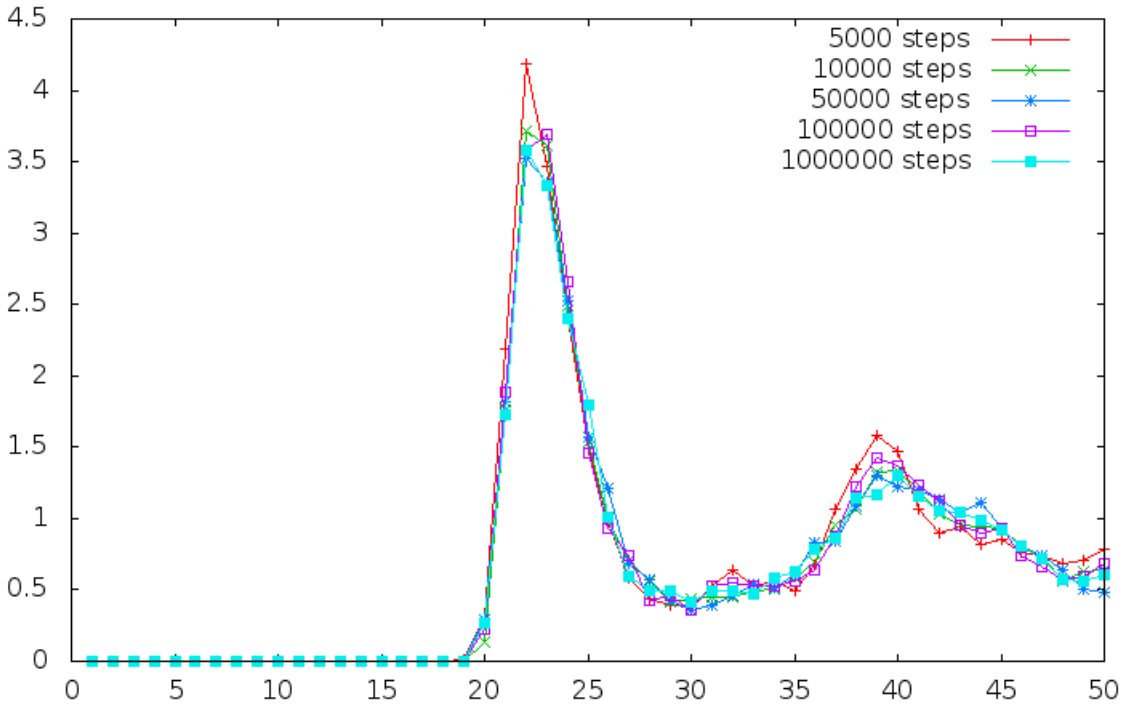

Figure 4: Radial distribution function plot from LAMMPS simulation

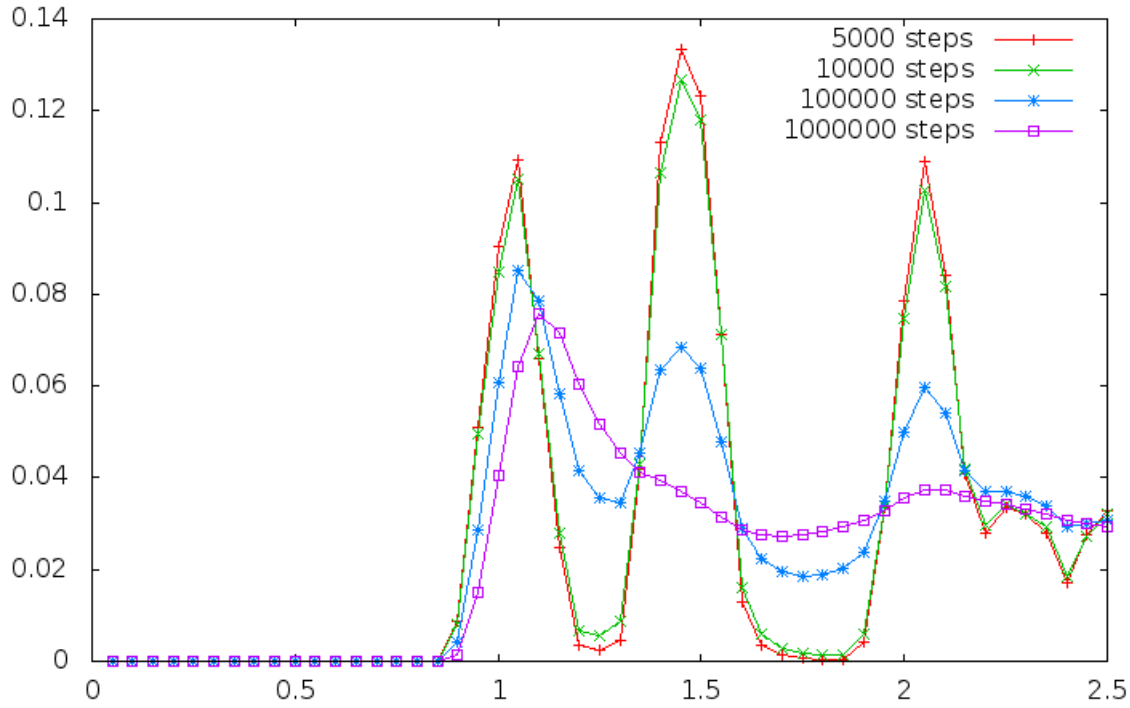

Figure 5: Radial distribution function plot from Monte Carlo program

2. Figure 1 shows the change of energy with respect to time. Energy , temperature(2) and pressure (**??**) plots are included in the report. Actual thermodynamic propertis (i.e energy, temperature and pressure) should be the average value of the data. Since MD simulation mainly deals with microcanonical ensemble.

1 Conclusion