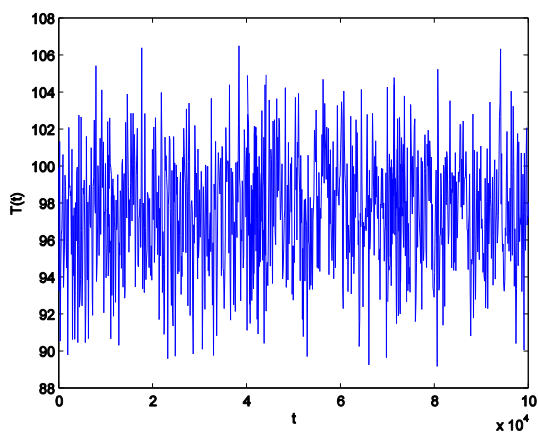
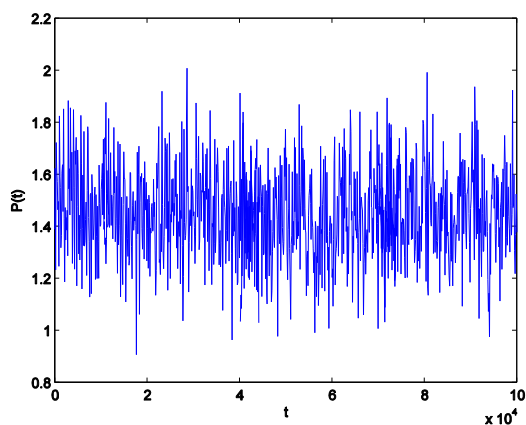


## Q1

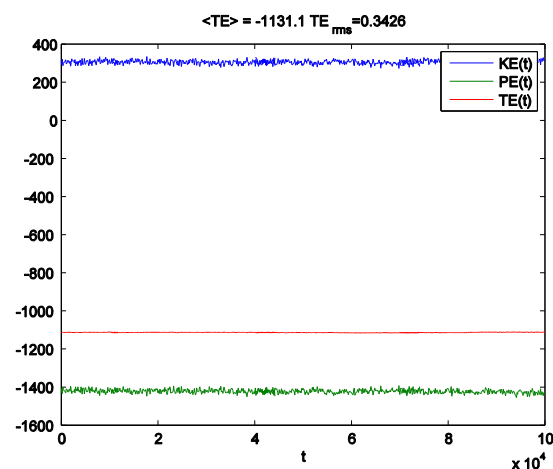
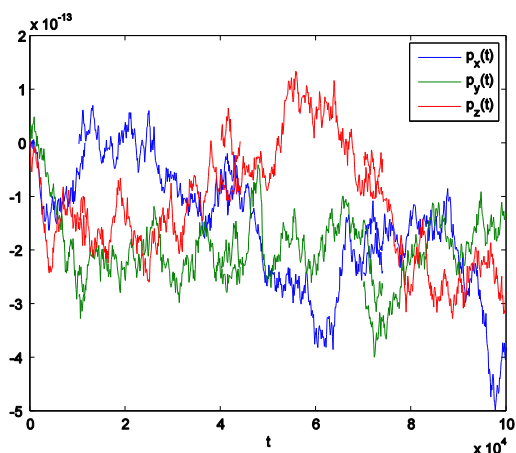
Below are plots of the temperature  $T(t)$ , pressure  $P(t)$ , momentum in the x,y,z directions, and the KE(t), PE(t), and TE(t).



$\langle T \rangle = 97.5821$  K       $T_{\text{rms}} = 3.2228$



$\langle P \rangle = 144.87$        $P_{\text{rms}} = 0.1801$



The momenta are conserved to within machine accuracy. The total energy is conserved such that the RMS fluctuations Terms/ $\langle TE \rangle \sim 10E-4$ .

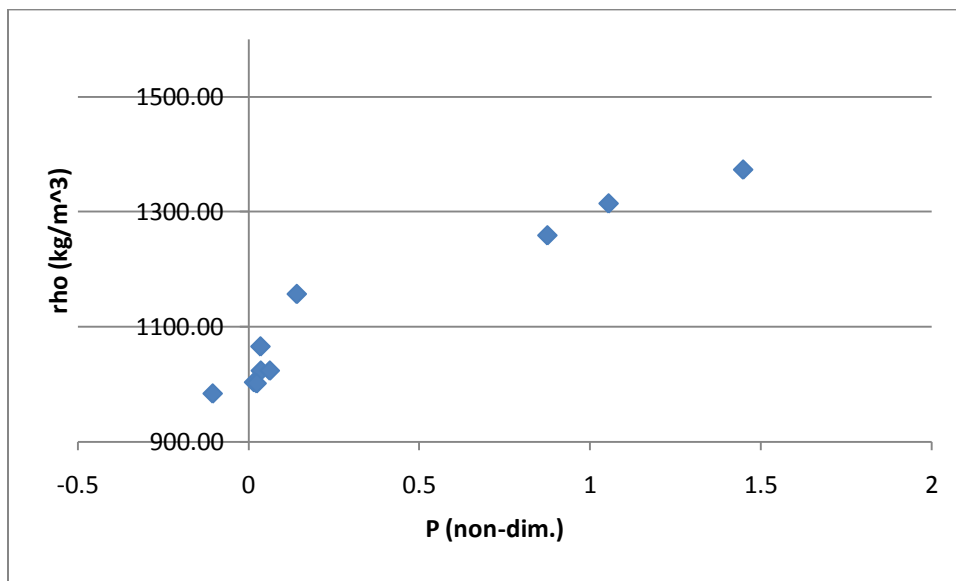
To produce this data, the structure given was “equillibrated” for 20,000 time steps at  $dt=0.002$  using a velocity rescaling at every time step which rescales the momenta by a quantity  $\alpha$  which is proportional to the current temperature  $T$  and the desired temperature  $T_{\text{set}}$ :  $\alpha \sim T_{\text{set}}/T$ . This is a crude way of enforcing a constant “temperature” for the Kinetic energy. Once this equillibration is done, the structure is then run in an NVE for 100,000 time steps, which is the above plotted data. This equillibration period is reduced to 5000 time steps for data taken in Q2.

## Q2

For this problem, data were collected for a given  $T, V$ , and  $P$  by the following procedure:

- 1) Equilibration by velocity rescaling to desired temperature for 5000-2000 time steps at  $dt=0.002$ . To vary  $T$ , the given structure was taken and equilibrated at the desired temperature. Progressively higher temperatures were achieved by taking the result of a previous run and equilibrating. For example, the result of running the given structure at 100K was taken and used as the initial conditions for a run at 200K.
- 2) The volume was changed in a similar way by varying the length of the simulation cube, starting with the given structure at  $L=6.8$ . Progressively larger (or smaller) simulations cubes were attained by changing  $L$  in small amounts (say  $dL=0.1$ ).
- 3) Data collection was taken over the “production” period of 2000-10000 time steps.

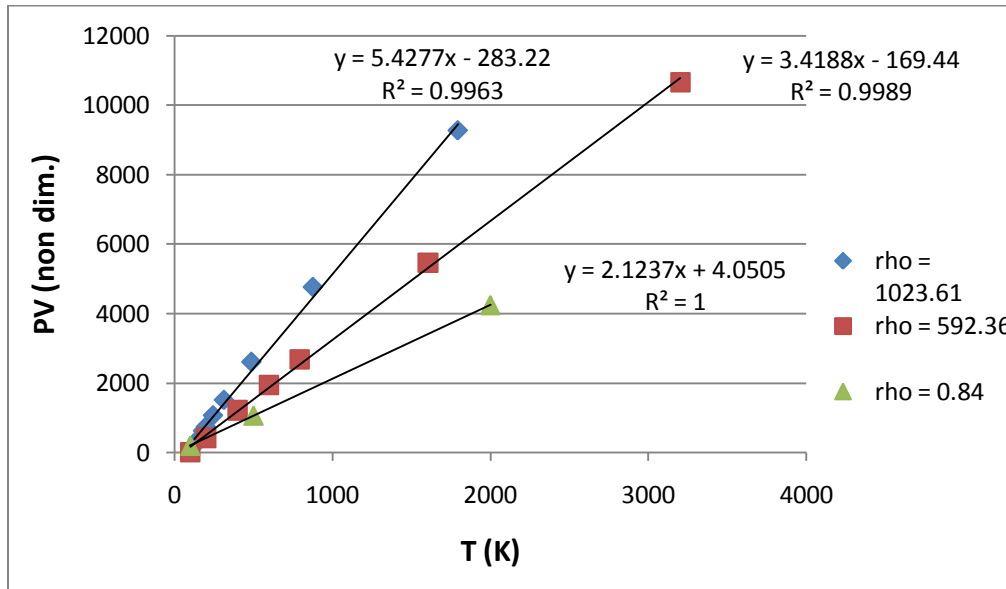
In this way, the 0 pressure density was found for a temperature  $T=100K$ . This value of the density was found to be approximately  $1000 \text{ kg/m}^3$  (see below plot). This corresponds to a value of  $L=7.55$ . Here, the value of the pressure is roughly %1 that of the pressure at  $L=6.8$ . This comparable to some references for liquid Ar at  $T=87K$  and  $P=1 \text{ atm}$  with  $\rho = 1430 \text{ kg/m}^3$  (see <http://physics.info/density/>).



The statement about the Ideal Gas law should hold in the limit that the interactions between atoms is negligible compared to the average kinetic energy, or when the virial contribution to the pressure is small compared to the ideal gas term. One might try to test the Ideal Gas equation of state for this Lennard-Jones Ar system first.

Below is a plot of  $PV$  vs.  $T$ , which for an ideal gas should be a straight line (ignoring Ideal Gas constants, etc.). One can see that linear fits to 3 different densities ( $\text{kg/m}^3$ ) show nearly Ideal

Gas behavior over a wide range of temperatures (about an order of magnitude), particularly for a diffuse  $\rho=0.84 \text{ kg/m}^3$ , which is to be expected.



However, the system mimicking the ideal gas equation of state is not a sufficient condition to claim ideal gas conditions. To investigate this further, the ratio(s) of  $\langle P_{\text{virial}} \rangle / \langle P_{\text{ideal}} \rangle$  and  $\langle PE \rangle / \langle KE \rangle$  are plotted below as functions of the density. One sees that around a density ( $\text{kg/m}^3$ ) of order 1 these 2 ratios are around 0.01, or  $P_{\text{virial}}$  and  $\langle PE \rangle$  are 1% of  $P_{\text{ideal}}$  and  $\langle KE \rangle$ , respectively. This is a more stringent test of the ideal gas condition than the equation of state measurement above. This value of  $\rho \sim 1 \text{ kg/m}^3$  is also close to references for Ar at  $T=300\text{K}$   $P=1 \text{ atm}$ , where  $\rho=1.449 \text{ kg/m}^3$  (see <http://physics.info/density/>).

