Molecular dynamics Project (Category –I)

Using the Python code that I have emailed earlier, calculate the mean square distance ($|\Delta r|^2$) of atoms in face centered cubic (FCC) argon solid with respect to time in a molecular dynamics simulation. The code used the Lennard-Jones Potential between pair of atoms:

$$V(r_{ij}) = V_0\left[\left(\frac{r_0}{r_{ij}}\right)^{12} - 2\left(\frac{r_0}{r_{ij}}\right)^{6}\right]$$

For argon V_0 = 0.01 eV and r_0 = 3.9 Å. Also the mass of each argon atom can be taken as 40 amu (atomic unit). Lattice constant for the argon crystal can be taken as 5.3 Å. We have discussed in the class that, the force derived from the above potential will be negligible at $r > 3r_0$. Build your simulation box considering this fact.

Also calculate the pair distribution function $g(r)$ for the FCC argon as defined in the slides that I have sent to you.

Now break the FCC arrangements of the atoms, then arrange the argon atoms randomly to simulate liquid. Calculate $g(r)$ to see if it behave like liquid.

Units used in the python code are:

Energy in V_0, length in r_0, mass in amu.

So the derived units are:

Time: $r_0\left(\frac{m}{V_0}\right)^{\frac{1}{2}}$; velocity: $\left(\frac{V_0}{m}\right)^{\frac{1}{2}}$; Force: $\frac{V_0}{r_0}$.

Modify and add to the Python code as necessary to analyze your results. Please provide the following:

(a) Necessary methodology and algorithm (30%)
(b) The Python code (20%)
(c) Results, plots and analysis (40%)
(d) Conclusions (10%)

I'll run you code as you send me. If it doesn't run, gives error message etc. you will not get credit on b, c and d.