ZCE 111
Assignment 7

Q1: Export data in *.xyz format

- Based on the steps instructed in http://www2.fizik.usm.my/tlyoon/teaching/ZCE111/1415SEM2/notes/exportformatedlist.nb
  develop a code that
- (i) generate the simulated data for *N* “Carbon” atom moving in a 3D box
- (ii) Cast the simulated data into XYZ format, and export them into a file named NP3D.XYZ. If Mathematica does not allow you to export the file with extension .XYZ you have to first export it as using the name NP3D.dat first, then use **RenameFile[]** command to rename the file name to NP3D.XYZ.
- (iii) Check that you can visualise NP3D.XYZ using the VMD software.
- You do not need to submit part (iii) in your assignment. Just do the practice on your own.

Q2 Detect NR and numberoftimestep in visualiseXYZ.nb automatically

- The code visualiseXYZ.nb imports NP3D.dat and visualise the simulation of NP particles in a box with size L = 1. The data file contains data simulated for a number of time step = numberoftimestep. Using the code visualiseXYZ.nb as a template:
- Determine the number of particles,NP, in the rawdata automatically instead of defining it 'by hand'.
- 2. Determine how many time step (or the number of 'block' in the rawdata), i.e., numberoftimestep, automatically?

Q3
Data Manipulation of *.lampstrj file

- The data file 1700.lammpstrj is yet another form of output file from a LAMMPS run. It's format is quite like the XYZ but slightly more informative. It contains additional information such as: the number index of all atoms, time step for each block, the size of the box, etc.
- 1700.lammpstrj is the result of a molecular dynamics simulation run using LAMMPS for a 2D sheet made up of silicon atoms in a new form of material known as 'silicene'.

Q3 (cont.)

- Write a code to

  (i) Abstract the coordinates of the atoms for all time steps in the data.

  (ii) Abstract the max and min of x-, y- and z-coordinates of the atoms in the box (take a hint from previous description about the *.lammpstrj file).

  (iii) Use Manipulate, Graphics3D[Points] to visualise the data.

Q3 (cont.) Comment

- Your code must be able to automatically abstract the data of number of particles involved in 1700.lammpstrj, to automatically identify where in the data file a time step begin and where it ends, and keep track of the time step of each block.
- Warning: this is going to be a tough exercise, mainly because the data file size is huge. You may experience occasional computer hang sessions during the coding process. In some event you may have to hard boot your computer.