ZCE 111
Assignment 7

Q1: Export animation of *N* Particle in a 3D box into a XYZ data file

Modify your code C4_simulate_Npbox3D.nb (which was already developed for the OTS assignement), which animates N free C atoms moving in a 3D box, to export the simulated data into a XYZ formatted file named NP3D.xyz.

Q2: Visualise XYZ data file in Mathematica

Develop a code to visualize NP3D.xyz using Mathematica automatically without manual intervention. Name your code as A4_visualiseXYZ.nb

Q3: Data manipulation of atom.lammptrj

Download the data file, atom.lammpstrj, which is yet another form of output file from a LAMMPS run. It contains the information of all coordinates of many atoms in a molecular dynamics simulation for a long sequence of time steps, along with some extra information other than the coordinates. Write a code to
(i) abstract the coordinates of the atoms for all time steps in the data.
After you have successfully done (i), continue to the next part:
(ii) visualise the data in Mathematica using Manipulate and Graphics3D[Points] (this part is similar to A4_visualiseXYZ.nb in Q2).
For (ii) to work, you have get (i) to work first.

Q3: Data manipulation of atom.lammptrj (cont.)

Hint: Your code must be able to automatically abstract the data of number of particles involved in atom.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.

Suggestion: use VMD to visualize atom.lammptrj.