Chapter 4

Data Manipulation and visualisation

A particle in a box

Algorithm to simulate a particle moving freely in a rectangular box with edge L:

Define the length of the box, L.
Specify the coordinates of the four corners of the box.
Draw the box
Generate a particle at a random initial position (x0,y0) located within the box.
Give the particles a random initial velocity, v0.
Let the particle's position to evolve in time at the constant initial velocity for a period of time defined in terms of the time scale of the system, T0= v0/L.
Simulate the trajectory of the particle as time evolves
When the particle touches the edges, impose a boundary condition: (a) fixed (b) or periodic boundary condition.

Simulate single particle in a 2D box

- See C4_simulate_1Pbox.nb
- Syntax:
- **Graphics[Point]**
- **Graphics[Line[{Table[coordinates[n], {n, 1, 5}]}]]**
- **Random[]**
- **Graphics[Point[coordxy[it]];**
- **Graphics[{PointSize[0.025], Point[coordxy[it]]}**
- **PlotRange -> {{0, L}, {0, L}}];**

Generalise to *N* Particle in a 2D box

The code comprises of 1 particle in a 2D box can be easily generalised to N particles, see C4_simulate_NPbox.nb.

Data in XYZ format

See http://openbabel.org/wiki/XYZ_(format) for data file in XYZ format.

Example File

```
12
benzene example
  C        0.00000        1.40272        0.00000
  H        0.00000        2.49029        0.00000
  C       -1.21479        0.70136        0.00000
  H       -2.15666        1.24515        0.00000
  C       -1.21479       -0.70136        0.00000
  H       -2.15666       -1.24515        0.00000
  C        0.00000       -1.40272        0.00000
  H        0.00000       -2.49029        0.00000
  C        1.21479       -0.70136        0.00000
  H        2.15666       -1.24515        0.00000
  C        1.21479        0.70136        0.00000
  H        2.15666        1.24515        0.00000
```

Visualising sample XYZ data

Download and install VMD at either

- http://www2.fizik.usm.my/tlyoon/Downloads/vmd191beta1win32.msi
- http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD

- Download the sample XYZ data files N3PD.xyz.
- Use VMD to visualise N3PD.xyz.

Exercise: Output snapshots of animation data into a XYZ data file

How would you export all the animation data generated by C4_simulate_NPbox.nb into a XYZ formatted file? To this end, let's do a simple exercise:

Modify the code C4_simulate_NPbox.nb so that the output is exported to a data file named data2D.xyz. I will call this modified code C4_simulate_NPbox_export.

For this case we shall learn to use a new command:

OpenWrite; **FormatType -> OutputForm**;

N Particle in a 3D box

- C4 simulate NPbox.nb can be generalized to animate N free particles moving in a 3D box.
- To this end, you need to use a new command:

Graphics3D[]

Exercise: do this, and name your code C4_simulate_NPbox3D.nb.

Exercise

Based on the code C4_simulate_NPbox3D.nb you have developed earlier,

(i) export the simulated data for N “Carbon” atom moving in a 3D box into a XYZ formatted file named NP3D.xyz
(ii) Use VMD to visualise your NP3D.xyz.

Name you code C4_simulate_NPbox3D_export.nb

Exercise: Visualise XYZ data file in Mathematica

Develop a code to visualize NP3D.xyz using Mathematica automatically without manual intervention. Name your code as C4_visualiseXYZ.nb

Exercise: log.lammps

- If you are given a data file with some fixed format other than XYZ, can you write a code to read in the data, process them and visualise the content according to your need?
- Try this out on the file log.lammps, which is part of an output produced by a Molecular Dynamics simulation software package LAMMPS.
- log.lammps is a formated file containing assorted information of the LAMPPS output, such as "Step" "Atoms" "Temp" "Press" "PotEng" "KinEng" "TotEng" "Volume" "Enthalpy

Exercise: log.lammps

- Write a Mathematica code to abstract the data of "Step" "Atoms" "Temp" "Press" "PotEng" "KinEng" "TotEng" "Volume" "Enthalpy from log.lammps.

Then plot

- Temp vs. Step
- PotEng vs. Step
- PotEng vs. Temp

See sample code: C4_loglammps.nb