A particle in a box

- To simulate a particle moving freely in a rectangular box with edge *L*.

Algorithm:

- 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.

Simulating Particle in a 2D box

- See 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 comprising of 1 particle in a box can be easily generalised to N particles, see simulate_NPbox.nb

Exercise: Generalise to *N* Particle in a 3D box

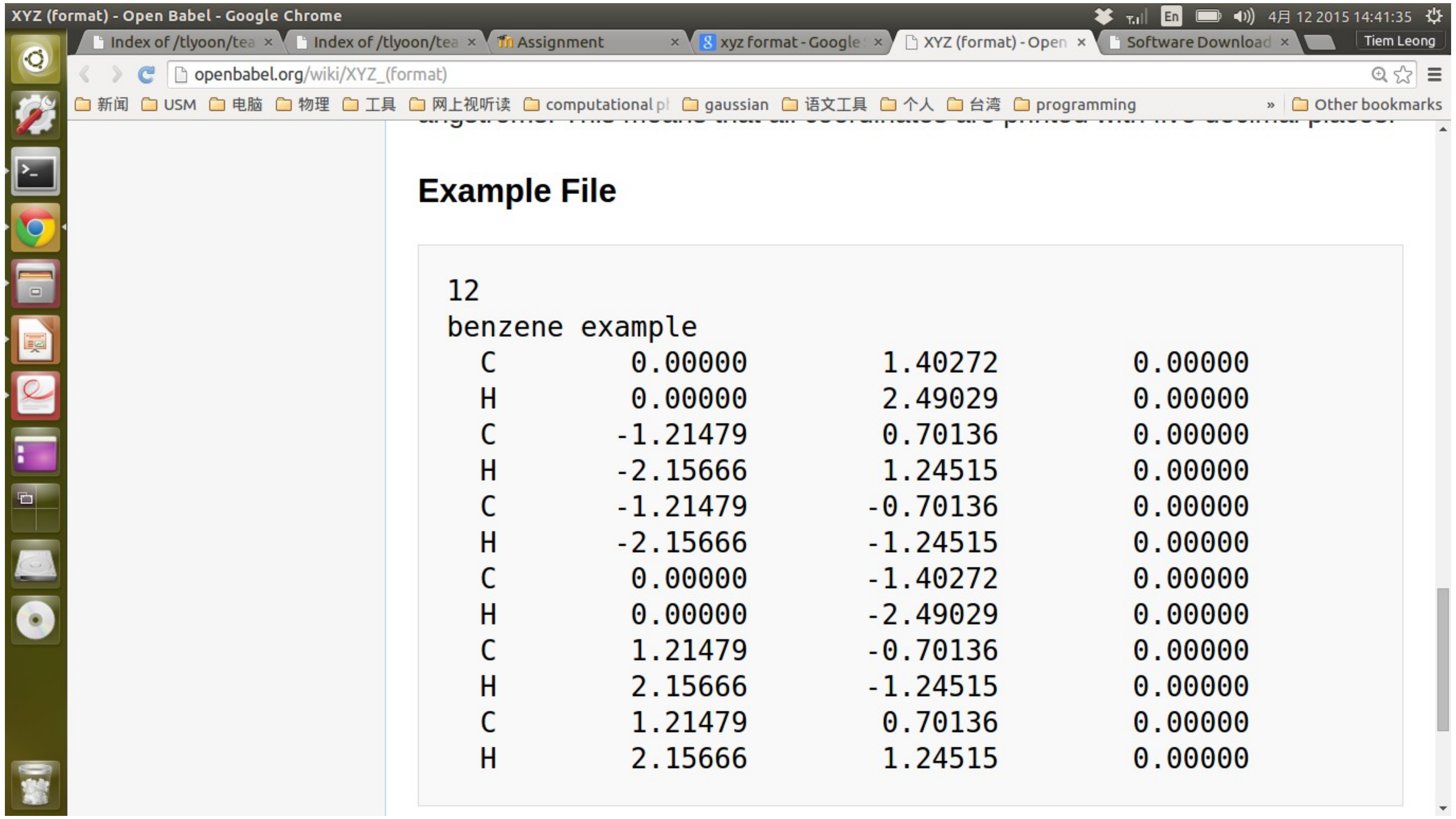
- Generalise the code comprising of N particle in a 2D box to a 3D box.
- Export your data as NPin3Dbox.dat in .xyz format
- Import NPin3Dbox.dat using Mathematica. Visualise it.

Manipulation of formatted data

How would you export the data of the simulation simulate_NPbox.nb into a *.dat file, and later retrieve it to display in Mathematica (or other visualisation software such as VMD?).

- Export them in the *.xyz format, see http://openbabel.org/wiki/XYZ_(format)

*.XYZ Format


XYZ (format) - Open Babel - Google Chrome
openbabel.org/wiki/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
```

- See exportformatedlist.nb   for how to export the data into *.xyz format.

Exercise

- 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.
- (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.

Visualise *.XYZ file in Mathematica

- I used the code Export_NP3Dbox_data.nb (not to be provided to you) to generate simulated particles data moving in a 3D box in XYZ format, and named the data file NP3D.dat.

  Import NP3D.dat into your mathematica.
- Now, write a code to visualise it.
- See visualiseXYZ.nb.

Exercise

- 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?

Data manipulation: 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

Data manipulation: 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 manipulate_data_LAMMPS.nb

Exercise

- If you can already manipulate an arbitrary format data file such as log.lammps, you can proceed to manipulate the data file 1700.lammpstrj, which is yet another form of output file from a ALMMPS 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 (which you do not need in this exercise).
- Write a code to

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

  (ii) Calculate the max and min of x-, y- and z-coordinates of the atoms in the box.

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