School of Physics & Astronomy

Modelling and Visualisation in Physics

PHYS10035 (SCQF Level 10)

Tuesday 28th April, 2015 09:30 – 12:30
(May Diet)

Please read full instructions before commencing writing.

Examination Paper Information

Answer all questions overleaf.
Completed codes should be uploaded via Learn as a single zip file immediately after the examination has finished. Alternatively, you can email the zip file to dmarendu@ph.ed.ac.uk.
Figures should also be submitted electronically, they should also be described in the script book.
You may use any resources available on the internet at the beginning of the examination, or present in your CPlab home directory but you may not communicate with any other person electronically or otherwise.

Special Instructions

- Only the supplied Electronic Calculators may be used during this examination.
- A sheet of physical constants is supplied for use in this examination.
- Attach supplied anonymous bar codes to *each* script book.

Special Items

- School supplied calculators
- School supplied Constant Sheets
- School supplied barcodes

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Let us consider a system of N particles of mass m in 2 dimensions. The positions of the particle centres are denoted by the vectors $\mathbf{r}_i$, with $i = 1, \ldots, N$; the vector joining the centre of the i-th particle to that of the j-th particle is denoted by $\mathbf{r}_{i,j} = \mathbf{r}_j - \mathbf{r}_i$. Any two particles, say the i-th and the j-th ones, interact with each other through the following Lennard-Jones potential,

$$U_{\mathrm{LJ}}(r_{i,j}) = 4\epsilon \left[\left(\frac{\sigma}{r_{i,j}} \right)^{12} - \left(\frac{\sigma}{r_{i,j}} \right)^{6} \right]$$

where $r_{i,j} = |\mathbf{r}_{i,j}|$ is the distance between the i-th and j-th particle centres, σ is the effective particle size, and ϵ is the interaction strength.

The Lennard-Jones particles can be connected to form a bead-and-spring chain, which is a simple model for a polymer. This is done, for example, by introducing the following finitely extensible nonlinear elastic (FENE) bond potential between the i-th and $(i+1)$-th particle,

$$U_{\mathrm{FENE}}(r_{i,i+1}) = -\frac{K R_0^2}{2} \log \left[1 - \left(\frac{r_{i,i+1}}{R_0} \right)^2 \right],$$

where $i = 1, \ldots, N-1$, and where K is the strength of the bond and R_0 is the maximal bond length. Note that U_{FENE} is only defined for $r_{i,i+1} < R_0$ (i.e. the bond length always needs to be smaller than R_0).

a. To set up a molecular dynamics algorithm, we need the forces resulting from the potentials we discussed. Show that the force on particle i due to the FENE potential $U_{\mathrm{FENE}}(r_{i,i+1})$ is given by (again only for $r_{i,i+1} < R_0$)

$$\mathbf{f}_{i,i+1} = \frac{K}{1 - \left(\frac{r_{i,i+1}}{R_0} \right)^2} \mathbf{r}_{i,i+1}. \qquad \textbf{[4]}$$

b. Write a Java program to simulate a polymer with N beads in the NVE ensemble, with periodic boundary conditions. Throughout this exercise you should set the following parameters: $m = \epsilon = \sigma = 1$, $R_0 = 1.6$, $K = 30$. When computing the interparticle distance to calculate the LJ potential, you should use the minimum image convention, i.e. the distance should be the minimum distance between all periodic images of the two particles. You should use a box size $L = 100$; this facilitates visualisation because most of the times the polymer fits within the box, and does not go through the periodic boundaries (provided that N is small enough). Your program should provide some means to change the value of the number of beads, N, and of the timestep, δt. It should also display the state of the system in real time as it is running. You should plot the bonds between particles, as well as spheres depicting their positions. This can be done, for example, either by plotting the lines connecting the sphere centres, or by plotting a few (say 5) spheres interpolating between the i-th and $(i+1)$-th beads, i.e. those which are connected along the polymer. To initialise the system with the desired number of particles, you should arrange the positions in a square lattice with nearest neighbour distance equal to 1, numbering the beads such that consecutive beads along the chain are nearest neighbours on the lattice. You should insert a check in your code which terminates the program with an error message if any bond length exceeds R_0 at any time. **[25]**

c. From now on, set $N = 30$. Compute the kinetic, Lennard-Jones and FENE potential energy and plot them versus time, for different values of the time step δt, equal to 10^{-4}, 10^{-3} and 10^{-2}. Show that, with a suitably small time step, the total energy is constant to a very good approximation within your NVE simulation. **[7]**

d. Generalise your code to simulate the polymer in the NVT ensemble, by using the Brownian thermostat. Write the code so that you can change the value of the temperature, T, while keeping $\epsilon = 1$. What is the typical configuration of the polymer for low temperature, $T = 0.1$? What is the typical configuration for high temperature, $T = 1.5$? Include a representative snapshot for each temperature to support your answer. **[6]**

e. A commonly used quantity to define the typical size of a polymer is the radius of gyration, R_g. Its square is defined as

$$R_g^2 = \frac{1}{2N^2} \sum_{i,j=1}^{N} \mathbf{r}_{i,j}^2.$$

Using the code for the NVT algorithm, plot the value of the radius of gyration, R_g as a function of temperature, for T between $T = 0.1$ and $T = 2.0$. Your graph should include error bars. What does the graph show, and how is it consistent with the snapshots you showed previously? **[8]**