

College of Science and Engineering
School of Physics and Astronomy



Modelling and Visualisation in Physics
SCQF Level 10, U01414, PHY-4-ModVis
Wednesday 21st April, 2010
9.30 a.m. – 12.30 p.m.

Chairman of Examiners
Professor R D Kenway

External Examiner
Professor M Green

Answer the question overleaf.

Completed codes should be uploaded via WebCT as a single zip file after the examination has finished.
If technical problems arise with the submission process, you should email the zip file to r.a.blythe@ed.ac.uk instead. Figures may also be submitted electronically provided they are 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.

The bracketed numbers give an indication of the value assigned to each portion of a question.

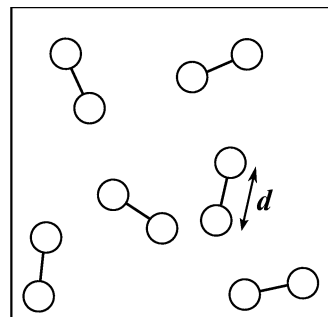
Only the supplied Electronic Calculators may be used during this examination.

A system of *dimers* can be modelled by starting with a collection of individual particles (*monomers*) that interact via the usual Lennard-Jones potential,

$$V(r_1, r_2, \dots, r_N) = \sum_{\langle k, \ell \rangle} 4\epsilon \left[\left(\frac{\sigma}{|r_k - r_\ell|} \right)^{12} - \left(\frac{\sigma}{|r_k - r_\ell|} \right)^6 \right],$$

where r_i are the monomer positions, and ϵ and σ set the energy and length scales respectively. To turn this into a model of dimers one must additionally ensure that pairs of particles begin a fixed distance d apart from each other, and remain so throughout the simulation, as shown in the figure.

This is achieved by numerically integrating the equations of motion as though the monomers were not bound, and then at the end of each timestep, adjusting the monomer positions so that bound pairs are the required distance d apart.



This adjustment entails adding a few extra lines to your existing molecular dynamics code. Questions (a)-(d) contain all the information that is needed to make these changes. You may benefit by spending 20–30 minutes on these questions to understand the required changes before implementing them.

- If particles i and j form a dimer, write down an equation for the constraint that must be satisfied by the coordinate vectors $r_i(t)$ and $r_j(t)$ at all times.
- Let $\underline{s}_i(t+h)$ and $\underline{s}_j(t+h)$ denote the positions of the particles obtained after one timestep in the absence of the constraining bonds. The adjustment to obtain the positions $r_i(t+h)$ and $r_j(t+h)$ is achieved by varying the parameter λ_{ij} in the equations

$$\begin{aligned} r_i(t+h) &= \underline{s}_i(t+h) + \lambda_{ij}[r_j(t) - r_i(t)] \\ r_j(t+h) &= \underline{s}_j(t+h) - \lambda_{ij}[r_j(t) - r_i(t)] \end{aligned}$$

until the particles i and j are the required distance d apart. Illustrate this adjustment with a figure, and explain its physical meaning.

- Show that the desired value of λ_{ij} is the solution of

$$[\underline{s}_i(t+h) - \underline{s}_j(t+h)]^2 - 4\lambda_{ij}[\underline{s}_i(t+h) - \underline{s}_j(t+h)] \cdot [r_i(t) - r_j(t)] + 4\lambda_{ij}^2[r_i(t) - r_j(t)]^2 = d^2$$

that is closest to zero. Assuming that λ_{ij} vanishes with the timestep h , argue that this solution can be calculated approximately via

$$\lambda_{ij} \approx \frac{[\underline{s}_i(t+h) - \underline{s}_j(t+h)]^2 - d^2}{4[\underline{s}_i(t+h) - \underline{s}_j(t+h)] \cdot [r_i(t) - r_j(t)]}.$$

- d. This adjustment step is most straightforwardly incorporated into the original Verlet algorithm (as opposed to the velocity version, which involves much more work). In this algorithm, $\underline{s}_i(t+h)$ is obtained from the two previous sets of positions using

$$\underline{s}_i(t+h) = 2\underline{r}_i(t) - \underline{r}_i(t-h) + \frac{h^2}{m_i} \underline{f}_i[\underline{r}_1(t), \underline{r}_2(t), \dots, \underline{r}_N(t)]$$

for each monomer i , where m_i is the mass of the monomer, and \underline{f}_i is the force acting on monomer i due to all the other monomers. Suppose that at $t = 0$ you prescribe the monomer positions $\underline{r}_i(0)$ and velocities $\underline{v}_i(0)$. Write down an expression for an estimate of $\underline{r}_i(h)$ in terms of the positions, velocities and forces acting at time $t = 0$ that can be used to get the Verlet algorithm started.

[2]

- e. Write a Java code that simulates the Lennard-Jones dimer system using the modification to the Verlet algorithm described above. The simulation should present a graphical display of the system's state as it evolves and allow you to vary the bond length d and the density.

[25]

Use your code to answer the remaining questions. For all of these questions, it is sufficient to simulate only the low density (fluid) phase. Graphs and relevant screenshots may be submitted electronically with your code, but you should also sketch and comment on them in the exam script, noting special features and parameter values.

- f. Demonstrate that your simulation is working correctly by showing for a few values of d , above and below the position of the minimum of the Lennard-Jones potential (*e.g.* d/σ between 0.5 and 2.0), that energy is conserved over time.

[3]

- g. Similarly, construct a measure of the accuracy with which the dimer constraint is satisfied, noting values that reflect good and poor accuracy. Plot this measure as a function of time for a few different d and densities. Which factor appears to affect the accuracy most strongly?

[5]

- h. Modify your code so that the dimer constraints are removed part-way through a simulation run so that it then reverts to a simulation of a monomer system. For various d , compare the mean kinetic energy in the equilibrium states that reached before and after the constraints are removed. Note and explain the changes you observe—and in particular any dependence on d —in terms of the partition of energy between kinetic and potential energy before and after the constraints are removed (no graphs are needed for this question).

[3]

- i. Use the equipartition theorem to deduce the possibility of the system's temperature decreasing while its kinetic energy increases after the constraints are removed. Note conditions under which this effect is seen in your simulation.

[2]