Intermediate Scientific Computing: Final Assessment

Deadline: Wednesday, 3rd May, 12:00pm

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Many common scientific problems require us to be able to track the behaviour of systems of particles. One common approach is to perform a so-called N-body simulation. In an N-body simulation we track the positions and velocities of individual particles, and use the forces between them to calculate their individual accelerations.

For this assessment, you will write an N-body code to simulate the behaviour of argon atoms confined within a box. You will then use this code to investigate how the pressure inside the box changes as you alter the system parameters. You will then write up your work, detailing how you set-up your code, demonstrating that it performs as expected for any relevant test cases, and showing your results. Your report should conclude with a discussion of any deficiencies and possible improvements that could be made.

You may use either C++ and/or python as you see fit, but your report must justify the choice.

Part 1 – Producing the N-body code

An N-body code must follow the trajectories of a fixed number of particles, N. Each particle, i, has an associated (vectore) position, $\vec{r_i}$, and velocity, $\vec{v_i}$. Particles interact with one another via the force between them. If the force on particle i due to particle j is given by F_{ij}, we can find the net force acting on particle i by summing over all particles (except for i!), i.e.

$$F_{\rm net} = \sum_{j \neq i} F_{ij}$$

We can then use Newton's second law to find the acceleration of particle i, a_i:

$$a_i = \frac{1}{m_i} \sum_{j \neq i} F_{ij}$$

where m_i is the particle mass. From the acceleration, we can then calculate the velocity and position and how they change over a given timestep, δt.

To perform the integration, we use a so-called Verlet 'leap-frog' integration scheme. For each particle i, we update the velocity based on the acceleration at the current timestep using half the step size:

$$v_i = v_i + \frac{\delta t}{2} a_i$$

and then use this new velocity to update the position across the whole time interval

$$r_i = r_i + \delta t v_i$$

Finally, we use the new positions to recompute the acceleration and then calculate the new velocity after the remaining half time step:

$$v_i = v_i + \frac{\delta t}{2} a_i.$$

The interaction between two atoms can be modelled using the Lennard-Jones potential:

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

where r is the separation between the atoms, and ϵ and σ are parameters that depend on the atoms. For argon, $\epsilon/k_B = 125.7\,\mathrm{K}$ (where $k_B = 1.38 \times 10^{-23}\,\mathrm{J/K}$ is the Boltzmann constant) and $\sigma = 0.3345 \times 10^{-9}\,\mathrm{m}$. You will need to convert this potential into a force, F, using $F = -\frac{dV}{dr}$!

Task 1: Create a piece of code that can perform the integration described above for a system of N particles. You will need to determine what is an appropriate size for your timestep. Demonstrate that the code behaves as expected for a system of two particles in close proximity (i.e. with a separation on the order of σ). You are strongly recommended to consider the efficiency of the code! Use array operations rather than for loops where possible – they are much, much faster!

Part 2 – Particles in a box

We now require some boundary conditions for the simulation. Assume our particles are going to be confined to a cubic box whose sides have a length of L. We will assume that the centre of the box is centred on the origin. Consider a particle travelling only in the x-direction. When it reaches the wall of the box at $x = L/2$, it rebounds elastically – i.e. its velocity in the x-direction is reversed, but its speed (and thus its kinetic energy is unchanged).

Task 2: Add a cubic box to your simulation so that all particles are confined within $-L/2 \leq x \leq L/2$, $-L/2 \leq y \leq L/2$ and $-L/2 \leq z \leq L/2$. Show that a particle hitting the walls of the box behaves as expected.

Part 3 – Investigate!

Task 3: You now have all the components you need to investigate the behaviour of the gas. How does the pressure of the gas change with changes in the volume of the box and the temperature of the gas? You will need to calculate the pressure of your gas and its temperature. Temperature is defined with respect to the total kinetic energy of the particles:

$$E = \sum_{i}^{N} \frac{1}{2} m_i v_i^2 = \frac{3}{2} N k_B T$$

where N is the number of particles, m_i and v_i are the mass and speed of the ith particle respectively. The pressure P is linked to the momentum flowing through a unit area in a unit time period (note you only need to consider particles passing in one direction through the area). Suppose we have an area, A, lying in the $y-z$ plane. The momentum crossing this plane in time Δt is the x-component of the momentum of any particle crossing this plane, $p_x = mv_x$ where v_x is the speed of the particle in the *direction*. The pressure in the x-direction is therefore:

$$P_x = \frac{1}{A\Delta t} \sum m_i v_x, i$$

where the sum is performed only over those particles crossing the plane in unit time. If we assume the pressure is isotropic, $P_x = P_y = P_z = \frac{1}{3}P$ where $Pisthetotalpressure$ (you might like to test if this is true in your simulations!). Note we only need to consider particles travelling in one direction, as pressure should be the same in both positive and negative directions when the system is in equilibrium.

It is up to you to decide on how many particles to use and how long to run the simulations for, and what you want your initial conditions to be. Your reasons for these choices should be justified in your report with valid scientific and/or computational reasons.

Hint: It is strongly recommended that you initialize the positions of your particles on a grid whose spacing is no smaller than the value of σ. The steep dependence of the potential for small r can lead to extremely large forces.

Submisssion

Your submission must consist of both your (documented) code and a report into your investigation of how the gas behaves. You must include working examples for the first two tasks which we must be able to run. It should be clear how these test cases are linked to the code you use in the final investigation of the gas. Your report should include details of how you tested your code to ensure that it is working as intended, how many particles you chose to use and the length of time you chose to run your simulations for.

Please submit your report as a PDF document via the submission point on Blackboard, along with a file containing your code and everything needed to run it.