

Statistical Physics TFY4230 - Computational Physics Project (Obligatory)

This computational project will explore the statistical mechanics of a collection of particles in two dimensions. The motion of the particles is determined by numerical integration of Newton's equations of motion. Consider N point particles with positions $\vec{r}_i = (x_i, y_i)$. The interaction potential between any two particles i and j is:

$$V(r_{ij}) = \epsilon \left[\left(\frac{a}{r_{ij}} \right)^{12} - 2 \left(\frac{a}{r_{ij}} \right)^6 \right] \quad (1)$$

where $r_{ij} = |\vec{r}_i - \vec{r}_j|$ is the distance between particle i and j , and the strength of the interaction is given by the parameter $\epsilon > 0$. The force is repulsive when $r_{ij} < a$, and attractive when $r_{ij} > a$. The potential energy increases fast when $r_{ij} < a$, and the length a therefore roughly defines the size (diameter) of particles. The particles are confined inside a rectangular container with dimensions L_x and L_y . The interaction between a particle i and the horizontal walls (parallel to x-axis) is modeled by a soft repulsive potential

$$V_x(\vec{r}_i) = \begin{cases} \frac{K}{2}(x_i - L_x)^2 & \text{if } x > L_x \\ \frac{K}{2}x_i^2 & \text{if } x < 0 \end{cases} \quad (2)$$

where $r_i = \vec{r}_i = (x_i, y_i)$. And exactly the same type of interaction for the vertical walls (which has length L_y). The total wall potential is $V_w = V_x + V_y$.

Newton's equations of motion is then:

$$m \frac{d^2 \vec{r}_i}{dt^2} = \vec{f}_i = -\frac{\partial V_w}{\partial \vec{r}_i} - \sum_{j \neq i} \frac{\partial V(r_{ij})}{\partial \vec{r}_i} \quad (3)$$

where the sum over j goes over all particles interacting with particle i . \vec{f}_i is the sum of all forces acting on particle i .

We shall use the velocity Verlet algorithm to numerically integrate the equations of motion. At time $t = 0$ we set the initial particle positions $\vec{r}_i(0)$ and velocities $\vec{v}_i(0)$, and update to new positions and velocities at each timestep using:

$$\vec{r}_i(t + \Delta t) = \vec{r}_i(t) + \vec{v}_i(t)\Delta t + \frac{1}{2} \frac{\vec{f}_i(t)}{m} \Delta t^2 \quad (4)$$

$$\vec{v}_i(t + \Delta t) = \vec{v}_i(t) + \frac{\vec{f}_i(t) + \vec{f}_i(t + \Delta t)}{2m} \Delta t \quad (5)$$

The first equation is simply the Taylor series expansion of the particle positions as a function of time. In the second equation we update the velocities using an average of the force (acceleration) at t and $t + \Delta t$.

In the following we rescale all equations so that the mass becomes $m = 1$ and the effective particle diameter $a = 1$.

In the folder 'course work' the file "verlet.py" gives an implementation of the velocity Verlet algorithm for a N particles. Notice that the relevant parameter is the kinetic energy per particle divided by the strength of the potential energy. You may therefore set $\epsilon = 1$ and vary the kinetic energy per particle. There is not necessarily a "perfect" value of K , but a very high K might result in numerical instability, and too low value will result in a very "soft" wall. The size of the box should not be too much larger than the size of the particles (otherwise it will take a long time for the particle to reflect).

We shall first consider the simple case of one particle.

1 One particle

a) Run the program and plot particle trajectories for different initial positions and initial velocities for one particle, $N = 1$. If the time-step Δt is too large the numerical solution will not be good. On the other hand making Δt small will slow down the simulations. Consider a fixed run time $T = \text{steps} * \Delta t$ (for example such that the particle is reflected ~ 10 times from the walls). Determine (approximately) the largest Δt that gives a good numerical solution to the particle trajectory.

b) Calculate numerically the total mechanical energy (kinetic and potential) $E = T + V$ as a function of time. It should of course be constant, but numerical errors will accumulate and there will always be a drift in the energy over time $E \rightarrow E + \Delta E$. This can be used as a criterion for the accuracy of your simulation. Plotting the energy as a function of time for different Δt will give an idea of the quality of the different solutions. We can of course never reach $\frac{|\Delta E|}{E} = 0$, but if $\frac{|\Delta E|}{E} \approx 0.2$ we know that the numerical solution is bad, and if $\frac{|\Delta E|}{E} \approx 0.01$ we can hope that it is good.

2 Two dimensional gas of interacting particles

Consider now N particles, the particle interactions are given by the pair potential Eq. (1). Choose the initial velocity conditions such that the kinetic energy per particles is somewhat larger compared to the potential energy ϵ . This will ensure that the system is in a gas phase. You choose the size of the container yourself, but the area fraction of particles should be small, such that we can consider it an ideal gas.

a) Plot the trajectories for short times and check that the particles scatter on each other (a few collisions). Start with $N = 2$, and then progressively change to larger N . It does not have to be Avogadro's number, you will see that even $N = 2$ is quite interesting. Plot the total energy as a function of time. If the total energy is conserved during collisions you have reason to trust your code.

b) Plot the trajectory of one particle over long times for $N = 2$, $N = 3$ and $N = 10$ (or larger N if you can). How does the dynamics differ from the $N = 1$ case? Plot the particle's positions as points (scatter plot) over long times, this will give you an impression of the time averaged particle density.

c) Try different initial conditions for the velocity, for example giving all the energy to one particle at $t = 0$. Calculate the time averaged kinetic energy of each particle. How is the energy distributed among the particles?

d) The simulations above corresponds to a micro-canonical system (total energy is conserved). If N is large we may consider that one of the particles is in the canonical ensemble (and the other $N - 1$ particles is the heat bath), this results in the Maxwell-Boltzmann probability distribution for the particle velocity:

$$P(v_x) = \sqrt{\frac{m}{2\pi k_B T}} e^{-\frac{mv_x^2}{2k_B T}} \quad (6)$$

Calculate numerically the velocity probability distribution for a single particle in a gas of $N = 10$ particles (or larger) and compare the result with the Maxwell-Boltzmann distribution. For a two-dimensional ideal gas the temperature follows from the equipartition theorem $k_B T = \langle \frac{1}{2} m \vec{v}^2 \rangle$.

3 Solid, liquid, gas

a) In the above exercises we assumed that the kinetic energy was large compared to the potential energy well ϵ . What happens when the kinetic energy is not large compared to the potential energy well? To study this we can place all the particles in an hexagonal packing (distance=1 between particles) at time $t = 0$, this will correspond to a minimum energy state (solid). First run simulations where the average kinetic energy per particle is much lower than ϵ . Then run simulations with progressively larger kinetic energy, and try to find for which kinetic energy the solid "melts". This is not a real phase transition since we have a finite number of particles, but it will give an idea of how it works.