Molecular dynamics of a mini-crystal

This computational project will explore the statistical mechanics of a mini-crystal in two dimensions. The particles have kinetic energy and are held together by potential energy (interactions). The motion of the particles is found by direct numerical integration of Newton's equations.

Simulation model:

We shall consider N point particles with positions given by the vectors $\vec{r}_i = (x_i, y_i)$. The interaction potential between any two particles i and j is:

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

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. Newton's equations of motion is then:

$$m \frac{\mathrm{d}^2 \vec{r}_i}{\mathrm{d}t^2} = \vec{f}_i = -\sum_{j \neq i} \frac{\partial V(r_{ij})}{\partial \vec{r}_i} \tag{2}$$

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 will 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:

$$\vec{r}_i(t + \Delta t) = \vec{r}_i(t) + \vec{v}_i(t)\Delta t + \frac{1}{2} \frac{\vec{f}_i(t)}{m} \Delta t^2 \tag{3}$$

$$\vec{v}_i(t + \Delta t) = \vec{v}_i(t) + \frac{\vec{f}_i(t) + \vec{f}_i(t + \Delta t)}{2m} \Delta t \tag{4}$$

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 velocites using an average of the force (acceleration) at t and $t + \Delta t$.

In the following we set the particle masss $m = 1$, distance $a = 1$, and interaction strength $\epsilon = 1$. This simply amounts to rescaling of the equations, or using different units. The free parameters that are left is the initial velocities and positions of the particles.

1.Two particles ($N = 2$)

1a) Write a program to simulate two particles. As initial conditions you may let the distance between particles be $r = 1.1$, and velocities can be zero.The timestep can be $\Delta t = 0.01$.

1b) Plot the distance between particles as a function of time. You should see oscillations. Do the same simulations with $\Delta t = 0.001$ and $\Delta t = 0.1$. Plot the distance between particles as a function of time (on the same graph) for the three different timesteps.

1c) Plot the total mechanical energy (kinetic + potential) as a function of time. The energy should be conserved to a good approximation when the timestep is low enough.

2. Mini-crystal

2a) Generalize your program for N particles. As initial positions put the particles ($N = 16$) in a perfect hexagonal packing with distance $r = 1$. The velocities of particles are taken as random vectors with module V_0. Start with a small velocity $V_0 = 0.01$. Plot the distance between two neigbouring particles as function of time, you should see oscillations[1]. Plot the total mechanical energy as a function of time, it should conserved to a good approximation (less than 0.1% error is preferred).

2b) Try to run with larger particle numbers, for example $N = 25$ and $N = 49$. Plot the distance between to neighboring particles again. You should be able to produce many oscillations (100 for example) in a reasonable time. Choose the number of particles that you feel works well on your computer and with your program. $N = 16$ is perfectly fine, but $N = 25$ or higher might give a little better statistics.

2c) Calculate the total average kinetic energy and potential energy (average over time) for different initial velocities V_0. Plot the total potential energy as function of kinetic energy. When the kinetic energy is low enough, there should be a linear dependence. Give an interpretation of the result.

2d) Make a histogram for the velocities v_x and v_y of one of the particles. Compare with the Maxwell distribution.

2e) If the initial velocities are increased to larger values there should be noticeably higher fluctuations (oscillations in distance between particles). Show that the crystal melts and becomes a gas (it evaporates) as V_0 is increased. Try to also find values of V_0 for which the particles appear in more liquid state (still together, but not in lattice structure).

2f) **optional question** (not obligatory) When the crystal evaporates the particles goes to infinity. In order to have a finite area, we can include a potential $\mathcal{V}(r)$ which is equal to $K(r - R)^2$ whenever $r > R$, and zero otherwise. The constant may be $K = 100$ for example, to ensure hard walls. This will amount to confinement in a circular container of radius R. At high V_0 you should see gas in confinement. Start with a high velocity and slowly decrease the velocity of all particles (cooling), you should now be able to see the opposite effect, formation of the crystal.

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[1]Notice that the oscillations need not be regular sinus waves, this is due to the complicated non-linear interactions between all particles (chaos).