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Computer Simulations in Statistical Physics

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Problem set 7

Proseminar

In this tutorial we will write a molecular dynamics (MD) simulation to numerically solve Newton's equations of motion for a system of interacting particles. The particles will interact with a pair-wise smooth repulsive potential, known as the Weeks-Chandler-Anderson (WCA) potential. The interaction between each pair of particles is given by

$$V(r) = \begin{cases} 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + \varepsilon & r \leq 2^{1/6}\sigma \\ 0 & r > 2^{1/6}\sigma \end{cases} . \tag{1}$$

where r is the distance between the particles. The two constants, ε and σ, determine the energy and length scale respectively. The potential is such that at $r_{\text{cut}} = 2^{1/6}\,\sigma$, $V(r) = 0$.

Problem 7.1 *WCA and LJ potentials*

Before performing simulations it is helpful to get a feeling for the potentials used in the MD simulations.

a) Plot the WCA interaction potential. What is the effect of changing ε and σ?

b) Choosing a larger cutoff $r_{\text{cut}} \gtrsim 3\sigma$ (and a different shift such that $V(r_{\text{cut}}) = 0$) includes an attractive tail to the interaction potential. It is then called the Lennard-Jones (LJ) potential. Do a small research on the physical motivation for choosing such a potential and which kind of interactions can qualitatively described by it.

c) From the potential defined above, find an expression for the distance-dependent force, $\boldsymbol{F} = -\boldsymbol{\nabla} V(r)$, one particle exerts on another.

Problem 7.2 *Molecular Dynamics Simulation*

Open the MD code snippet provided. This program initializes the positions of the particles in a 3D lattice, and assigns the initial velocities with a random direction, and a magnitude according to a specified input temperature. Apart from the initialization of the velocities, the code only provides functions you have already written yourself for the Monte Carlo simulations.

a) In the function "calculate_potential()", calculate the total potential of the system. Chose $\varepsilon = 1$, $\sigma = 1$ and mass $= m = 1$, so that the units of length in the simulation will be σ, and energy will be ε. The units of time are then $\tau = \sqrt{m\sigma^2/\varepsilon}$. Use the cell lists provided when identifying neighboring particles. Check that the result behaves as expected when changing the number of particles and the density.

b) In the function "calculate_forces()", calculate the force on each particle, using the expression found in Problem 7.1. Use the cell lists provided when identifying neighboring particles.

c) Newton's equations of motion can be integrated numerically with the Verlet algorithm:

$$v\left(t + \Delta t/2\right) = v\left(t\right) + \frac{\Delta t}{2m} F(t) \tag{2}$$

$$x\left(t + \Delta t\right) = x\left(t\right) + \Delta t v\left(t + \Delta t/2\right) \tag{3}$$

$$v\left(t + \Delta t\right) = v\left(t + \Delta t/2\right) + \frac{\Delta t}{2m} F(t + \Delta t). \tag{4}$$

Write a function "md_step()" to increment all particle positions and velocities by one time step using this algorithm. Calculate the acceleration of each particle using your force function (remember to update the forces between Eqs. (3) and (4)). Once the particles have been moved, map their positions back to the central periodic box and recalculate the cell lists.

d) Write a function "calculate_kinetic()" to calculate the kinetic energy of the system. Run the MD program, and output the kinetic energy, potential energy and total energy. Plot kinetic energy and potential energy as a function of time. How long does the system take to equilibrate?

e) Assuming $\varphi = 0.3$ and $T = 1$, run the simulation with different time step sizes, $\Delta t = 0.001, 0.005, 0.01$, and look at how the total, kinetic, and potential energy changes with time. What is the effect of changing Δt?