PHYS-E0412 Computational Physics :: Homework 5

Due date 12.2.2019 at 10 am

Molecular dynamics with Lennard-Jones potential

This week's problem is to simulate molecular dynamics (MD) using the Velocity Verlet iteration of N particles in a three-dimensional box with volume $V = L^3$ in periodic boundary conditions using the Lennard-Jones (LJ) pair potential where $r_m = 2^{1/6}\sigma$ is the potential minimum, and we set $\epsilon = 1$, $\sigma = 1$. An example molecular dynamics code written in Python can be found in MyCourses in the file hw5_md.py It should be useful for solving this homework. Note that the code uses Python 3 (not 2)!

1. Implement a function that evaluates the force based on the Lennard-Jones potential, see also lecture slides and hw5_md.py. Use the analytical formula for the force. Test that your forces are implemented correctly by testing that the total energy (kinetic + potential) is conserved in a NVE MD run for a two particle system and check that your total energy value is correct. This is relatively easy if you start near the potential minima. Submit a plot containing total, kinetic and potential energies for one run. (NVE microcanonical ensemble, i.e. constant N, V and E.). (1p)

2. Implement the sampling of the pair-correlation function (radial distribution function, RDF) $g(r)$ and implement velocity initialization at given temperature T. Test these by initializing a simulation $N = 108, \rho = 0.8442, T = 0.728$ with simple cubic lattice and plotting RDF. Explain the location of the first peak in RDF. (2p)

3. Identify the phase in previous assignment and find the two missing phases by plotting and analyzing resulting radial distribution functions $g(r)$. In addition to temperature and density you should pay attention to the initial configuration. (2p)

4. How many hours did you spend working on this exercise?

Hint. The equipartition theorem can be used to relate the velocities v and temperature T

$$K = \sum_i \frac{1}{2} m v_i^2 = \frac{3}{2} N k T, \tag{1}$$

where we set $m = 1$ and $k = 1$. To control the temperature, you can scale the velocities of the particles to match the target temperature at the beginning of the simulation.

Hint. Implement $g(r)$ by accumulating a histogram of interparticle distances (the suitable choice for a bin width will depend on both N and the simulation time). Note the use of periodic boundary conditions. The normalization condition for $g(r)$ is

$$\rho \int g(r) d\mathbf{r} = N - 1 \approx N. \tag{2}$$

Note that the integral is over three dimensional space.

Hint. In addition to simple cubic structure, also a more closed packed structure might be good for finding phases. E.g. face centered cubic (fcc) structure.

Upload your solution in MyCourses (mycourses.aalto.fi) to the corresponding assignment. Please remember to attach your figures and codes as well!