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Computer Simulations in Statistical Physics

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Problem set 8

Proseminar

Problem 8.1 *Observables in molecular dynamics simulations*

In this exercise we will calculate a number of static properties from our MD simulation. Start with a copy of your simulation code from problem set 7, or use the solution provided. In each case, ensure that your system has first equilibrated, before sampling configurations to calculate the averages. As input parameters take $N = 10^3$ (number of particles), $\varphi = 0.45$ (packing fraction), $\sigma = 1$ (diameter of a particle).

a) Calculate the static structure factor of the WCA fluid:

$$S(q) = 1 + \frac{1}{N} \left\langle \sum_{i \neq j} \sum e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \right\rangle \tag{1}$$

For $\mathbf{q}$ use vectors with length given by an integer multiple of $2\pi/L$, and direction along the x, y, or z axis. Plot the function and compare it to the static structure factor of liquid sodium (provided in the lecture script). Note that to obtain good enough statistics, you may need to leave this calculation running in the background while you work on the subsequent problems.

b) In the microcanonical ensemble, the heat capacity can be calculated from fluctuations in the kinetic energy. This is given by

$$\frac{C_V}{k_B} = \frac{3N}{2}\left(1 - \frac{2\left\langle \delta E_k^2 \right\rangle}{3N(k_B T)^2}\right)^{-1}, \tag{2}$$

where E_k is the total kinetic energy of the system,

$$E_k = \frac{m}{2}\sum_i^N \mathbf{v}_i^2. \tag{3}$$

The temperature is calculated in the simulation as

$$k_B T = \left\langle \frac{2E_k}{3N} \right\rangle \tag{4}$$

and the variance in the kinetic energy can be calculated as

$$\left\langle \delta E_k^2 \right\rangle = \left\langle E_k^2 \right\rangle - \left\langle E_k \right\rangle^2 \tag{5}$$

Calculate the heat capacity in your simulation.

c) The pressure can be calculated from the virial expression as

$$PV = Nk_B T + \frac{1}{3}\left\langle \sum_{i<j} \mathbf{r}_{ij} \cdot \mathbf{f}_{ij} \right\rangle \tag{6}$$

where $\mathbf{f}_{ij}$ is the force that particle j exerts on particle i, and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$. Write a function to calculate the pressure. To meaningfully compare pressure and density, we need to set the average temperature in our system to a specific value. Modify your code so that during the equilibration period, the velocities are periodically rescaled so that the average temperature matches the input temperature. Run your simulation at a few different values of the density, and then plot pressure against density.

Problem 8.2 *Time reversibility*

For this exercise, use your code from problem set 7, or the solution code provided.

a) Set $\Delta t = 0.0005$, $N = 6^3$. Run your simulation for 10^4 timesteps. Then change Δt to -0.0005, and continue running your simulation for another 10^4 timesteps. This is equivalent to time running backwards. Plot the potential and kinetic energy throughout the process. Plot the x-y positions of the particles initially, after the first 10^4 timesteps, and then again after the reversed 10^4 timsteps.

   Repeat the above procedure with 10^3 and $4 \cdot 10^4$ timesteps.

b) Repeat one of the simulations from a), however now, when reversing the timestep, also rotate the x-y direction of one particle's velocity by 10 degrees. Explain your findings.