COMPUTATIONAL PHYSICS - EXERCISE SHEET 03
Radial distribution function

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The following is the report for the Exercise Sheet 03. The goal of this exercise is to enrich the molecular dynamics implementation of Exercise 02 with routines for computing the radial distribution function (RDF), the isothermal compressibility k_T and the running coordination number $n_c(r)$. Along this report, python scripts were also handed in. Additional code can be found at the github repository given at the end of this page.

I. CODE IMPLEMENTATION

The following are the new routines implemented in the new code.

A. Radial distribution function (RDF)

The radial distribution function is used to characterize the structure of simple fluids and it gives the probability of finding a pair of atoms at a distance r. In the simulation the $g(r)$ is computed with the following formula

$$g(r) = \frac{V}{N^2}\Big(\sum_i \sum_{i \neq j} \delta(r - r_{ij})\Big) \tag{1}$$

where r_ij is the distance between particle i and j, V is the volume of the box and N the number of particles

B. Running coordination number

The radial integration of the RDF in spherical coordinates gives the running coordination number n_cr, which represents the number of particles within a specific distance r from a given particle. The running integration number over the entire volume yields the total number of particles - although in simulations the results may not be accurate due to errors in the integrations. The $n_c(r)$ is given by

$$n_c(r) = 4\pi\rho \int_0^r g(r')r'^2 dr' \tag{2}$$

where ρ is the system number density.

C. Isothermal compressibility

The isothermal compressibility, namely the response to a change of pressure in terms of relative volume change, can be calculated in the following way

$$k_T = \frac{1}{k_B T \rho} + \frac{1}{k_B T} \int_V dr[g(r) - 1] \tag{3}$$

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II. SIMULATING A 3D SYSTEM WITH $N = 8^3$ ATOMS

For this part of the exercise I simulated a system with $N = 8^3$ particles and number density $\rho = 0.5\sigma^{-3}$. The system was equilibrated for 3000 timesteps and the RDF, running coordination number, and isothermal compressibility were then computed.

A. Radial distribution function

The following plot shows the radial distribution function. The maximum peak is found at distance $r_{max} = 1.16\sigma$ with RDF value of $g(r_{max}) = 1.78$. The radius of the first solvation shell is found at $r_{min} = 1.86$ with value $g(r_{min}) = 0.83$.

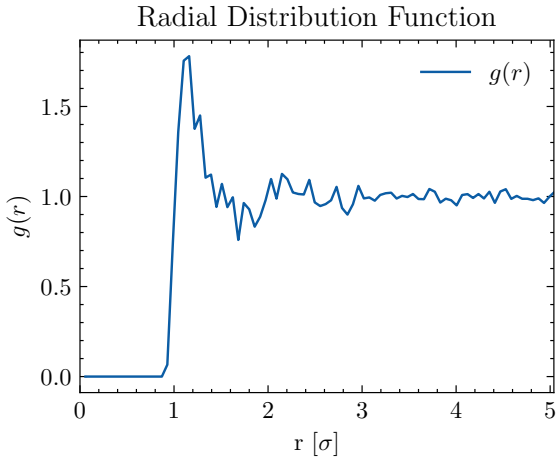

FIG. 1. The figure shows radial distribution function (RDF) of the system.

B. Running coordination number

The following plot shows the running coordination number. The value obtained for the first solvation shell is $n_c(r_{min}) = 13$ (particles). It is to be noted that the bin size at which the $g(r)$ is computed as a great impact on the values of $n_c(r)$, due to more precise numerical integration.

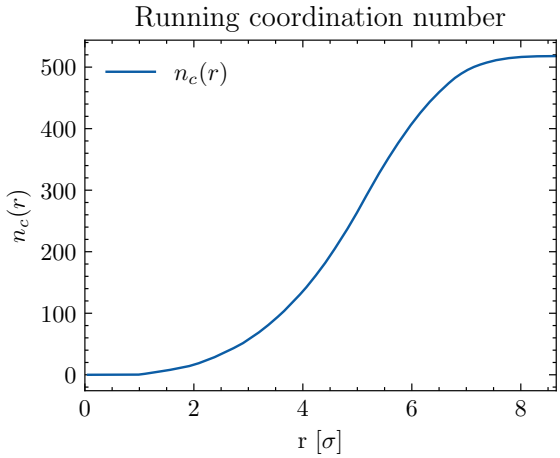

FIG. 2. The figure shows the running coordination number

C. Isothermal compressibility

We then computed the isothermal compressibility of the system, comparing the results with different values of number density rhoρ. The following are the values obtained. It is to be noted that a negative value was not expected, suggesting some errors in the calculation/implementation as well as due to the integral computation.

$$\rho = 0.25\sigma^{-3} \qquad k_T = 0.055 \text{ [red. units]} \tag{4}$$

$$\rho = 0.5\sigma^{-3} \qquad k_T = -0.658 \text{ [red. units]} \tag{5}$$

III. SIMULATING A 2D SYSTEM WITH $N = 400$ ATOMS

The second part of the exercise considers a 2-dimensional system with $N = 400$ particles and a number density of $\rho = 0.5\sigma^{-3}$. The main system parameters are the usual and reduced units were also used.

A. Simulation procedure: equilibration, production, and cooling

The simulation consisted in four main phases:

- Equilibration (2000 iters): the system is equilibrated at a given temperature by rescaling the velocities
- Production (2000 iters): the system is free to evolve
- Cooling (10000 iters): the system is cooled to 10K by rescaling the temperature every 100 iterations
- Production (2000 iters): the system is again free to evolve without velocity rescaling

The radial distribution function is computed after the first and second production run. Together with the RDF, ovito snapshots of the system are provided.

B. Radial distribution function

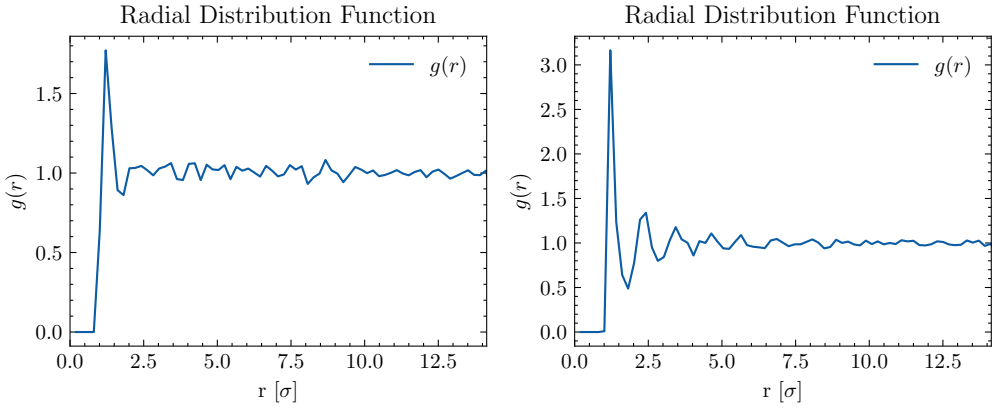

FIG. 3. The figures show the radial distribution function (RDF) of the system after the first (left) and second (right) production run.

C. Positions snapshots

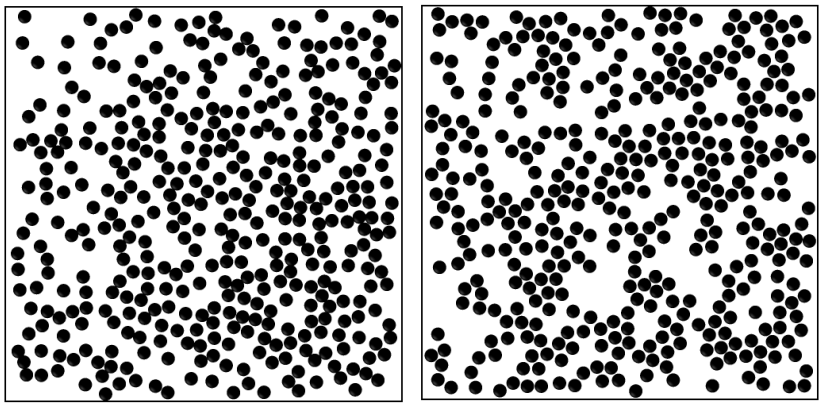

FIG. 4. Ovito snapshots of the system after the first (left) and second (right) production run. The particle radius is representative and has no physical meaning.