Universität Freiburg – Institut für Physik
Applied Theoretical Physics
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Exercise 3 for '*Computational Physics - Material Science*', SoSe 2021
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Please provide a well documented submission of your solution. Your submission should include

- A pdf file containing the solution to the questions with the corresponding equations that are implemented in your codes. Figures must contain axis titles with corresponding units and a caption.
- The source code should be commented, and the equations given in the pdf file have to be referenced in the source code.
- There is no need to provide the trajectory files.
- In case your code is not working properly, please provide a description of the debugging attempts you did.

Exercise 3.1: The radial distribution function, RDF

The structure of simple fluids can be characterized by the Radial Distribution Function (RDF), $g(r)$. This function gives the probability of finding a pair of atoms at a distance r relative to the probability expected for a totally random distribution at the same particle density. In computer simulations employing pair potentials, $g(r)$ can be computed

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

where $\mathbf{r_{ij}} = \mathbf{r_j} - \mathbf{r_i}$ is the vector between atoms i and j, $\mathbf{r}$ is the vector with respect to the origin, $r = |\mathbf{r}|$, and V and N are the volume simulation box and the number of atoms in the simulation box, respectively. The objective of this exercise is to calculate and analyze the RDF of a LJ fluid.

a) Enrich the MD implementation of Exercise sheet #2 with a function that calculates, on-the-fly, the RDF, $g(r)$. Generate the trajectory of an equilibrated system of $N = 8^3$ atoms included in a periodic system of volume, V, such that the number density $\rho = N/V = 0.5\sigma^{-3}$, and calculate the corresponding RDF. Plot the result, and answer the following questions: At which distance, r, you find the maximum peak? What is the height and the meaning of this peak? What is the size of the first solvation shell, defined by the first minimum (disregarding the global minimum at $r = 0$)?

b) The radial integration of the radial distribution function in spherical coordinates yields the running coordination number, $n(r_c)$, around a particle within the distance r_c. Plot the result as $n(r_c)$ versus r_c. Which coordination number do you obtain for this system in the first solvation shell?

c) The isothermal compressibility, κ_T, can be calculated from the RDF, $g(r)$, using the compressibility equation and the Kirkwood-Buff integral, which writes

$$\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T = \frac{1}{k_\mathrm{B}T\rho} + \frac{1}{k_\mathrm{B}T}\int_V \mathrm{d}\boldsymbol{r}\,[g(r)-1]\ ,$$

where p is the internal pressure of the system. Calculate the isothermal compressibility, κ_T, for your system. What is the change of the isothermal compressibility when decreasing the number density from $0.5\sigma^{-3}$ to $0.25\sigma^{-3}$?

d) Reduce the dimensionality of your MD implementation to 2D. This operation can be done by (i) initializing the atoms' velocity along the z-direction to 0, (ii) cancelling the time integration along the z-direction, and (iii) correcting the normalization factor of the RDF. Construct a simulation setup consisting of $N = 400$ atoms distributed on a 2D lattice in the xy-plane such that the number density is $\rho = 0.5\sigma^{-2}$. Initialize the atom velocities to obtain a temperature $T_{init} = 300K$. The atoms are interacting through a LJ potential, with $\epsilon = 0.5k_BT_{init}$ and $\sigma = 2.55$ Å. Perform the following computer experiment:

i) Equilibrate the system at $T = T_{init}$ during 2000 time steps.

ii) Generate a trajectory for 2000 time steps while keeping the temperature $T = T_{init}$, and calculate the corresponding RDF.

iii) Cool down your system during 10000 time steps to 10K without altering the well depth of the LJ potential.

iv) Generate a trajectory at $T = T_{init}$ during 2000 time steps, and calculate the corresponding RDF.

Plot the RDFs at the end of (ii) and (iv), and provide representative ovito-snapshots obtained in (ii) and in (iv).

Numerical values of quantities to be used:

quantity	value (units)
k_B	1.38×10^{-23} ($\mathrm{m^2\ kg\ s^{-2}\ K^{-1}}$
ϵ	0.5 k_BT
σ	2.55×10^{-10} (m)
T	300 (K)
m	105.52×10^{-27} (kg)
Δt	10^{-15} (s)
t_{eq}	2000 Δt
t_{prod}	2000 Δt