Exercise 1 Radial distribution functions for different phases of water

Molecular Dynamics (MD) is a tool for sampling an atomic system by evolving it in time by integrating the equations of motion. In practice, a trajectory of the system in phase space (the positions and momenta of all particles) is recorded at regular time intervals which allows us to compute many physical observables.

Several software packages allow us to visualize the trajectory of atomic systems. We will use the visualization and analysis program VMD (Visual Molecular Dynamics) that also allows us to compute useful averages by analyzing system trajectories. In this exercise we will compute the radial distribution function (RDF) of pairs of atomic species $g_{AB}(r)$, which is defined for atomic species A and B as follows:

$$g_{AB}(r) = \frac{1}{4\pi r^2 N_A} \left\langle \sum_{j=1}^{N_A} \sum_{k=1}^{N_B} \delta(r - r_{AB}^{jk}) \right\rangle$$

where $\langle \ldots \rangle$ denotes the average value for the ensemble of configurations in the simulation, r_{AB}^{jk} is the scalar distance between the j^{th} particle of species A and the k^{th} particle of species B, and N_A and N_B are the total numbers of particles of species A and species B in the system, respectively. Notice that the normalization factor $\frac{1}{4\pi r^2 N_A}$ ensures that the average number of B particles between distances r_1 and r_2 from an A particle can be computed using the expression $\int_{r_1}^{r_2} 4\pi r^2 g_{AB}(r) dr$.

The $g(r)$ is an important observable since it can also be measured experimentally through neutron and x-ray scattering; consequently, it is often used as a benchmark for simulations of atomic systems.

(a) Compute the radial distribution functions $g_{OO}(r)$, $g_{OH}(r)$ and $g_{HH}(r)$ for the following systems:
- Ice at 273 K.
- Liquid water at 300 K,
- Liquid water at 580 K,
- Water vapour at 580 K,

You can get trajectories obtained from MD simulations in the assignment folder.

(b) Look at the RDF for ice. Comparing the plot with the structure of ice, can you identify which structural feature(s) each of the first few (2-3) peaks of the RDF correspond to?

(c) How does radial distribution function of liquid water change as the temperature is increased? Can you rationalize this change?

(d) Explain how (and why) the $g_{AB}(r)$ differ for the different phases of water. In your answer, you should comment on the degree of "structural order" in the three phases.