6th Tutorial on MD - Radial Distribution Function and Scattering Function

Using LAMMPS we will simulate a single chain and calculate its radial distribution function (RDF) using our own Python code. Then we will Fourier transform the RDF to obtain the scattering function of the system. You receive the initial LAMMPS scripts and data files and a `jupyter notebook`.

Radial Distribution Function

1.) Simulate a single isolated chain of length $N = 100$ for a few million steps by first equilibrating it and then, during the production run, write out the coordinates in suitable time increments (Hint: use the `dump` command of LAMMPS).

2.) Write the code to read in the coordinates of the simulated chain. You can use the material from previous exercises, e.g. the 2nd exercise on MD.

3.) Iterate through the coordinates at each timesteps and calculate the radial distribution function $g(r)$ of the system. Plot the function and save it to a text file.

Relation to the Scattering Function S(q)

One can obtain the scattering function $S(q)$ of a system by Fourier transformation of the radial distribution function $g(r)$. This is possible by using the formula

$$S(q) = 1 + 4\pi\rho \int_0^\infty r(g(r) - 1)\frac{\sin qr}{q} dr.$$

4.) Create a python code that reads in your radial distribution function $g(r)$ and performs this Fourier transformation in a discretized manner to obtain $S(q)$. Plot the resulting function and save it to another text file.