Algorithm for calculating the Radial Distribution Function (RDF) for a given position configuration

Decide on bin size (delta)
Take distances up to L/2
length = int(0.5L/delta): Length of RDF array
rho = N/(L*L) : Mean number density

RDF function (positions, length):
    Initialize distribution array of length `length'
    loop over all pairs:
        calculate relative position of pair and correct it (torus)
        calculate pair distance
        determine which `bin' this distance corresponds to
        if the bin index <= length - 1:
            add 1 to the bin
    divide the individual entries by rho*2*pi *r*delta (Note: r will be different for different entries).
    return the distribution array

Strategy for plotting RDF

1. Run the Verlet algorithm with the thermostat to initially `thermalise' the system to equilibrium.
2. Run the Verlet algorithm further for t = 100 *without* the thermostat (the system will now be isolated with conserved energy).
3. Further run from t=100 to t=200, but now gather data.
4. Initialise the distribution array.
5. Every 10 cycles of the loop (this number is flexible), compute the RDF and add the data to the distribution array.
6. Divide the array by the number of data samples (set a sample counter)

Create an array of radii. This will have length `length'.
Plot the RDF array vs the array of radii.