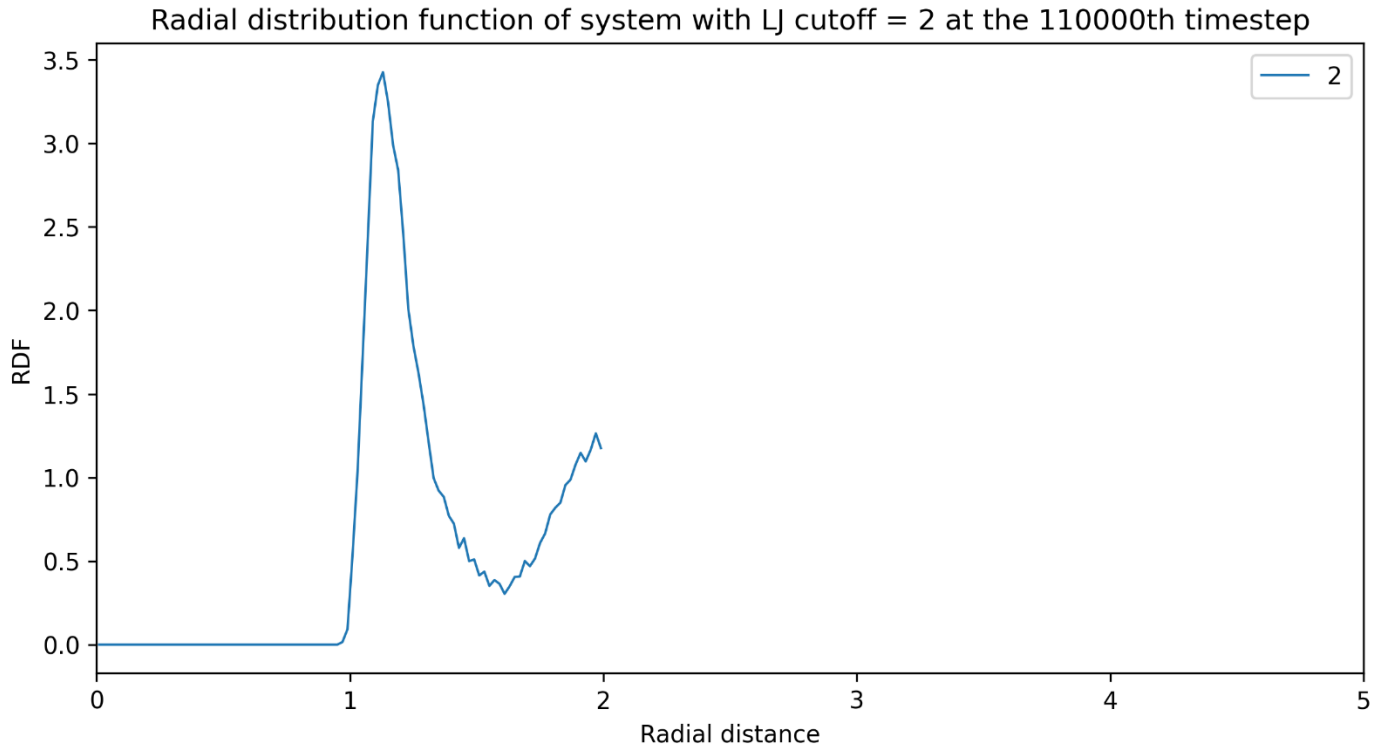
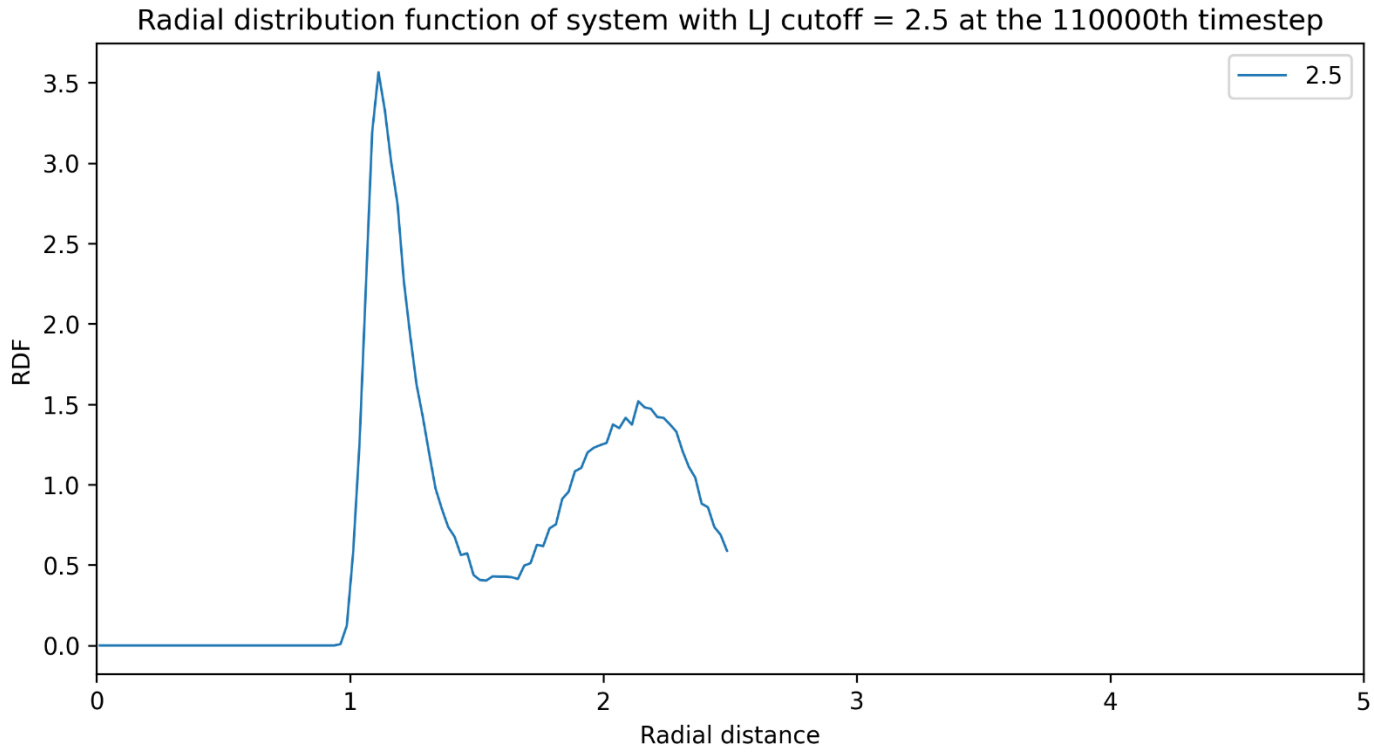
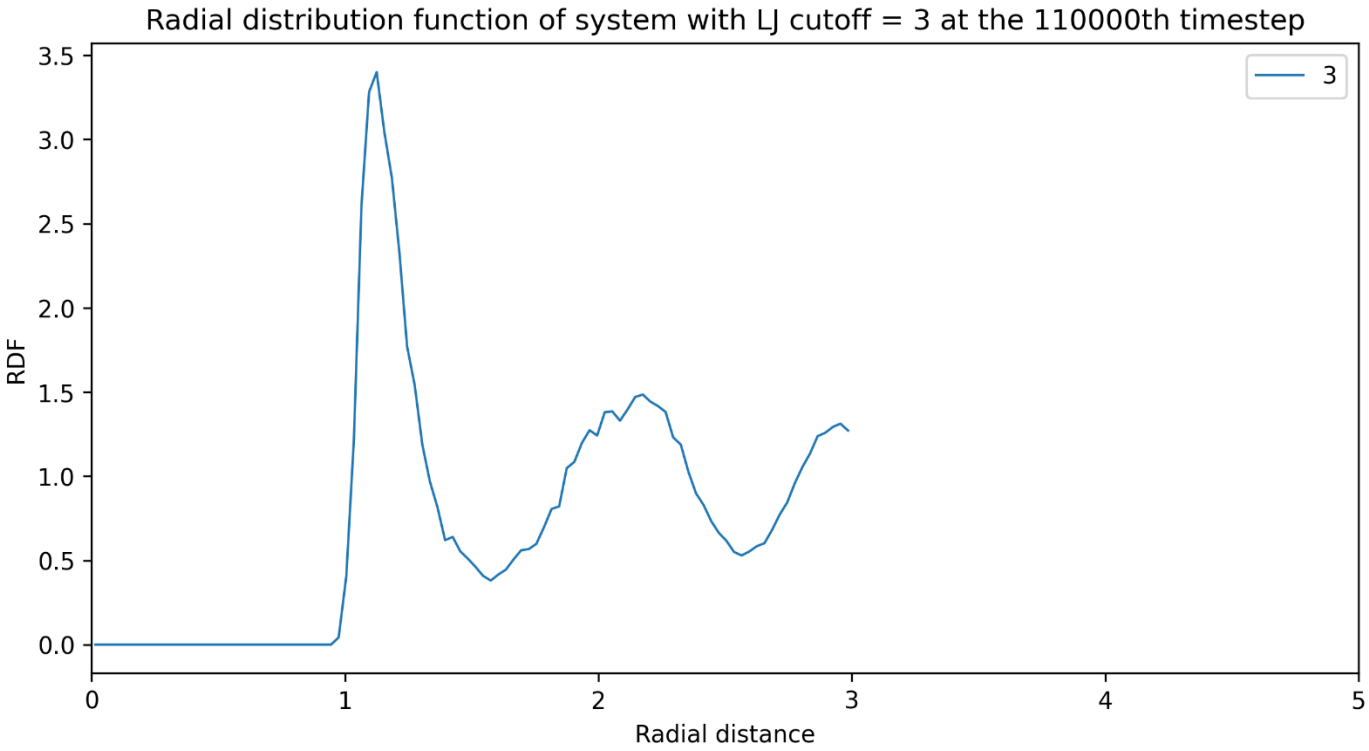
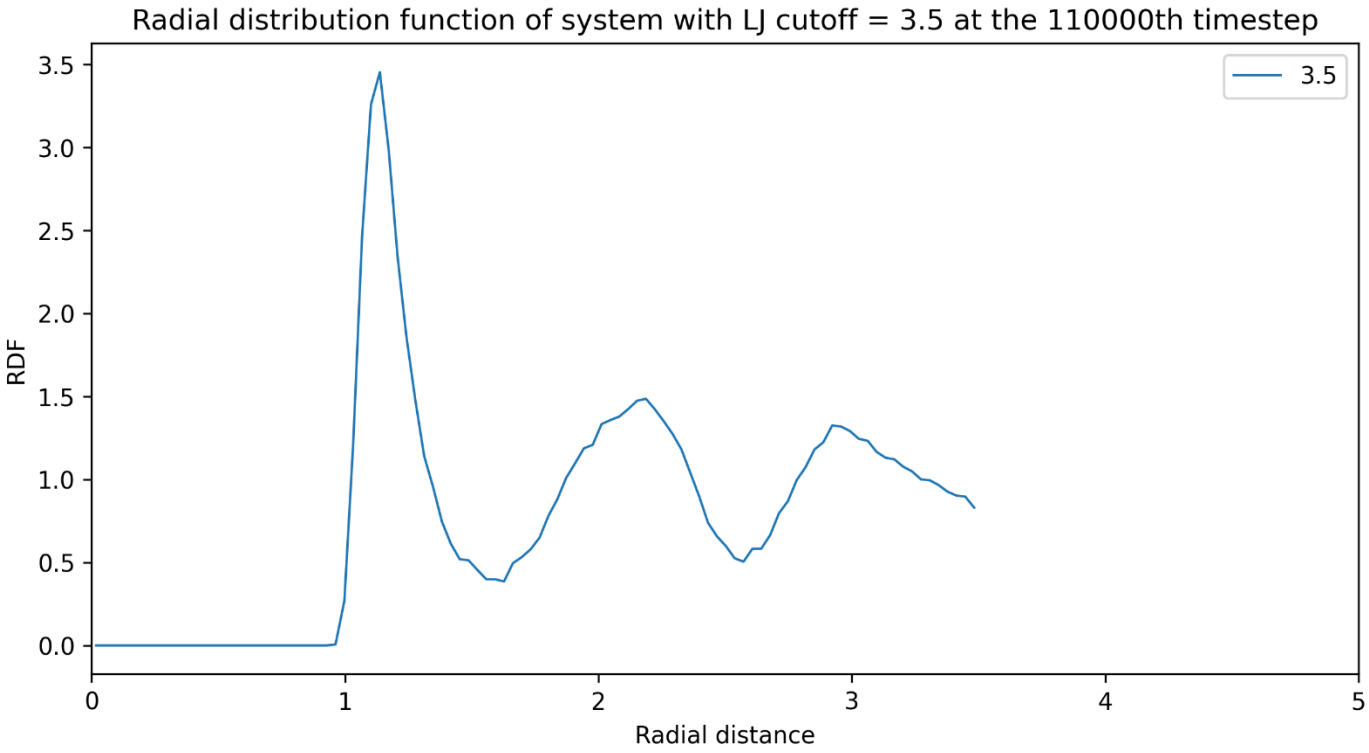
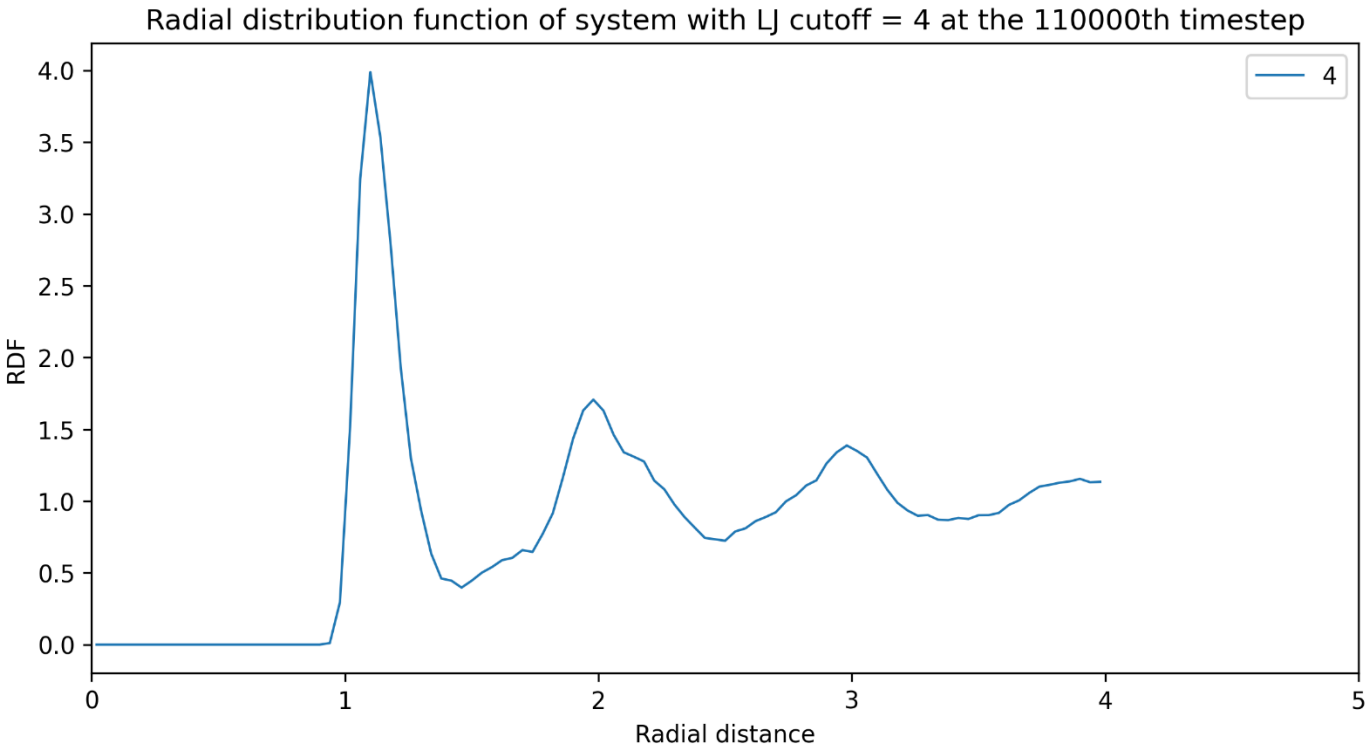
Following are various plots of RDF versus time. First, I have shown RDF-time curves at the final simulation timestep for varying LJ cutoff values. Then, I have shown combined plots across different timesteps to illustrate how RDF varies with simulation time. The numbers in the legends signify the cutoff distances as applicable.

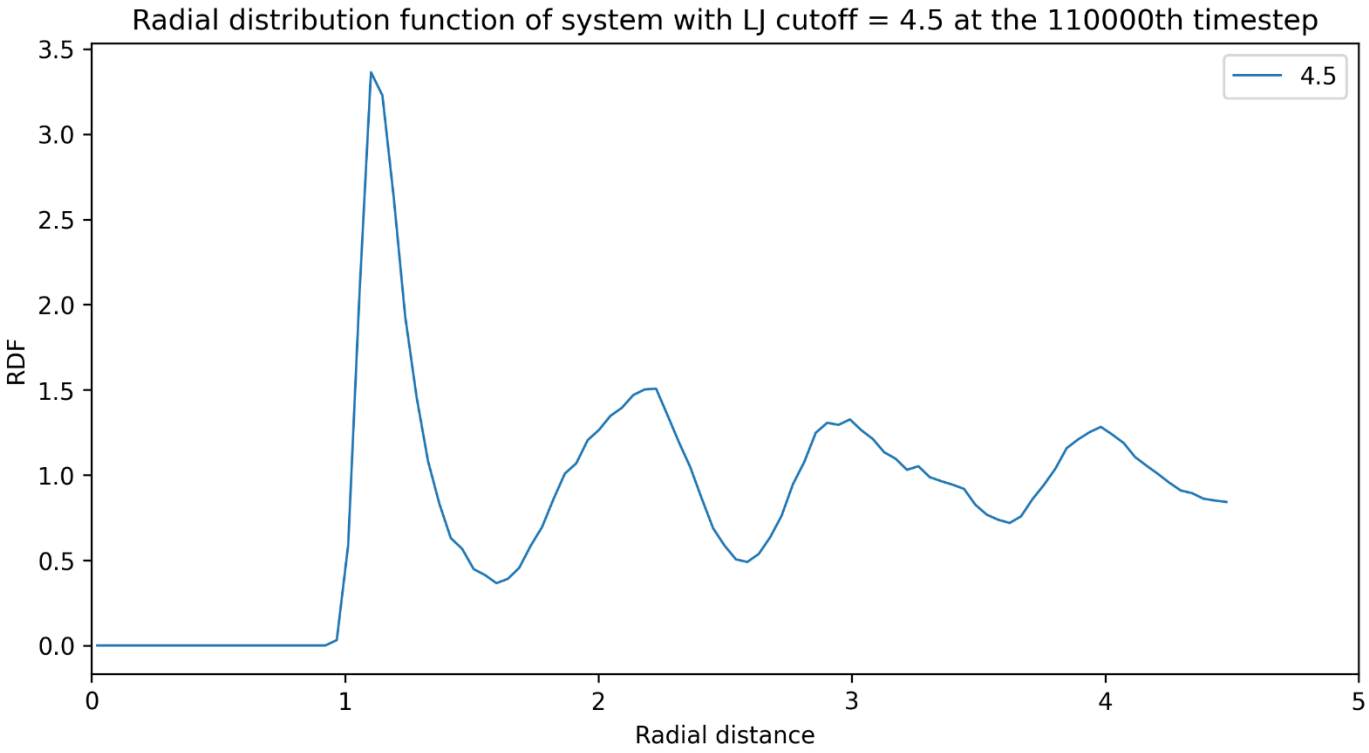


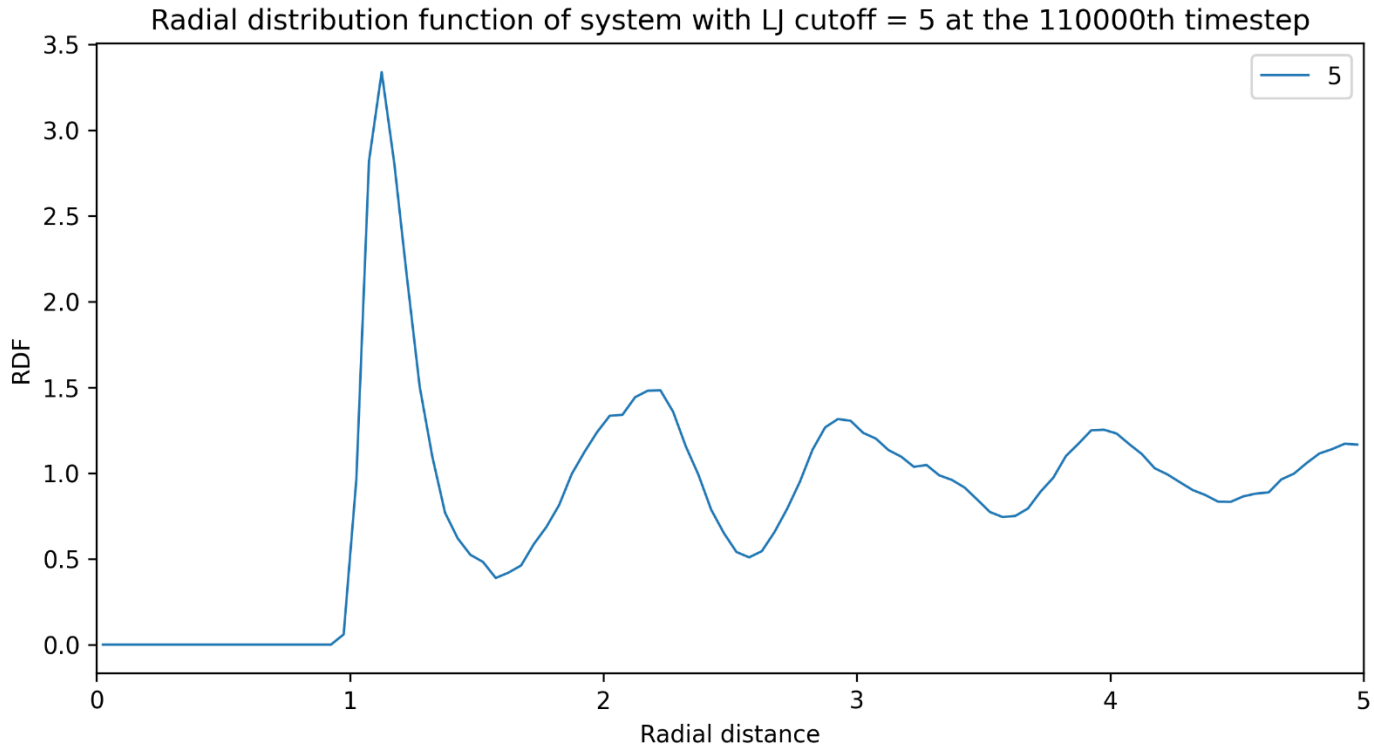




Radial distribution function of system with LJ cutoff = 3 at the 110000th timestep
3
RDF
Radial distance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
1
2
3
4
5

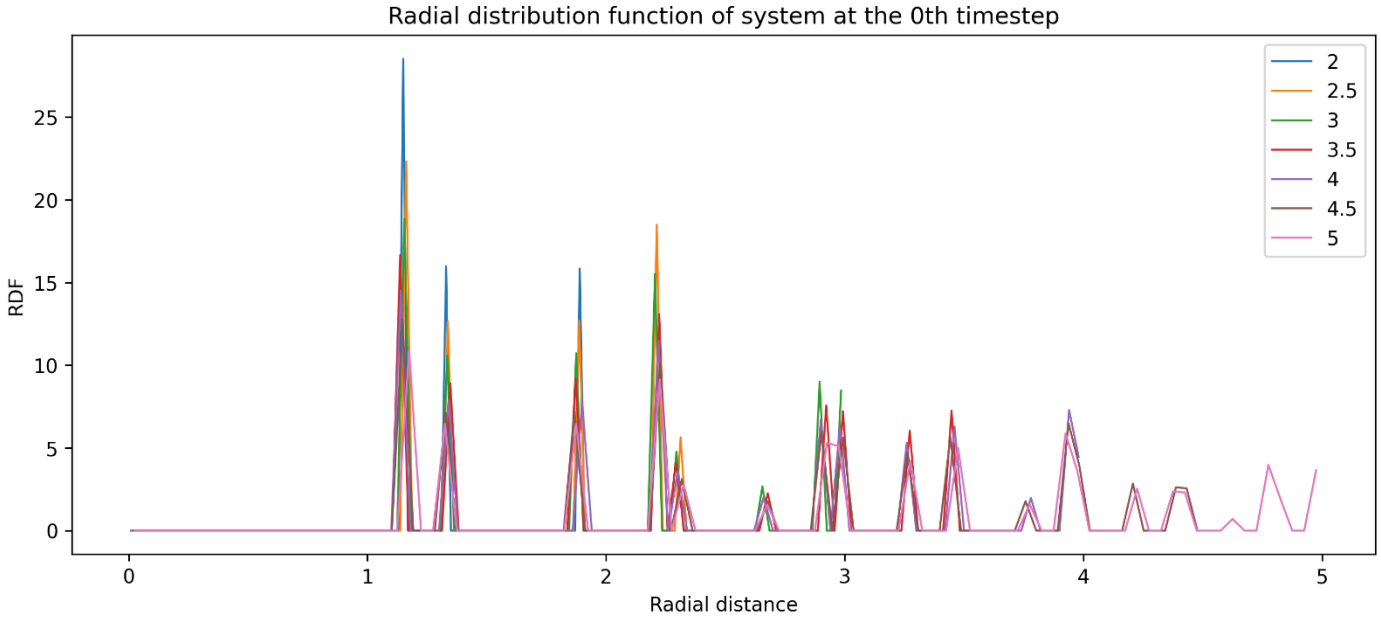

Radial distribution function of system with LJ cutoff = 3.5 at the 110000th timestep
3.5
RDF
Radial distance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
1
2
3
4
5

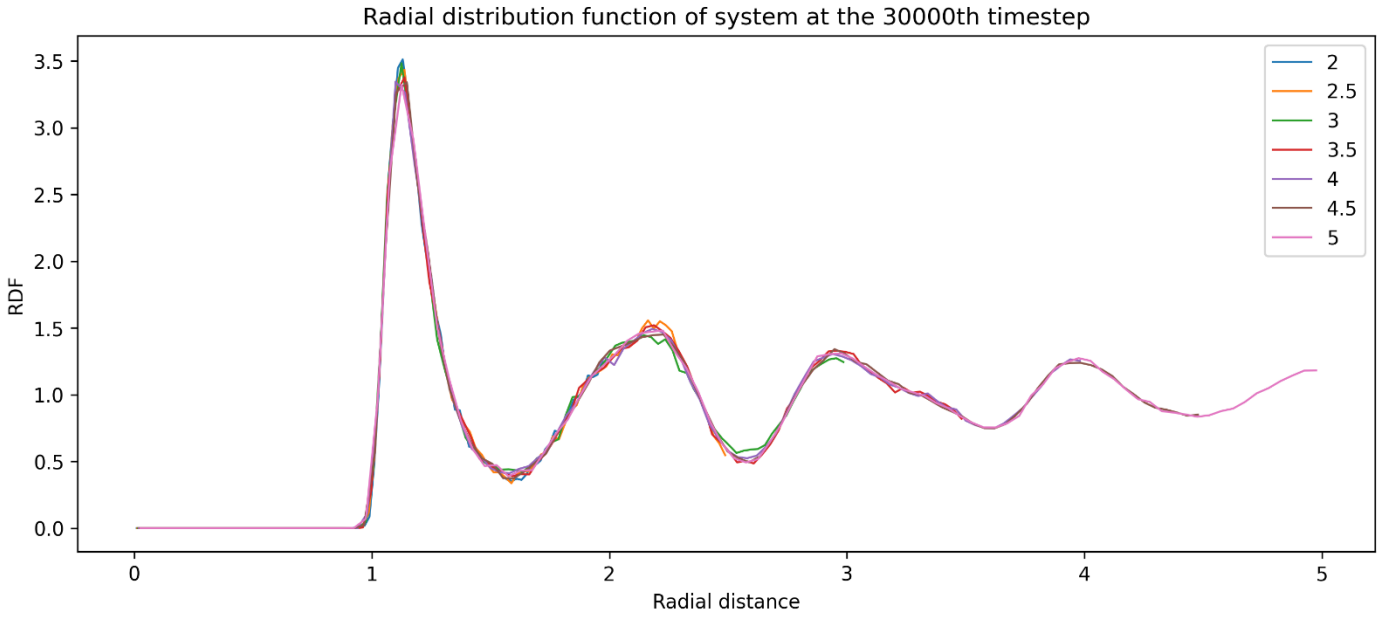

Radial distribution function of system with LJ cutoff = 4 at the 110000th timestep
4
RDF
Radial distance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
0
1
2
3
4
5

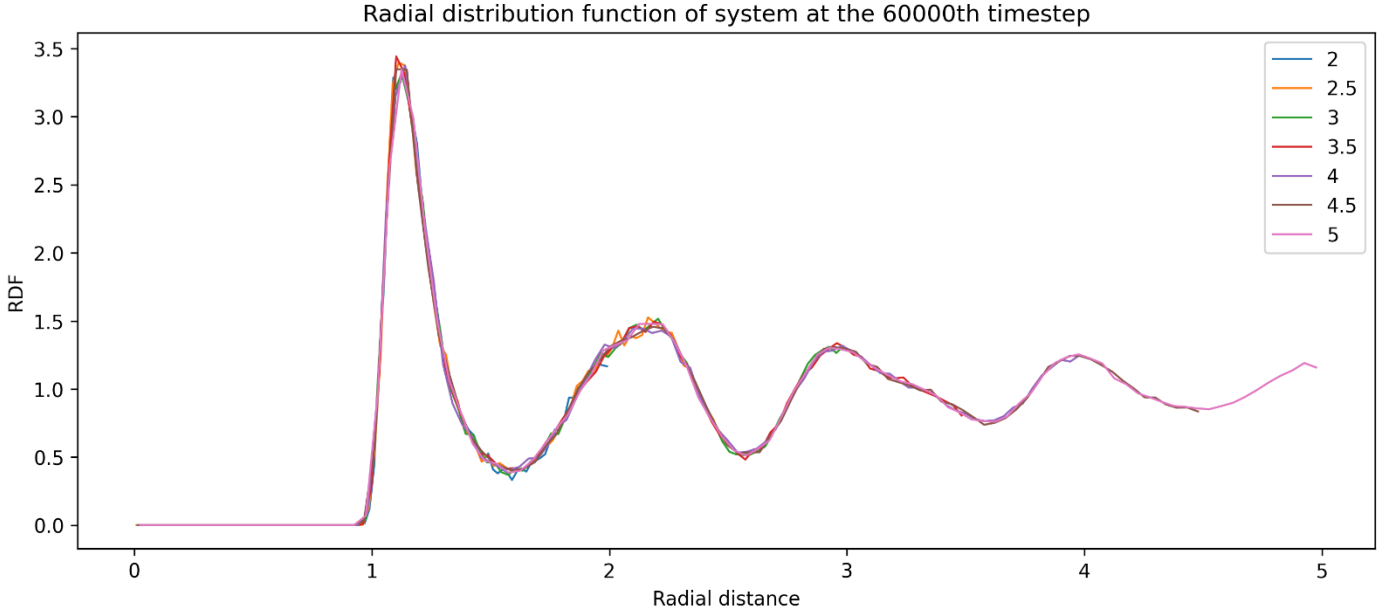

Radial distribution function of system with LJ cutoff = 4.5 at the 110000th timestep
4.5
RDF
Radial distance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
1
2
3
4
5

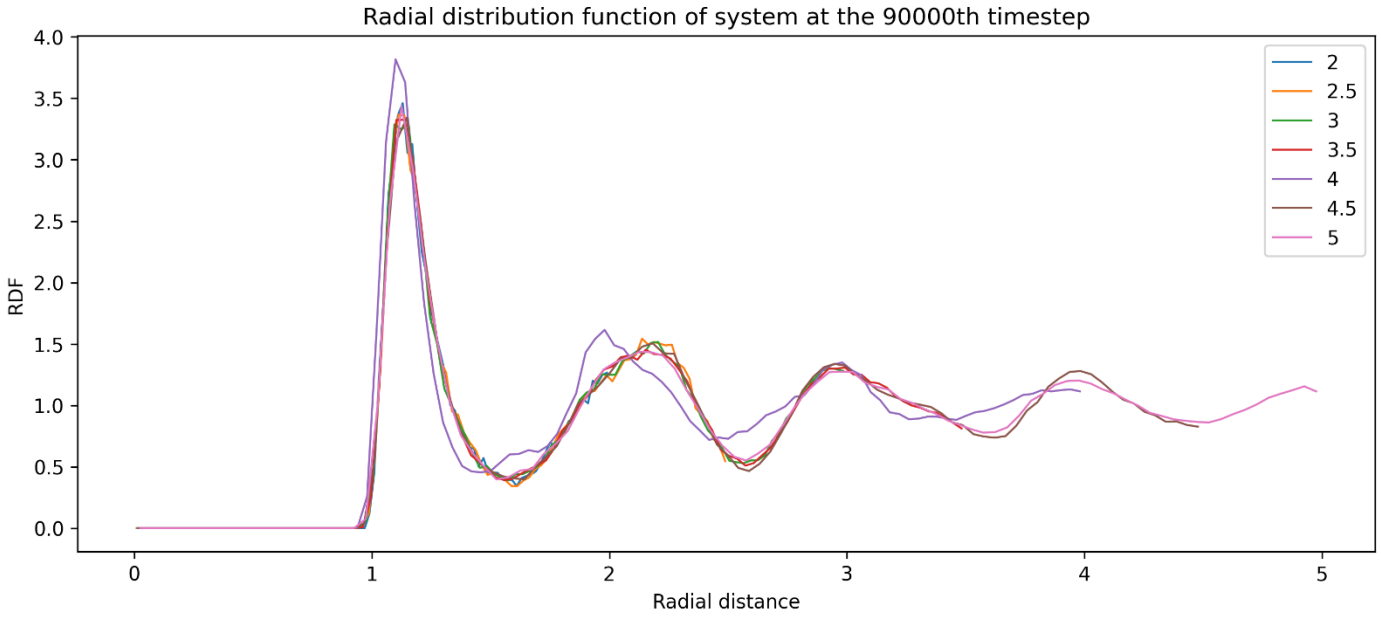


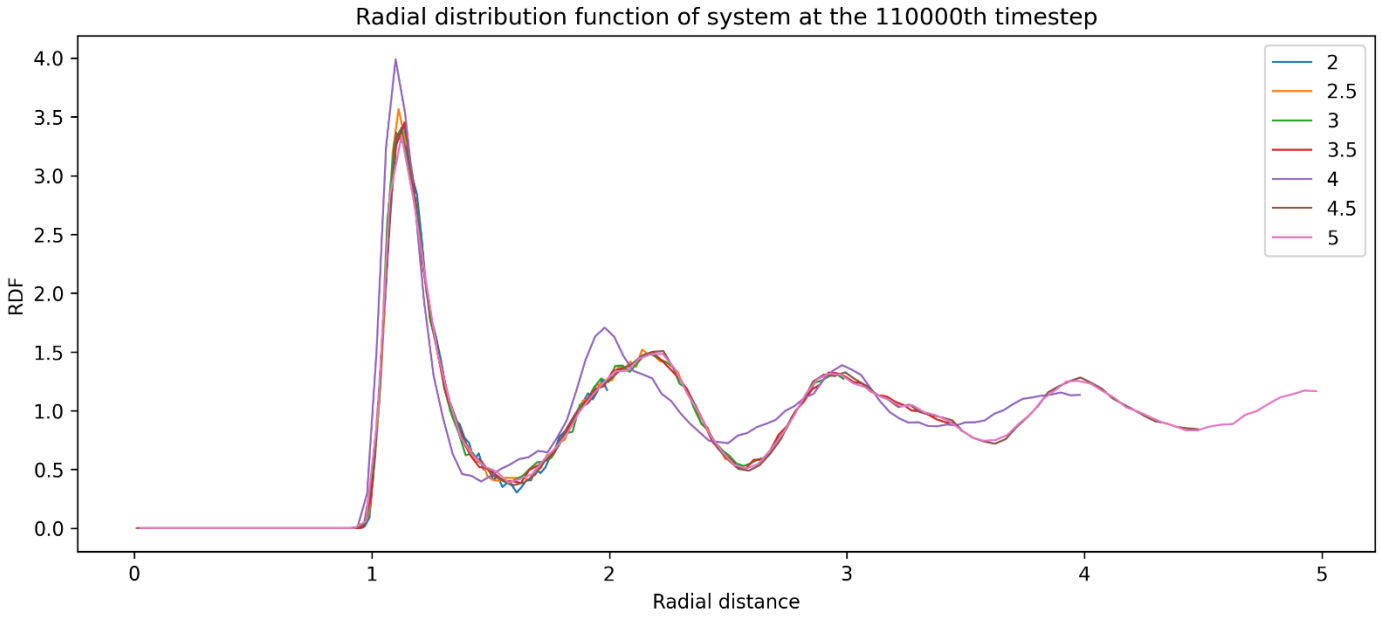

We see the major peak around a radial distance of 1 – 1.5 which corresponds to the first shell of the coordination sphere. While the plots look roughly the same, I present combined plots over different timesteps for a clearer comparison. The time variance is shown to illustrate how the system evolves; we see that the RDF changes shape as the lattice ‘melts’ and the atoms move around their lattice positions. The numbers in the legends signify the cutoff distances.




Radial distribution function of system at the 30000th timestep
RDF
Radial distance
2
2.5
3
3.5
4
4.5
5


Radial distribution function of system at the 60000th timestep
RDF
Radial distance
2
2.5
3
3.5
4
4.5
5




The curves overlap extremely well for common radial distances. The curve for cutoff = 4 seems to be an outlier, which might be due to simulation variability.

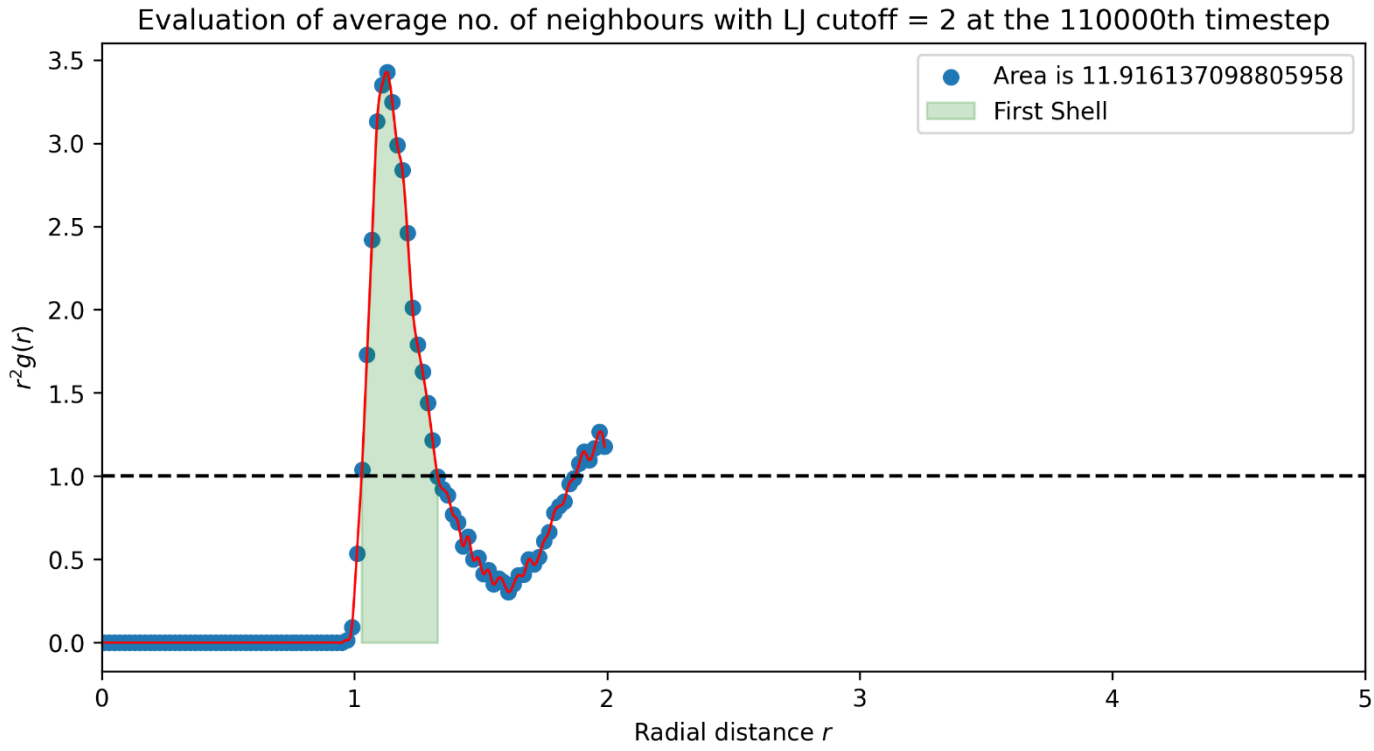
**Calculation for average number of nearest neighbours**

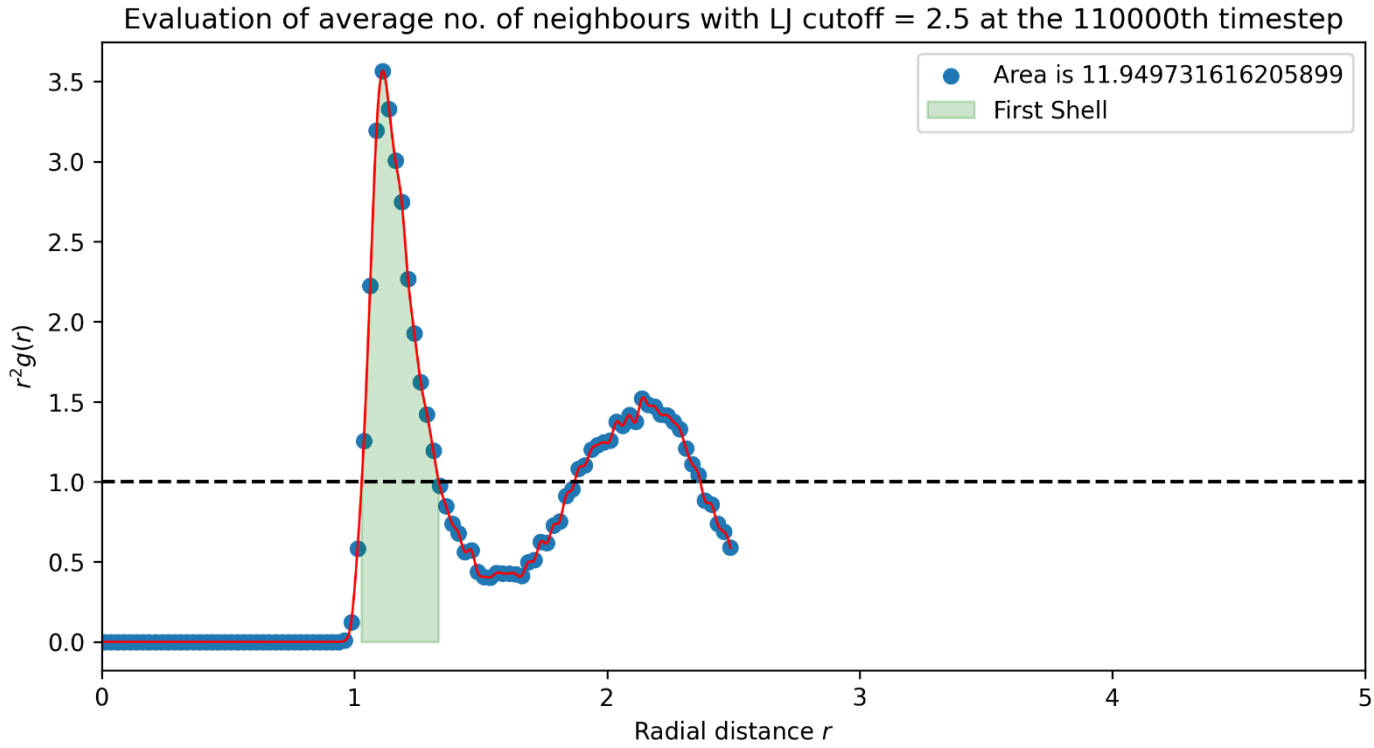
The following equation is invoked:

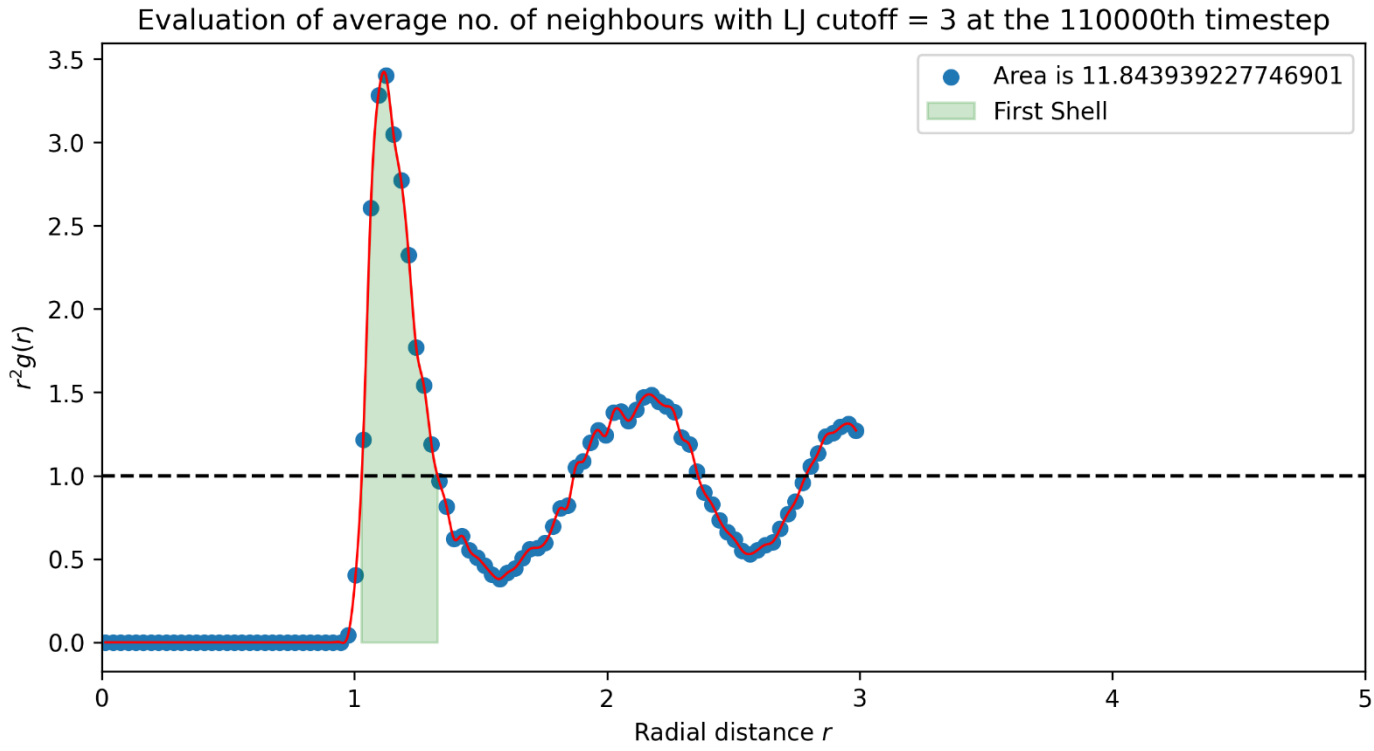
$$n = 4\pi \frac{N}{V} \int_{r_{in}}^{r_{out}} r^2 g(r) dr$$

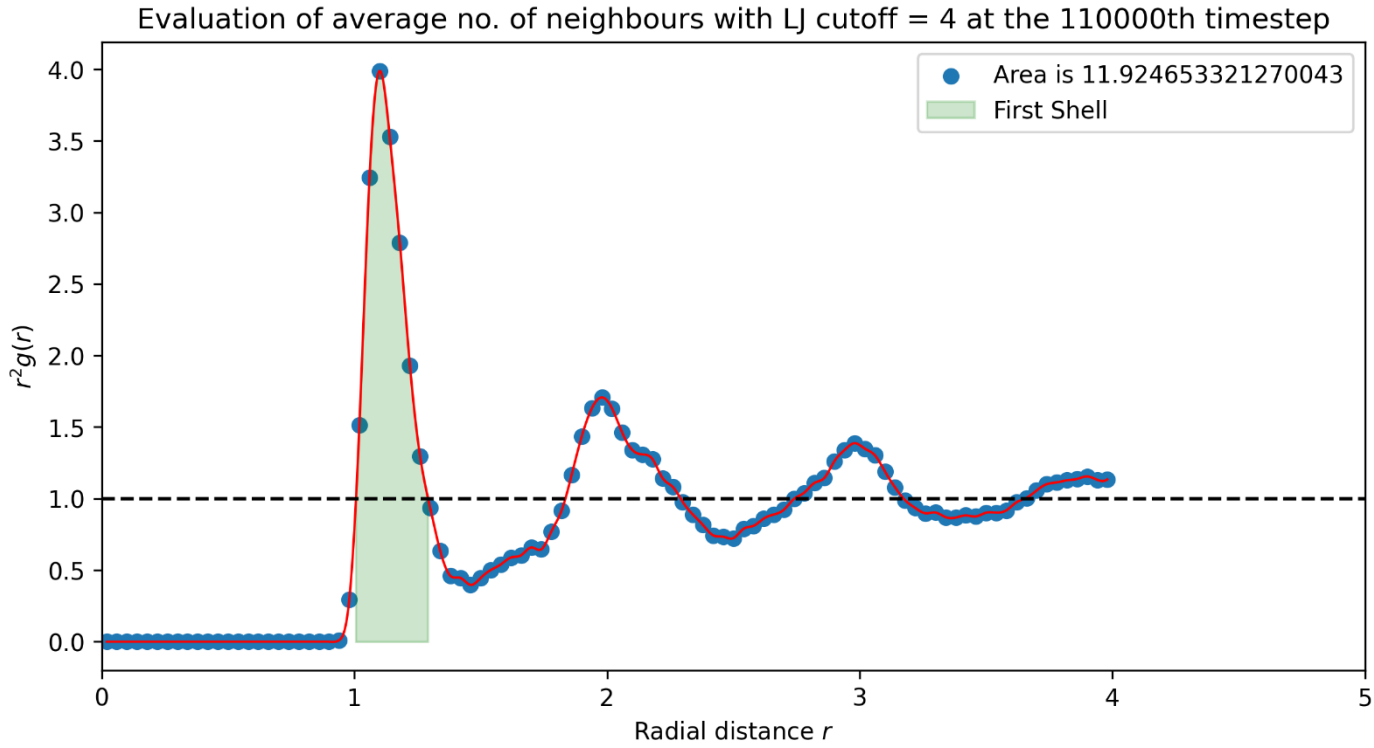
Here, N/V is the density of the liquid. For our simulations, this is evaluated to be (2000 atoms / simulation volume of 1000) = 2. The integral is computed numerically from the RDF ($g(r)$) curves scaled with the $r^2$ factor.

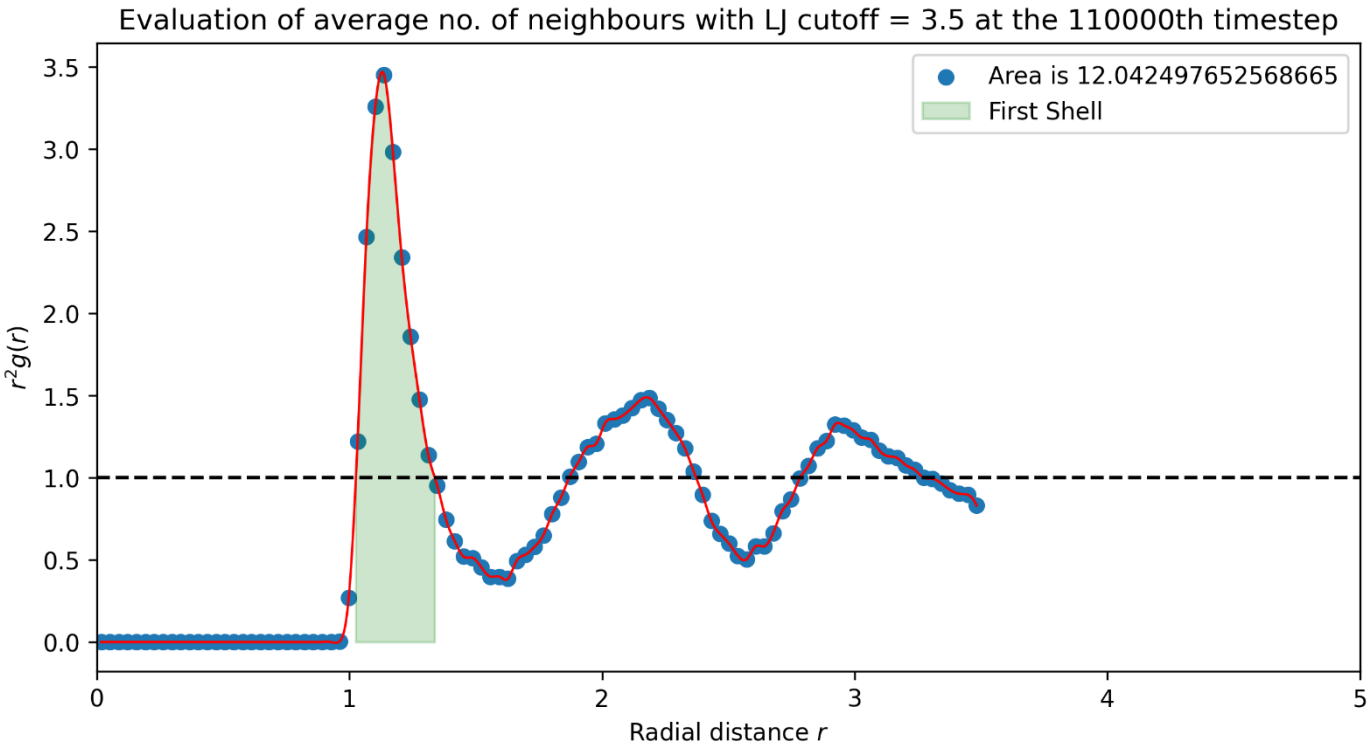
Due to a sparsity of points in the region of interest, a spline curve was generated to interpolate the data points. In the following plots, the solid line indicates the spline curve while the scatter data correspond to the true data:

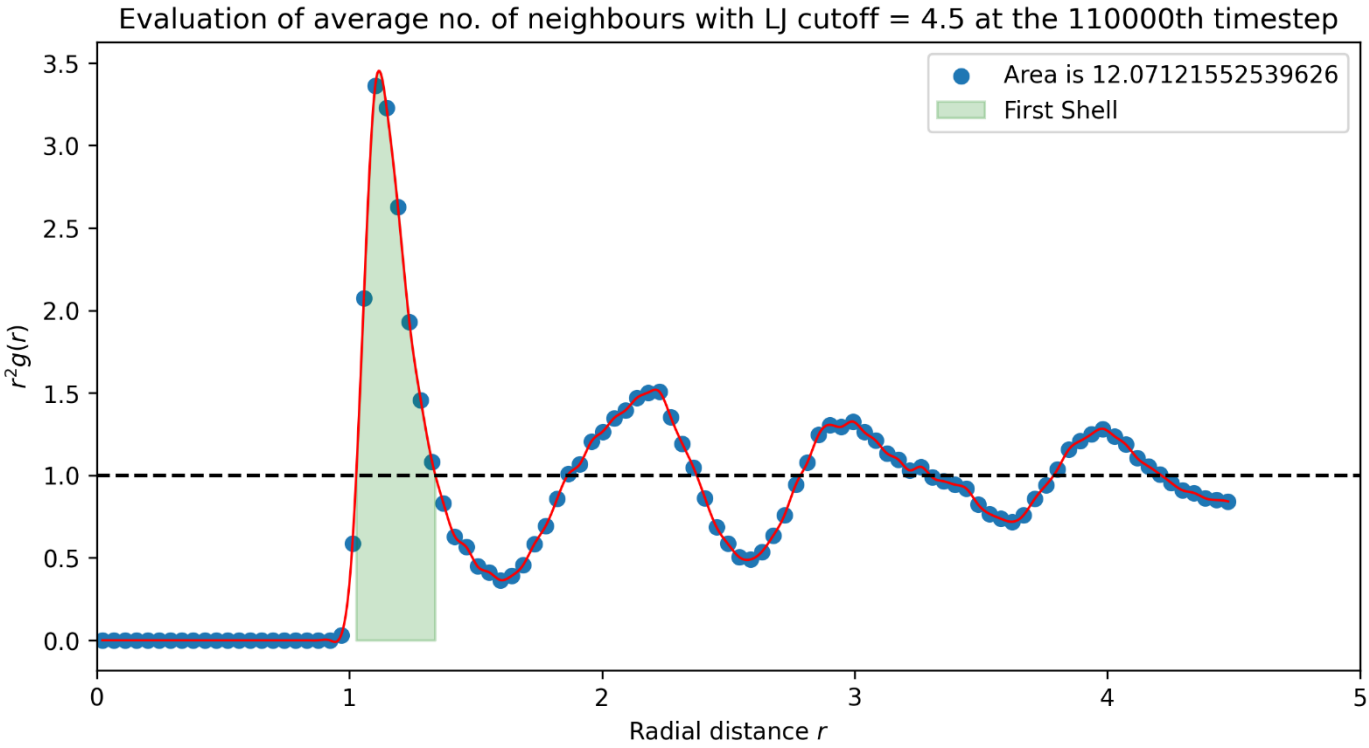

Evaluation of average no. of neighbours with LJ cutoff = 2 at the 110000th timestep
Area is 11.916137098805958
First Shell
$r^2g(r)$
Radial distance $r$

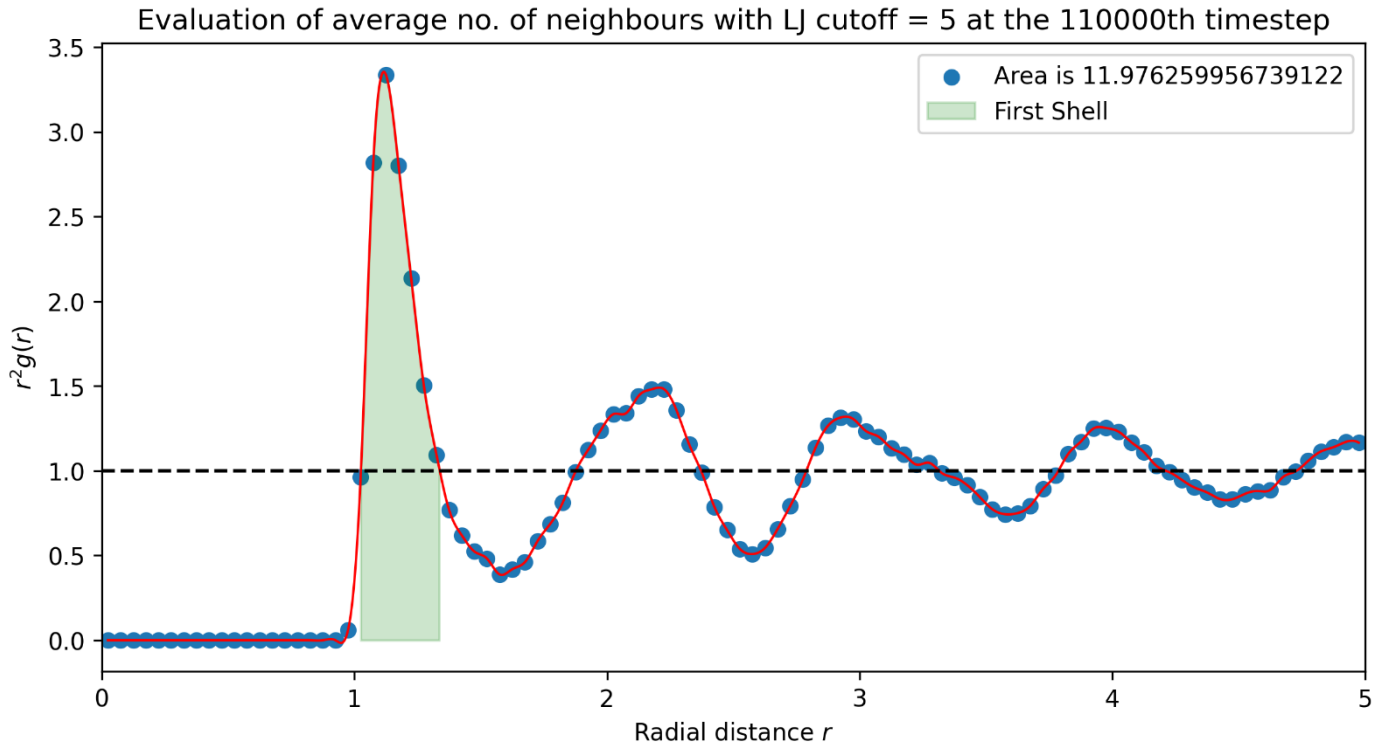

Evaluation of average no. of neighbours with LJ cutoff = 2.5 at the 110000th timestep
Area is 11.949731616205899
First Shell
$r^2g(r)$
Radial distance $r$


Evaluation of average no. of neighbours with LJ cutoff = 3 at the 110000th timestep
Area is 11.843939227746901
First Shell
$r^2g(r)$
Radial distance $r$


Evaluation of average no. of neighbours with LJ cutoff = 4 at the 110000th timestep
Area is 11.924653321270043
First Shell
$r^2g(r)$
Radial distance $r$


Evaluation of average no. of neighbours with LJ cutoff = 3.5 at the 110000th timestep
Area is 12.042497652568665
First Shell
$r^2g(r)$
Radial distance $r$


Evaluation of average no. of neighbours with LJ cutoff = 4.5 at the 110000th timestep
Area is 12.07121552539626
First Shell
$r^2g(r)$
Radial distance $r$




To summarize the data,

| Cutoff distance | Value of $n$ |
|---|---|
| 2 | 11.9161 |
| 2.5 | 11.9497 |
| 3 | 11.8439 |
| 3.5 | 12.0425 |
| 4 | 11.9246 |
| 4.5 | 12.0712 |
| 5 | 11.9762 |

We see that, on average, atoms in the system seems to have 12 nearest neighbours.