Week 7: Radial Distribution Functions

2MMN40: Introduction to Molecular Modeling and Simulation
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Contents

1 Introduction

You have implemented everything for your molecular dynamics code. Today you will only add a bit of functionality to analyze your trajectories. It is a shorter exercise, afterwards you can work on your code and prepare your final report.

2 Radial distribution functions

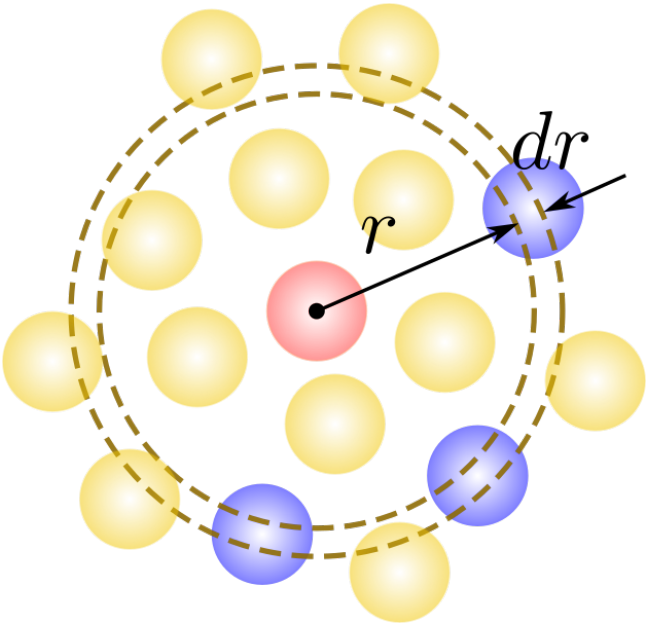

Figure 1. RDF calculation with distance from central atom r and infinitesimal dr ring. Taken from https://en.wikipedia.org/wiki/Radial_distribution_function

The radial distribution function is defined as the ratio of density of atoms at distance r (in control area rdr) divided by the overall density. It is calculated by counting how many atoms are in a ring with radius r and thickness dr around the atom of interest. For a discrete system dr has to be a finite value. Hence the calculation can be done as a histogram where every bin represents a ring of thickness dr (note that NumPy has a function `np.histogram` that computes histograms given some data and the bins).

Implement this functionality either in your md code or write a program that reads in your md trajectories and calculates the RDF from it. How can you use averages and which kind of averages? How large should you choose dr? How big can r become?

Of course you can also look at element specific RDFs, where you only look of atoms of a certain kind.

Tip: Don't forget the PBCs in your calculations for the RDF.