Week 1: Trajectories and Distances

2MMN40: Introduction to Molecular Modeling and Simulation
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Contents

1 The Assignment

This weeks assignment consists of three parts

1. Load a few of the trajectories in VMD and see what happens,
2. Write a small program that can read trajectory (.xyz) files and
3. Write a function that calculates the distances between all the atoms.

There are four trajectories you can test your code on: waterSmall.xyz (only one time step), hydrogen.xyz, water.xyz and methane.xyz. For the first trajectory we will provide you with the correct distances so you can quickly check if your code calculates the right numbers. The distances are represented in a matrix where entry (i,j) is the distance from atom i to j.

```
[[0.         0.9571889  0.96136413 2.97819977 3.08586955 3.64431369]
 [0.9571889  0.         1.49174449 3.63838878 3.80324848 4.38048156]
 [0.96136413 1.49174449 0.         3.574232   3.45996945 4.19310287]
 [2.97819977 3.63838878 3.574232   0.         0.95166474 0.95486255]
 [3.08586955 3.80324848 3.45996945 0.95166474 0.         1.50441861]
 [3.64431369 4.38048156 4.19310287 0.95486255 1.50441861 0.        ]]
```

2 Visual Molecular Dynamics (VMD)

There is a short VMD tutorial available on canvas. It will show you how to install and use VMD in about 5 or 10 minutes.

3 Trajectory Files (.xyz)

Trajectory files are relatively simple, they contain the type and position of every atom in the simulation. The basic file format is

```
<number of atoms>
<a line for comments>
<atom type> <x> <y> <z>
<atom type> <x> <y> <z>
```

To allow for multiple time steps, the frames are simply put one after the other in the file. An example for two time steps of a single hydrogen molecule.

```
2
This is a comment about hydrogen
H   0.0   0.0   0.367
H   0.0   0.0  -0.367
2
```

```
Another comment
H    0.0    0.0    0.361
H    0.0    0.0   -0.361
```

Note that there are quite some ommissions in a .xyz file. For starters there is no timestep present. Secondly there are no bonds specified, how should we know how the atoms are connected? If you have already loaded a trajectory in VMD, how do you think VMD does it?

> **TIP:** The time step problem is easily solved by adding the timestep to the comment line. As an example, you could add `t=<number>` and use python to search for the t= in the comment and read the number. For now you don't need to worry about this, but it might come in handy later on.

4 Programming with Python

To help you get started with programming in python we have made a few python tutorials that are available on canvas. These python tutorials are not meant as a reference, but as a time saver. They will cover most of the features you will need in this course, but there is way more to learn than just these tutorials.

We also have a page on canvas with general programming tips and tricks and a page with good python resources to learn python in more detail or as an alternative to our tutorials. These pages can be found in the Additional Resources module.

If you want to use the tutorials start with the one called "Basic Python".