Task for first week

1.- **Reading materials**:

Understanding DNA: The Molecule and How it Works. Authors: Chris Calladine, Horace Drew, Ben Luisi, Andrew Travers.

2.- **LAMMPS installation with oxDNA**:

Instructions are provided in the additional pdf file: **README*lammps*installation.pdf**

LAMMPS scripts and simple initial configuration can be found in the LAMMPS folder: *examples/PACKAGES/cgdna/examples/oxDNA2/*. There, you will see examples of double stranded rings (inside dsring) or linear double stranded DNA (inside duplex1).

3.-**oxView**

a) Read the description of oxView on their github site: *https://github.com/sulcgroup/oxdna-viewer*

b) Watch their youtube tutorial: *https://www.youtube.com/watch?v=arhmT0LStUQ*

c) Use the website tool of oxview *https://sulcgroup.github.io/oxdna-viewer/* to create your own initial configuration of a linear double-stranded DNA with the following sequence:

AACGGAATTCGCATGGATCCCCACGATCG

Save that configuration as an oxDNA type. This will create two files (usually on your *Downloads* folder) called: **output.top** (this is the topology files with information about the bonds) and **output.dat** (thi is the file with the positions and orientations of the nucleotides in your system).

4.-**tacoxDNA**

Convert the previous two files into a format that can be read by LAMMPS using tacoxDNA website: *http://tacoxdna.sissa.it/oxDNA_LAMMPS*

5.-**Run and compare two simulations**

a) Using the LAMMPS script mentioned in point 2, but with the initial configuration you created, run the simulation for at least 2x10^7 timesteps. You have to modify a little bit the script for this:

Replace:

> variable ofreq equal 1000
>
> variable efreq equal 1000
>
> read_data data.duplex1
>
> run 1000000

By the following:

> variable ofreq equal 50000
>
> variable efreq equal 50000
>
> read_data *NameOfYourInitialCongigurationFile*
>
> run 20000000

Finally, chek the trajectory with vmd.

b) If you have enough time, create an initial configuration with the same sequence as before, but this time instead of creating a double-stranded DNA, create a single-stranded DNA. Run a simulation and check the thrajectory with VMD. Dou you notice any difference? which?

c) With oxview, try to create a ring double-stranded-DNA instead of a linear one.