LAMMPS installation with the oxDNA package

Download the last stable version of lammps from the website *https://www.lammps.org/download.html* and unzip the file. Alternatively, you can use a terminal to download the github repository:

```
1.- git clone -b stable https://github.com/lammps/lammps.git mylammps
```

The following are the steps to install LAMMPS with the oxDNA package

```
2.- Go to *src/STUBS* and type *make*

3.- Go to src/ and load the required packages for oxDNA:
    cd ..
    make yes-rigid yes-molecule yes-asphere yes-USER-CGDNA

4.1.- In order to produce serial excecutable, in src/ type:
    make serial

4.2- In order to produce a parallel executable:
     make -j4 mpi
```

This will create the executables **lmp_serial** and **lmp_mpi** respectively. Copy this executable to your home directory.

Run the examples of oxDNA that come with the LAMMPS distribution:

Inside the LAMMPS folder you download (or clone) in the previous section go with a terminal to the following path: **examples/PACKAGES/cgdna/examples/oxDNA2/duplex1/**. You will find the initial configuration file (data.duplex1) and the LAMMPS script (in.duplex1). Review the LAMMPS scritp and see if you understand what the script is doing. It might be helpful to take a look to the paper about the oxDNA implementation into LAMMPS: *Coarse-grained simulation of DNA using LAMMPS : An implementation of the oxDNA model and its applications*

Finally, to run a simulation you need to use the LAMMPS executable previously created, for example **lmp_serial** (that is located in your home directory). Open a terminal inside the folder **examples/PACKAGES/cgdna/examples/oxDNA2/duplex1/** and type:

```
~/lmp_serial -in in.duplex1
```