Task for first week

1.- Reading materials:

Increasing valence pushes DNA nanostar networks to the isostatic point. Nathaniel Conrad. PNAS.

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

If you want to know more about the oxDNA model, chapter 1-2 from Thomas Ouldrige thesis is a good place to start: Coarse-grained modelling of DNA and DNA self-assembly. https://ora.ox.ac.uk/objects/uuid:b2415bb2-7975-4f59-b5e2-8c022b4a3719

2.- Initial configurations (n=0) At this point you should have initial configurations of DNAnanostars with valence f=3,4,5,6. Each of these nanostars has n=0 nucleotides at FJC (flexible joint at the core). Remember to check that:

a) The total number of nucleotides is the one you expect: (47 f).

b) That the molecule-id of particles in the initial configuration runs from 1 to f.

c) That the sequence is the correct one, from 3' to 5', in the initial configuration file.

3.- Run simulations (n=0) Run simulations for each DNAns with the following parameters in the oxDNA lammps script:

a) seqdep: sequence dependent interactions.

b) tem=0.1: at a temperature 0.1 (in simulation units).

c) sc=0.15: salt concentration of [NaCl]=0.15 M.

d) runtime1=10^8 timesteps with tdamp=0.03 (default in the oxDNA model)

e) runtime2=10^8 timesteps with tdamp=2.5.

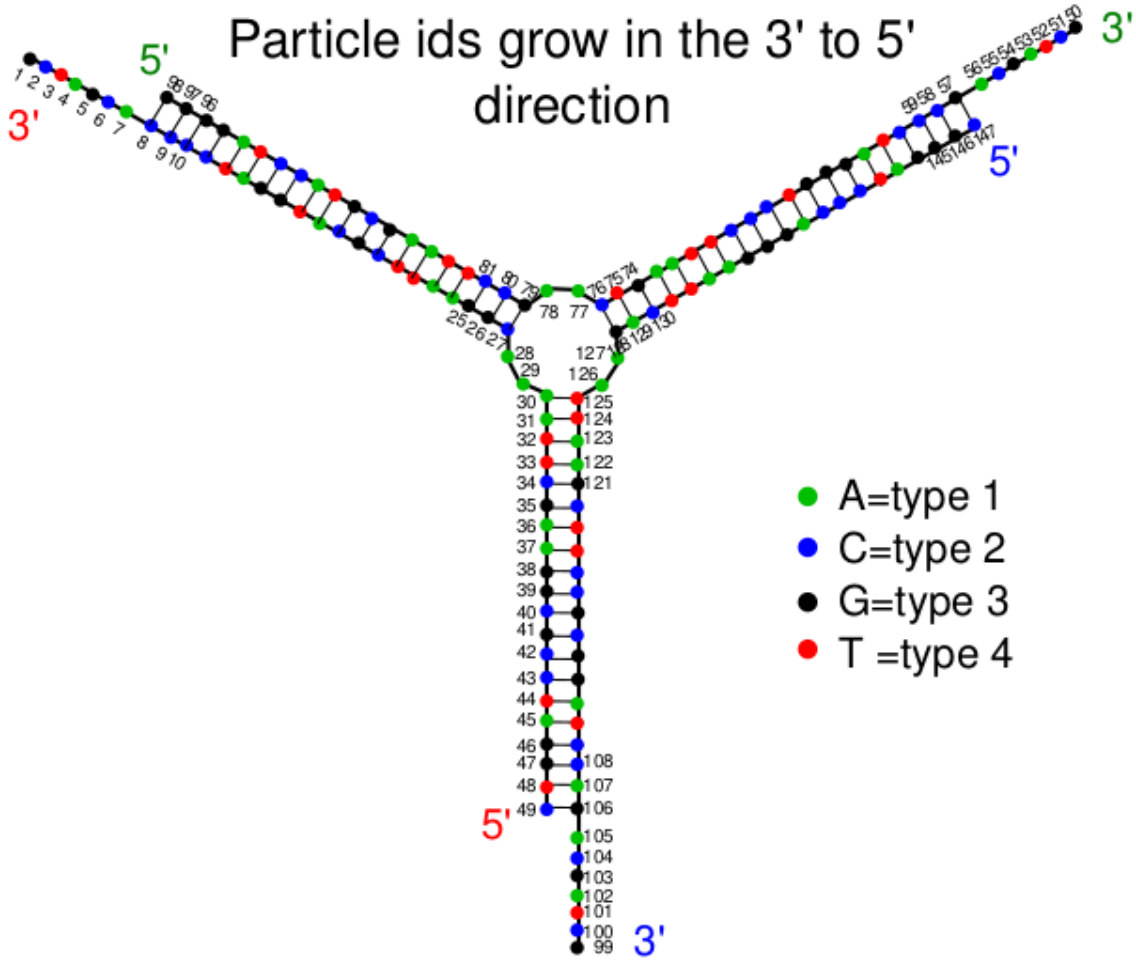
Note: Sequences for nanostars with different valence and n=2 (two nucleotides at FJC) can be found in the Supplementary Information of the PNAS paper (reading material for this week).

4.- Post processing You have to compute two important quantities:

a) The distance (dp) from the core of the molecule to the plane touching the end of the arms forming the DNA nanostar. The definition of this variable can be found in the file attached (dp.pdf)

b) The angle between the arms of the molecule.

Note that to define the orientation of the arms, you will have to find (for each of the arms), the id of the two particles forming the base-pair closer to the core of the molecule (27,79; 76,128; 30,125), and the id of the two particles forming the base-pair closer to the sticky end (8,98; 57,147; 49,106). See figure below with the id of each particle forming a DNAns with f=3.



I attach a c++ programm to do this calculation for DNAns with valence f=3. You will have to generalize this code to compute the planarity and angles between all possible pair of arms, for DNAns with different valence.

To run the programm *cv_evolution.cpp* easily I use the bash script called **script*cv*evolution.sh**. Both files have to be in the same folder (any folder). Then you need to set the value of certain variables in the bash script:

a) **mainpath:** Provide the path to the folder where your lammps-script and initial-

configuration are. You can find this information by opening a terminal inside that folder and typing **pwd**.

b) **outputpath:** provide full path to the folder where you want to store the output.

c) **multi=0:** because we are not reading results from multiple simulations, just one.

d) **conf=4:** since multi was set to zero in the previous step, this variable does not have a meaning for the computation. You have to set any integer.

e)**start=0:** start the computation from this timestep (always set it to 0).

f)**dumpfreq** the frequency of dumping used in the lammps-script to tun the simulation. Usually 100000

g)**last=:** the last timestep of your simulation. This should be set equal to runtime1+runtime2 (set in the lammps-script).

h)**N=147:** The total number of nucleotides in your system.

i)**version:** the oxdna version you use to run your simulation (always set to 2).

Once you have set all the previous variables, open a terminal and make your bash script executable by typping: **chmod a+x script*cv*evolution.sh** and then run the script: **./script*cv*evolution.sh**. This will generate a file called: **N147.oxDNA2.colvar*vs*time** in the folder specified in **b)**.