Task for first week

1.- Reading materials:

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.- Create a DNA nanostar with valence three

Use the tools you learned last week (oxView and tacoxDNA) to create a DNA nanostar (DNAns) with three double stranded arms. The sequence of each of the 3 single strands is he following:

5′– CTGGATCCGCGGAAGCTTAA AA CGGAATTCGCATGGATCCCC A CGATCG –3′

5′– GGGGATCCATGCGAATTCCG AA CTGAATTCCCTGGGATCCCG A CGATCG –3′

5′– CGGGATCCCAGGGAATTCAG AA TTAAGCTTCCGCGGATCCAG A CGATCG –3′

Each ssDNA is 49 bases long and consist of five regions (see table below and Figure1 attached). The segments I and II (20 nucleotides long each) are designed to form the three dsDNA arms. In between the two segments there are two A-nucleotides acting as a spacer and forming the flexible joint at the nanostar core, (FJC). The sticky end is formed by 6 bases and has the same sequence for the three oligonucleotides.

Segment I	FJC	Segment II	FJ	Sticky end
$5'-$ CTGGATCCGCGGAAGCTTAA	AA	CGGAATTCGCATGGATCCCC	A	CGATCG $-3'$
$5'-$ GGGGATCCATGCGAATTCCG	AA	CTGAATTCCCTGGGATCCCG	A	CGATCG $-3'$
$5'-$ CGGGATCCCAGGGAATTCAG	AA	TTAAGCTTCCGCGGATCCAG	A	CGATCG $-3'$

Table 1 Strand sequence used in the nano star design with valence $f = 3$. Each row represents a different ssDNA oligonucleotide. Segments with the same colour have complementary sequences to form the double stranded arms as shown in Fig. **1**.

3.- Check initial configuration file Before running a simulation check that the initial

configuration has the correct format. Quick checks to do:

a) That the molecule-id is the following:

> 1 for particles with atomid 1-49
>
> 2 for particles with atomid 50-98
>
> 3 for particles with atomid 99-147

b) That the sequence of each of the strands is given from 3' to 5' direction as the atom-id increases. Remember the relation between atom-type and nucleotide type: A(1), C(2), G(3) and T(4)

4.- Please complete any pending tasks from last week. Feel free to send a message if you need help