oxDNA users and developers workshop: Programme

Monday 2 September 2019

Location: Simkins-Lee Room, Beecroft Building, Department of Physics, OX1 3PU

9:30-10:00 Arrival and coffee

10:00-10:10 Ard Louis: Welcome
10:10-10:30 Jonathan Doye
A brief history of oxDNA
10:30-11:00 Will Kaufhold
Rapid In Silico Prototyping of Proximity Sensitive DNA Nanostructures

11:00: Coffee

11:30-12:00 Enrico Skoruppa
Torsional Properties of DNA
12:00-12:30 Antonio Suma
Accessibility of endonuclease to DNA origami: role of local and global fluctuations
12:30-1:00 Ard Louis
Modelling thymine dimers in oxDNA

1:00-2:00 Lunch

2:00-2:30 Oliver Henrich
Using oxDNA in the LAMMPS code
2:30-3:00 Matthew Patitz
A web-based front end for oxDNA
3:00-3:30 Michael Matthies
General-Purpose analysis package for coarse-grained simulations of DNA/RNA nanotechnology

3:30-4:00 Coffee

4:00-4:45 Carlos Castro
Design Automation for DNA Origami Mechanisms
4:45-5:15 FabianKohler
Cryo-EM Studies of Multilayer DNA Origami Objects
5:15-5:45 Megan Engel
Internal forces in oxDNA

Tuesday 3 September 2019

Location: Simkins-Lee Room, Beecroft Building, Department of Physics

9:30-10:00	Thomas Ouldridge Non-equilibrium information processing: modelling with oxDNA
10:00-10:30	Erik Benson Evolutionary refinement of DNA nanostructures using coarse-grained molecular dynamics simulations
10:30-11:00	Flavio Romano
11:00-11:30	Coffee
11:30-12:15	Petr Sulc Towards simulations and design of large DNA/RNA systems with oxDNA/oxRNA
12:15-1:00	Christopher Maffeo: A Python framework for multi-resolution modeling of nanoscale DNA objects
1:00-2:00	Lunch
2:00-2:30	Ferdinando Randisi FabricNano: a DNA-nanotech/bio-catalysis startup
2:30-3:00	Rahul Sharma The cgDNA family of coarse grain models of DNA: cgDNA+, cgDNAweb, and cgDNAmc
3:00-3:30	Discussion 1: oxDNA where next? The model
3:30-4:00	Coffee
4:00-4:30	Elisa de Llano Adenita: Customizable modeling and visualization of DNA nanostructures
4:30-5:00	Lorenzo Rovigatti
5:00-5:30	Discussion 2: oxDNA where next? The codes

Workhsop Dinner: Jesus College, OX1 3DW

6:30 Drinks
7:00 Dinner in hall

Wednesday 4 September 2019

Location: Lindeman Lecture Theatre, Clarendon Laboratory, Department of Physics

9:30-10:00	Joakim Bohlin Converting from structure design to course-grained simulation
10:00-10:30	Domen Prešern Pleated DNA nanotubes

10:30: Coffee

11:00-11:30	Discussion 3: oxDNA where next? The infrastructure
11:30-12:00	Jiaming Yu Numerical study on the effect of flexibility in DNA linker mediated hydrogel
12:00-12:30	Behnam Najafi Characterising DNA T-motifs

1:00-2:00 Lunch

Location: Freeman Room, Beecroft Building, Department of Physics

2:00-2:45	Christopher Maffeo mrDNA tutorial
2:45-4:15	oxDNA users clinic
4:15-5:00	Discussion group: Tutorials

Social Event:

5:00 Tolkien walk: start at Beecroft

8:00 Wine tasting at Ard’s home: 1 Southmoor Place, OX2 6NZ

Thursday 5 September 2019

Location: Freeman Room (3rd Floor, Beecroft)

9:30-10:30 Discussion group: ASU oxDNA Web-server and sharing protocols

10:45-11:15 Discussion group: Nanostructure relaxation algorithms

11:30-12:00 Discussion group: oxDNA + proteins

12:15-1:00 Discussion group: Sequence-dependent structure and mechanics

Lunch: Not provided / local establishments

2:00-2:30 Discussion group: Improving ion-specific electrostatics / non-canonical DNA/RNA structure

2:30-3:00 Discussion group: Analysis tools

Location: Simkins-Lee Room

3:00-5:00 Carlos Castro and Chao-Min Huang
magicDNA tutorial