Potential Supervisors

Peter Minary

Motivated by grand challenges in structural and molecular biology, our research combines the development of enabling methods in applied statistics and scientific computing to perform novel applications in computational structural biology. Our work on algorithmic development is equally driven by our research interest in nanoscale design, experimental refinement, molecular genetics and related collaborations with both computational and experimental laboratories.

One major area of our methodology development is addressing the challenges in exploring the conformational space of large biological macromolecules. Besides the development of numerous novel optimization and sampling algorithms, we introduced a linear complexity chain closure algorithm that enabled the use of arbitrary user defined degrees of freedom in a protocol called (Hierarchical) Natural Move Monte Carlo or (H)NM-MC. All these and other relevant algorithms have been implemented into our software package, MOSAICS.

Software Tools Developed

MOSAICS - **Methodologies for Optimization and SAmpling in Computational Studies** is a software package written in C++ for the conformational optimization and modelling of nucleic acids, proteins and their macromolecular complexes. Molecular entities/biopolymers can be described at different resolution from one centre per monomer (residue/nucleotide) to all atom description with solvent effects. After registration, the software is free of charge for academic use. MOSAICS enables the use of a rich variety of user-defined degrees of freedom (DoFs) in combination with a variety of state-of-the-art conformational sampling algorithms (e.g. Multicanonical Markov Chain Monte Carlo) facilitating the rapid exploration of the conformational space of molecular complexes. The benefits of custom tailored DoFs have been demonstrated by notable works such as a comprehensive investigation of the protein fold universe, aiding the design of RNA nanostructures and fitting molecular structures against their Cryo-electron microscopy images. Some selected publications and completed project highlights are available online.

Involvement of DTC Students

Several former DTC students have contributed to the MOSAICS project either by doing short rotations or by pursuing research for longer term as a DPhil student or a postdoctoral fellow.

- Samuel Demharter (DPhil Student)
- Konrad Krawczyk (Postdoctoral Fellow)

During his DPhil Samuel developed novel applications and protocols using Natural Move Monte Carlo. Currently Samuel is a postdoctoral fellow at the University of Copenhagen. Konrad Krawczyk developed PyMOSAICS (Graphical User Interface to MOSAICS), by combining MOSAICS with one of the most used molecular visualisation software, PyMOL. Konrad is currently an impact software engineer at the Department of Statistics at Oxford. *Note: Further research contribution in the application of MOSAICS was made by Bernhard Knapp, a former associate director at SABS-DTC.*

Industrial links

UCB, **Pfizer**, **Evotec**, **Roche**. *Note: I was named supervisor on short project proposals for which at least one of these companies was named as an industry partner. Shorts projects with UCB, Pfizer and Evotec was also chosen for rotation but I have not yet had a DPhil student co-supervised by industry.*