

Molecular Dynamics, Movements and Evolution

by Thomas Darden, Jotun Hein and Mark Sansom.

The scholarship is only available to Home and EU students who meet the residency requirements!!! Potential applicants should contact Maureen York (york@stats.ox.ac.uk) for more information.

Comparative Biology is a major contributor to biological understanding and can be applied to any biological objects that are homologous. The large application area presently is sequences, but other rising areas include structures, networks, organs and more. The strength of evolutionary comparison is the ability to detect features of functional importance and thus select properties that demands a functional explanation from a sea of noise. The only requirement for evolutionary comparison is that the objects to be compared are homologous. In this sense movements are perfectly homologous as the movements associated an ancestral molecule would be inherited with modification, when the molecule evolved over evolutionary time. Movements of molecules have a series of special properties that singles them out compared to other comparative traits. If we imagined to compare the movements of globins over time, this would involve about 3000 atom positions, that could be observed in 10^9 time steps of size 10^{-15} seconds. One could imagine 2-10 globins had been observed and the total data set would be of the order 10^{10} spatial positions. Due to the increase in use of molecular dynamics, this kind of analysis has great potential and it is clear that analysis of such data would need entirely new approaches.

Thomas Darden, Jotun Hein and Mark Sansom have a series of specific projects fitting this framework, but we will first formulate a plan for the complete Dphil after a dialogue with the successful applicant. Thomas Darden is a mathematician with main expertise in methodology development within Molecular Dynamics. Jotun Hein is a bioinformatician/geneticist interested in expanding the domain of evolutionary modelling and analysis. Mark Sansom is a biochemist with focus on the application of molecular dynamics to especially membrane proteins. For further information please visit their web-pages:

<http://dir.niehs.nih.gov/dirlsb/cchome.htm>

<http://mathgen.stats.ox.ac.uk/bioinformatics/>

<http://sbc.bioch.ox.ac.uk/>

The student will be jointly supervised by Thomas Darden (NIEHS, North Carolina, USA), Jotun Hein (Oxford, UK) and Mark Sansom (Oxford, UK). The scholarship starts October 2007 and is of 4 years duration. The first year will be focused on following courses given by the Systems Biology Doctoral Training Centre (Oxford). In the following 3 years the students will be based in both the US and UK. The project has great potential, but is also demanding as it covers Molecular Dynamics, Statistical Models of Evolution and also Software and Algorithm Design. Applicants must have strong qualifications in the relevant areas.