

My PhD thesis is devoted to a single project: Studying the Evolution of Molecular Movements by Molecular Dynamics (MD) Simulation of homologous proteins. I am supervised by Tom Darden, Jotun Hein and Mark Sansom.

MD is being used with greater and greater success. Simultaneously, such studies are being performed on homologous systems. Thus questions concerning conservation, rate of evolution of molecular movements will be asked increasingly often. It will be the aim of my DPhil to develop appropriate statistical methods analyze such data and apply them to interesting examples. The data are daunting – a simulation can trace the positions of a thousand atoms over millions of time steps. An evolutionary analysis will have to compare such a data point to another data point of roughly the same dimensions. The main challenges are

- Finding which positions (atoms) in one simulation should be compared with which positions in the other. One way to solve this is pairwise alignment, but that is not fail proof. This could be called the spatial matching problem.
- The two movements might be of register time wise, creating a temporal matching problem. Finally, some groups of atoms could almost independently of other.
- Finding movements that are conserved over evolutionary time.
- Finding a meaningful measure expected neutral evolutionary rate of molecular movements.
- Possibly moving to a set of homologous molecular movements at the end of my DPhil.

Applying these techniques to interesting and increasingly challenging examples. More distantly related is harder than very similar. Finding proteins where structure is conserved, but movements has change would be very interesting. The reverse would also be of great interest.

Refer to CV, publications and projects. I did a summer project with Jotun Hein on how to use biological knowledge to constrain the search space in systems biology identification problems to make them more tractable. The report can be found [here](#).