The aim of my interdisciplinary PhD project is to perform a computational study of protein unfolding due to force. Many proteins, such as those found in muscle, cell adhesion complexes and baroreceptors, have to maintain structure and function when stressed by an external force. Other proteins have evolved to change conformation or even unfold when stressed to a certain level; and it is known that force directly modulates biological function. Consequently, studying the manner in which proteins unfold when subjected to force is of considerable scientific importance.

Protein unfolding due to force is typically modelled using computationally-expensive molecular dynamics simulations. In collaboration with our colleagues at Arizona State University we have developed a new technique to simulate unfolding which agrees with molecular dynamics for 9/12 of the proteins studied but produces unfolding pathways at a fraction of the computational cost. This work, for which I am joint first author (Protein Unfolding Under Force: Crack Propagation in a Network. Adam M. R. de Graff, Gareth Shannon, Dan Farrell, M. F. Thorpe and Phillip M. Williams) is to be published in Biophysical Journal next month (August, 2011).

The model being published is completely deterministic and so to make the model more physical I am currently introducing a great deal of stochasticity and making other changes which will slow the code down considerably. In order to tackle this I intend to edit the code to make it run in parallel. I hope this course will provide me with the tools I need to do this as though I am a competent developer; I have no prior parallel programming experience. I also hope the course will improve and add to my general programming/computational skills which will consequently be of benefit to my PhD and stand me in good stead for my future career as a computational scientist. It is worth noting that I still have over 2 years with which to complete my PhD.

Gareth Shannon