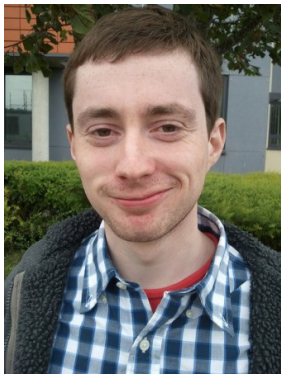
Ciaran Hughes Internship Report



Name: Ciaran Hughes

Current Status: PhD student at DAMTP

Website: To appear once I start the PhD.

Where I worked: Cambridge University centre for computational chemistry CUC³

Supervisor: Professor David Wales

Summary of Work: The diversification internships allow students with a variety of backgrounds the great opportunity to experience a field of research or an industrial placement that would otherwise remain elusive. Interested applicants originally specify their availability and where they would most enjoy spending their time. By organising the placement oneself or through the diversification internships administrative contacts, most applicants had their work plans organised before the time approached where one starts worrying about exams. Everyone that I know of that has participated in this internship has been given the chance to meet and collaborate with experts in fields that they would not otherwise have access to. Since this internship allows students to experience work that can be unrelated to their academic background, both supervisor and supervisee can bring different skills and contacts in order to bridge gaps between fields. Continuing these partnerships can lead to interesting results including new perspectives on a problem, access to a wealth of knowledge in a different subject or simply increasing relations between the host institution and the Cambridge university mathematics department for future projects. (http://www.maths.cam.ac.uk/)

For my internship, I contacted Professor David Wales of the Cambridge university centre for computational chemistry. The research and modelling carried out at CUC³ covers an exceptionally broad range of topics in theoretical and quantum chemistry, condensed matter physics, surface science, and statistical mechanics of complex and disordered systems including macromolecular aggregates.

In particular, certain aspects Prof. Wales and his group studies involve computer simulation of protein folding and misfolding including aggregation of misfolded proteins, giving new insights and rise to further experimental research. Prof. Wales' group is also interested in optimisation algorithms and the study of the dynamical properties of structural and spin glasses using the potential energy surface. A spin glass (http://en.wikipedia.org/wiki/Spin_glass) describes certain types of magnetism which can decay over long periods of time. They are difficult to explore experimentally. Also, it is known that spin glass models are NP hard problems meaning that they are difficult to solve by computational means. My diversification internship was spent studying a particular spin glass model called the XY model (http://en.wikipedia.org/wiki/Classical_XY_model). The potential energy surface can be investigated to explain and predict the complicated properties of spin glasses. Given the potential energy, Prof. Wales' group have created computer software (link to software: http://www-wales.ch.cam.ac.uk/software.html) that can examine the potential energy landscape in

order to find stable and unstable configurations of the magnets intrinsic constituents leading to a understanding of the physically realised properties. So far, this work has led to some interesting results and I will accumulate more in the near future. When the data is analysed further, I will update this page. To reiterate my main point, I believe that the diversification internships award great opportunities that students would not otherwise have and can forge links between industry or academic departments and the Cambridge University Mathematics department through its students.