My PhD project involves large-scale exploration of the potential energy surfaces of metallic clusters, with a view to determining thermodynamic information and generating important structures. Working with a range of simulation techniques (Basin-Hopping, Monte-Carlo, Genetic Algorithms), a detailed picture of characteristic regions of this high-dimensional surface can be obtained. With the produced data, one may track transition pathways between minima, gather information on the kinetics of such a path, and map out the connectivity of stable minima, in order to characterise the topology of the surface in general.

Even with the use of empirical potentials, designed to retain important information whilst keeping the computational cost low, there is still a very high associated cost for full statistical explorations. These calculations therefore require efficient and effective use of high performance computing facilities. In order to maximise accuracy, higher level calculations are also performed, using Density Functional theory (DFT), which increases cost by orders of magnitude. I use a local supercomputer within the university for such a purpose, and so must have an understanding of the workings of such a system.

To better exploit the above mentioned methods and minimise the computational expense, interfacing and code development is a major focus of my studies. By combining methodologies, one may extend the scope, and allow for more efficient calculation of the properties of interest. As most of these codes are written in the Fortran language, an improved understanding of programming with Fortran will be an invaluable skill for this work

Collaborative projects, such as a current HPC-Europa-funded project with a group in Stuttgart, require me to develop serial and parallel codes, as well as porting code between HPC systems, making parallelisation a vital technique. The behaviour of different supercomputer architectures, and how best to treat them with regards to parallelisation, is, however, not a subject of which I have any prior knowledge.

Aside from running large scale simulations, maintenance and improvement of in-house serial and parallel programs within the group is a continual requirement, and one I would certainly be better equipped for after an intensive course in this area. In addition, the mixed background of the members of the group means a varied level of experience with computational and programming techniques. I feel to have the opportunity to learn and disseminate this information would be a great value to my group on the whole.

In conclusion, my project requires familiarity with a wide range of areas within scientific computing, some of which are entirely new to me, and this course will significantly improve my readiness for many of the tasks I am to face.

Chris Heard