EPSRC CENTRE FOR DOCTORAL TRAINING IN

COMPUTATIONAL METHODS FOR MATERIALS SCIENCE

BULLETIN ISSUE 1

Welcome to our first newsletter. We hope to produce these three times a year to keep you informed of activities in our CDT. If you have suggestions for content or topics for future newsletters do send these to admin@csc.cam.ac.uk. The main purpose of this edition of the newsletter is to introduce the students in our first cohort who started in October 2014. It has been very encouraging to see how well this cohort has bonded together. In the four months they have been here, they have been very busy with lectures, examinations, the first short project and an entrepreneurship course - and there is plenty more to keep them busy for the rest of the academic year! Michaelmas term was heavy on lectures and computing practicals. They had mock exams before Christmas and "live" exams once they got back from the Christmas break. They are currently working on their two written assignments, actively engaging with supervisors. These assignments are due at the end of the month when their main research project will start.

In this newsletter, we also have some pictures from the 1st meeting of our Steering Panel which met on Thursday 3rd July 2014 and from the Launch Event in October. The Steering Panel is Chaired by Professor Peter Gumbsch who is Executive Director and Director of the Fraunhofer IWM in Freiburg. The Steering Panel provides advice and guidance on the CDT training programme and it meets annually in the morning of the first Thursday in July – so the next meeting will be on Thursday 2nd July 2015. That afternoon will be an opportunity for everyone associated with the CDT to get together and to meet the students and find out more about their projects. We hope that many of you will join us for this event – you are very welcome to bring colleagues with you - so please put this date in your diary. If there any issues or suggestions relating to the CDT that you would like the Steering Panel to consider please send them to admin@csc.cam.ac.uk.

We are about to start recruiting our second cohort of students so it is not too late to propose potential PhD projects to start in October 2015. If you, or any of your colleagues, would like to discuss possible PhD projects, want to find out more about the CDT or would like me to visit please feel free to get in contact with me at mcp1@cam.ac.uk.

Mike Payne

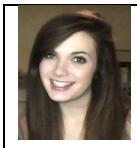
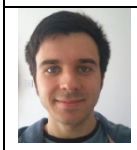
Photos from the first CDT CMMS Steering Group Committee AGM in July 2014

Meeting in progress

Steering Committee with some academic and student members of 2013/14 MPhil cohort

Photos from launch in October 2014

Our 12 new CDT students in Year 1 cohort

	**Alice Allen** I am currently studying for an MPhil in Scientific Computing as part of the Centre of Doctoral training in Computational Methods for Material Science. Prior to this I was studying for a BSc in Physics at Imperial. At the moment I am completing two short projects. One of which is using a density functional theory code to study simple molecular and crystalline structures. The other is using statistical inference in order to find correlations in amino acid sequences of proteins. This information can then be used to give the tertiary structure of the protein.
	**Kevin Duff** I completed my Masters degree in Theoretical Physics at the University of York. The degree was highly computational, giving me an interest in the development and implementation of theory aimed at solving computational problems. My main project in the CDT will involve the search for quantum mechanical simulation techniques for metals on the multi-nanometre length scale. Currently, linear scaling within DFT is possible for materials with nonvanishing band gaps, but the 'long-range' nature of quantum mechanics in metals limits studies of systems such as catalytic or magnetic nanoparticles, which are of interest to industry and display characteristics very different to their bulk counterparts. This project will be carried out in collaboration with one of the industrial partners of the CDT.
	**Andrew Fowler** I am currently in my first year of a combined Masters and PhD course in the Laboratory for Scientific Computing at The University of Cambridge. My previous studies were for an undergraduate Masters in Physics at The University of Warwick. Understanding materials is an important challenge to many aspects of industry and academia and often a picture of the properties of interest is necessary at many length and time scales. The phenomena seen and computational methods used in Physics and Chemistry that span atomistic and macroscopic length scales, for example are equally as diverse and bridging the gaps between these length and time scales is an interesting feat. My research specifically is to apply multi-scale descriptions of Carbon Nano Tube fibres to develop a rigorous and more insightful image of properties which are of both academic and industrial importance.
	**Benedict Irwin** I am undertaking a CDT in scientific computing at the University of Cambridge. Before this I studied Physics with Nanotechnology at the University of Leicester. My focus of study is computational water models, which are used in large molecular dynamics simulations of proteins interacting with drugs. As water makes up a large part of the simulation a complicated model can quickly become computationally expensive. However, water can play a pivotal role in the chemistry around protein active sites, and an oversimplified model can lose vital information. The aim is to include the quantum mechanical effects of water in such simulations and compare to existing water models.

(Arndt) Ryo Koblitz

I am a postgraduate student at the Laboratory for Scientific Computing based at the Cavendish Laboratory, University of Cambridge. I have previously studied Mechanical Engineering at University College London where I worked on direct numerical simulations investigating vortex decay in ambient turbulence.

My research is aimed at using continuum methods alongside high-performance computing to study the physics of fluids containing non-colloidal particles. Complex fluids are used in a wide range of applications in the oil and gas industry and often possess non-Newtonian characteristics. I aim to use resolved continuum simulations to perform case studies to investigate suspension flows, including effects such as particle migration, effective rheology changes, sedimentation and bed formation.

Edward Linscott

I am in the first year of a joint MPhil and PhD within the Laboratory for Scientific Computing in the Cavendish Laboratory at the University of Cambridge. I completed my undergraduate studies at the University of Otago (New Zealand) and the University of California, Berkeley.

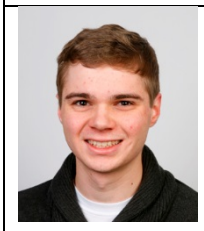
My research is focused on the application of quantum mechanics to biological systems. Biological systems are difficult to simulate with computers due to (a) the sheer number of atoms that make up these systems, and (b) the irregularity with which these atoms are arranged. However, these challenges can be overcome using clever linear-scaling electronic structure methods and high performance computing. I am using these approaches to investigate the behaviour of electrons within a photosynthetic light-harvesting complex found in plants and bacteria, and in an enzyme associated with HIV.

Felix Mocanu

I am a first year student in the joint Scientific Computing MPhil and PhD at the University of Cambridge. I have completed my undergraduate studies with an M.Sci in Natural Sciences in the Chemistry Department at the University of Cambridge. As a part of M.Sci thesis I worked on computer simulations of phase-change materials used for non-volatile computer memory in the Chemical Physics Group of Prof Stephen Elliott. My current research hinges on making use of the large amount of DFT data in a Machine Learning approach. The goal is to obtain a hierarchy of faithful empirical potentials with techniques developed by the Csányi group in the Department of Engineering. This will allow more detailed study of this system within larger and longer simulations. If the process proves to be robust and reliable it may be the basis for high-throughput simulation of such materials with figures of merit being calculated quickly and reliably from these simulations. The phase-change materials that I'm investigating are a serious candidate for non-volatile computer memory, they are capable of both storage and processing of information and are naturally well suited for "brain-like", neuromorphic computing. They could be an important part of fast, reliable, energy-efficient electronic devices, they may bridge the gaps in the current memory hierarchy improving the performance of our computers and smartphones and may also shed light on the way our brains process information in parallel networks.

Verena Neufeld

This is my fifth year in Cambridge as I have done my undergraduate degree here as well. Before joining the Centre for Doctoral Training, I have studied the Natural Sciences Tripos focussing on physics. I really enjoy physics and programming so I am very happy to be part of this program now. My research interest lies in multiscale modelling. Often a simulation focusses on processes at a certain length scale, e.g. the atomistic scale or the lengthscale where dislocation movements can be observed. My aim is to be able to run simulations looking at more than one length scale so it is possible to gain a deeper understanding of the processes involved. I am especially looking at electronic-atomistic-dislocation length scales.



Martin Schlegel

I am a student at the Centre for Doctoral Training in Computational Methods for Materials Science in Cambridge. I am currently in my first year as an MPhil student in Scientific Computing under the supervision of Dr Gábor Csányi from the Department of Engineering. I graduated with a BSc in Physics from Heidelberg University, Germany in 2013 and with a MASt (Master of Advanced Study) in Physics from the University of Cambridge in 2014.

During my first master's degree, I worked on an atomistic analytical description of the bulk and shear modulus of soft amorphous solids. My current research aims to understand the temperature driven phase transition in titanium with an atomistic approach using the relatively recently proposed nested sampling algorithm. With this understanding, we hope to make possible further work to gain insight into shape memory alloys and their superelasticity (in particular the alloy nickel titanium, also known as nitinol). Nitinol is very biocompatible and therefore used in many medical applications. However, many other fields of applications exist ranging from eyeglass frames to planes.

Max Veit

I am a student in the CDT in Computational Methods for Materials Science at Cambridge. Currently I am in the MPhil in Scientific Computing, which is the first year of the CDT.

I graduated in 2014 from the University of Minnesota with a Bachelor of Science in physics and in computer science. I also did an exchange year at the TU Munich from 2011-2012. My research so far has been in various applications of computing to physics: During a summer fellowship at Los Alamos National Laboratory in 2013 I analyzed Monte Carlo simulations of nuclear reactors. During my last year at the U of M I worked on simulating genetic regulatory networks in cells. Now, in Dr. Gábor Csányi's research group, I will be taking machine learning atomistic simulation methods into a new area by applying them to materials with strong electrostatic interactions. Examples include hydrocarbon compounds mixed with water and most biological molecules. A machine learning method uses accurate quantum mechanical calculations to inform much faster molecular dynamics simulations, which can be used to calculate a material's macroscopic properties. However, in systems with strong electrostatic interactions, the long length scales over which these interactions take place make machine learning difficult. The goal of my project is to use machine learning to construct an electrostatic force field that will account for these interactions. This research will potentially enable the calculation of the macroscopic properties of these materials from first principles.

	**Simon Wilkinson** After attending the European School of Varese, in Italy, he attended the University of Southampton to study particle physics. He won a DAAD scholarship to undertake a summer research internship at TU Berlin, Germany. In his final year, he moved to CERN, Geneva to do his Master's project on the Level-1 Trigger of the ATLAS experiment on the LHC. He has worked in the Laboratory of Hybrid Photonics in Southampton on the numerical solution of the Gross-Pitaevskii equations. He is now a member of the CDT, where his research interests are in computational fluid dynamics and the simulation of detonations.
	**Jamie Wynn** I am a first-year student at the EPSRC CDT for Computational Methods for Materials Science. My research focuses on first principles crystal structure prediction, using a technique known as AIRSS (Ab-Initio Random Structure Searching). AIRSS is a powerful and flexible technique that uses the power of density functional theory to predict the ground state phases of materials, as well as their low-lying structural defects. I will be focusing on further developing the AIRSS method, as well as applying it to technological problems such as designing materials for batteries ab initio.