EPSRC CENTRE FOR DOCTORAL TRAINING IN

COMPUTATIONAL METHODS FOR MATERIALS SCIENCE

BULLETIN ISSUE 3

Welcome to our third 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 second cohort who started in October 2015. It has been very encouraging to see how well this cohort has bonded together. In the few months they have been here, they have been very busy with lectures - 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 will sit mock exams before Christmas and "live" exams once they return from the Christmas break.

The first Lennard Jones Centre lecture of the year, by Prof. Igor Abrikosov of the Materials Modelling and Development Laboratory, “MISIS” in Moscow, entitled, "Materials modeling using modern computers: from the Earth’s core simulations towards accelerated knowledge-based materials design" was held on 3 November in the Department of Materials Science (West Cambridge).

We are about to start recruiting our third cohort of students so it is not too late to propose potential PhD projects to start in October 2016. 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

Our 10 new CDT students in Year 2 cohort

	**Brett Abram** Earlier this year, I graduated from the Cambridge Natural Sciences Tripos (BA & MSci), in which I specialised in Materials Science. As part of my final year, I conducted a research project on the "Atomistic modelling of twinning modes in *alpha*-uranium" using the LAMMPS molecular dynamics package. I also have industrial experience of finite element simulations from an internship with Frazer-Nash Consultancy. I am currently studying for the MPhil in Scientific Computing as part of the CDT. My focus is now on numerical simulations for impact and fracture; happily combining the computational skills from the MPhil with my knowledge and experience as a materials scientist.
	**Benedetta Bianchi** Hi! I come from Rome, Italy, and I am currently studying towards an MPhil in Scientific Computing as part of the EPSRC CDT in Computational Methods for Material Science. Prior to this I lived in London where I attained a MEng degree in Chemical with Nuclear Engineering at Imperial College London. My research interest lies in Nuclear Fusion. As part of the CDT I will be involved in the modelling of Navier Stokes equations combined with Maxwell's equations in Inertial Confinement Fusion applications. Ultimately my goal is to derive estimates of the impact of strong magnetic fields on liquid metals' heat transfer properties for Fusion power generation applications. Besides research I love experimenting new dishes in the kitchen and travelling.
	**Matthew Evans** I am a new member of the EPSRC CDT for Computational Methods for Materials Science, currently completing an MPhil in Scientific Computing before starting my PhD studies. As part of Dr Andrew Morris' group inside TCM, my research will involve extending and applying the methods of *ab initio *random structure searching (AIRSS) to improve our understanding of the effects of disorder, particularly on carbon nanotubes and anode materials for Li-ion batteries. Prior to joining the group, I completed an MPhys in Physics with Theoretical Physics at the University of Manchester, where I wrote my MPhys thesis on the electronic structure of defects in graphene/h-BN superlattices. My interest in computational physics flourished whilst embedded in the quantum fluids group at Manchester, where I wrote simulations to model the microscopic dynamics of vortex rings in superfluid helium under the vortex filament model.

Tomé Gouveia

I am a student at the EPSRC Centre for Doctoral Training in Computational Methods for Materials Science. Prior to coming to Cambridge, I completed a Bachelor's degree in Physics at the University of Coimbra, in Portugal. I attended the Master in Advanced Studies in Physics at the University of Cambridge in the academic year 2014-2015. I chose to focus the taught component of this degree in theoretical condensed matter physics, as that is one of my main interests. Understand how materials' properties and structure on a fundamental, first-principle level is highly appealing to me. The research component of this degree was in computational fluid dynamics. In my research project, I used geometric algebra to describe classical hydrodynamics and then simulated the propagation of waves and studied the formation of shock waves in (initially homogeneous) ideal and van der Waals gases. A short digression on the quantisation of elastodynamics was also included in the final project report.*

*This year, I am enrolled in the MPhil in Scientific Computing, as part of the CDT program, with a focus on Continuum Mechanics. My research project is focused on the modelling of fracture of three-dimensional materials within a two-dimensional framework. The aim is to come up with a model for fracture based on two dimensional PDEs, which, although still remarkably hard (in some cases impossible) to solve analytically, are far simpler than 3D PDEs, allowing for faster and easier simulations.

William Grant

I have just graduated from the Natural Sciences Tripos at Trinity College, Cambridge, focussing on solid state physics. As part of the CDT, I hope to apply my physics background to solving research problems in the field of biological modelling. My project will involve the application of network analysis to the study of protein structure. This should allow for new coarse-graining of molecular dynamics simulations, and provide new approaches to classifying proteins. This should hopefully build on my prior Part III project, which used graph theory in the modelling of epidemics through a random lattice.

When not attending lectures or programming, I can be found playing water polo, running, or playing guitar.

Haran Jackson

I've just begun the CDT in Computational Methods for Materials Science, having spent the past year working in a couple of research institutes in Lisbon and Bangalore, and a tech company in the Cambridge Science Park. Prior to my year out, I graduated from Oxford University with an MMath in Mathematics, and it was in the final year of this course that I developed a particular interest in the computational side of the subject; an interest that would eventually lead me to where I now find myself.

My project, orchestrated by BP, will focus on the development of a CFD-based cement displacement simulator with fast simulation time for real wellbore conditions. In the MPhil year of the CDT I will complete projects on the projection method, the ghost fluid method, and other methods of numerical simulation of non-Newtonian flows.

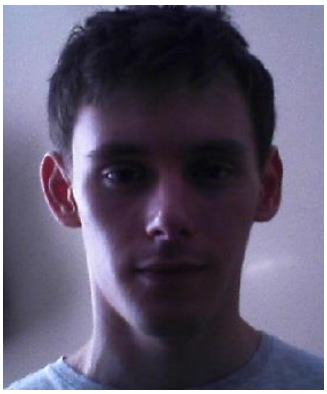
Mark Johnson

I have recently graduated from an MPhys in Physics at Oxford, where I specialised in theoretical physics and condensed matter. My current area of research is the atomistic simulation of carbon nanotube formation. I am simulating the catalytic effects of iron nanoparticles on short carbon chains, and the action of sulphur to prevent the conglomeration of the nanoparticles.

The processes that I am simulating have been experimentally demonstrated, but the mechanisms driving them are not fully understood. I hope that my research will lead to an improvement in this understanding, with potential industrial applications if such an improved understanding can be used to refine the process.

Knut Kleppestoe

I have a background in physics from the University of New South Wales (BSc) and the Norwegian University of Science and Technology (MSc), and am particularly interested in solving PDEs describing fluid dynamics systems. While at the CDT, I will be working with Hari and representatives from BP on developing a massively parallel CFD-based cement displacement simulator which can be used to make real-time wellbore decisions. When I'm not programming (i.e. on extremely rare occasions), I like to have Bene tell me how to cook Italian food and Brett tell me about the sporting events he frequents in London.



Liam Pattinson

I recently started studying scientific computing at the University of Cambridge as part of the EPSRC Centre for Doctoral Training in Computational Methods for Materials Science. As an undergraduate, I studied natural sciences at Cambridge with a focus on physics. I will be investigating the electrodynamics of high-frequency copper transmission lines in collaboration with BT. Though optical fibres allow higher bandwidths and minimal noise, modern society remains highly reliant on copper networks for practical and economic reasons. Despite concerns that the bandwidth of copper wiring would become prohibitive, copper technology has been steadily improving for decades to keep up with increasing data demands. My work will aid in understanding the underlying physics of the copper network and hopefully allow further progress to be made.

Matthew Smith

I completed my Masters degree in Theoretical Physics at the University of York. My main project in the CDT will involve the study of anharmonic atomic vibrations in crystalline solids. Such vibrations can significantly affect the structure of some solids and therefore their inclusion, beyond the usual harmonic approximations, is necessary if computational models are to be improved. The project will utilise various techniques, including AIRSS (Ab-Initio Random Structure Searching) – a code implementing density functional theory to predict the ground-state structures of materials.