Title of the Tutorial:
CCP5 Summer School in Molecular Simulation 2012

Organisers
The Summer School was held at the University of Cardiff. The School was organised by the CCP5 Summer School Working Group, which comprises John Harding (Chairman), John Purton (Secretary) and David Willock (CECAM applicants) and members of the lecturing team. The lecturing team included Philip Camp, Jamshed Anwar, Rebecca Notman, Keith Refson, Ian Halliday, Mark Seaton. The local organisation was handled by David Willock from the School of Chemistry at Cardiff University.

Aims of the Tutorial
The CCP5 Summer School in Molecular Simulation has run annually since 1989. Over the last five years the number of students attending has averaged about seventy. (This is about the maximum number that the School can accommodate) The 2012 School was held at the University of Cardiff. The website www.ccp5.ac.uk/SSCCP5/main.html gives full details of the 2012 school.

The objectives of the Summer School are as follows:

1. To introduce the participants (particularly PhD students) to the theory and practice of computer simulation through a combination of formal lectures and "hands-on" sessions.

2. To inspire the participants to see what simulation can accomplish through a set of plenary research lectures given both by established practitioners in the field and by "rising stars"

3. To enable and encourage the participants to meet their peers and establish contacts (and even collaborations) in an informal atmosphere and in particular through a poster session and the opportunity to give short seminars.

Report on key lectures and hands-on sessions (one page)

The details of the course lectures can be found on the course website given above. The programme of the School consisted of two parts. The course content was reviewed after the summer school of 2011 and the student responses were taken into account this year, as far as was practical. The only significant change from the original application is that the Biomolecular Simulations course was given by Jamshed Anwar and Rebecca Notman rather than by Xavier Daura as proposed.

The **basic course** is designed to introduce students to the fundamentals of molecular simulation. It covers the basic elements of statistical mechanics and gives a thorough grounding in the methodologies and applications of Monte Carlo and molecular dynamics simulations. All students were required to attend the basic course and were presented with prepared course notes beforehand. Following the lectures in the morning, the afternoons were devoted to **computational workshops.** In these the students were required to complete exercises based on the topics covered in the basic course. The exercises expanded on the material presented in the basic course while giving the students opportunity to study the underlying computational methodology and allowing them to experience problems and solutions in actual computational work. One afternoon was devoted to a `mini-project' on diffusion of methane in a zeolite cage (Willock). The material for the exercises was supplied by the current and past lecturing team. The exercises were done on desktop personal computers using the Virtual Box software to obtain a Linux operating environment (with both C and Fortran compilers). Also available were CCP5's DL_POLY program, visualisation tools such as VMD and JMol and standard graphics packages. An additional multiprocessor platform was available for the advanced courses.

The **plenary lectures** are an integral feature of the School and are intended to demonstrate to students what science may be accomplished by molecular simulation methods. This year the plenary lectures were given by: Paul Mulheran (Strathclyde), Robert Best (Cambridge), Patricia Hunt (Imperial), Nicola Spaldin (ETH Zurich), David Manolopoulos (Oxford) and Charles Laughton (Nottingham). A plenary session was also dedicated to short (15 min.) talks given by the students. The four talks selected this year were:

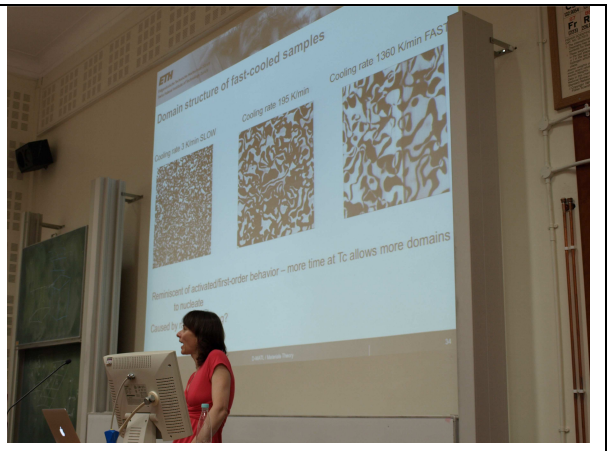
- Micha Kunze (University College London) *Loop dynamics tune the structure of the human histone deactylase for ligand binding and release*
- Alexey Lukoyanov (Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences) *Investigations of materials with strong electron correlations using LDA+DMFT method*
- Jeff Rodgers (University of Bristol) *Understanding the reaction mechanisms of CVD diamond thin film growth through 3-dimensional kinetic Monte Carlo* (*kMC*) *simulations*
- Donguk Suh (Keio University) *Molecular Dynamics analysis on edge effects of nanoparticle growth*.

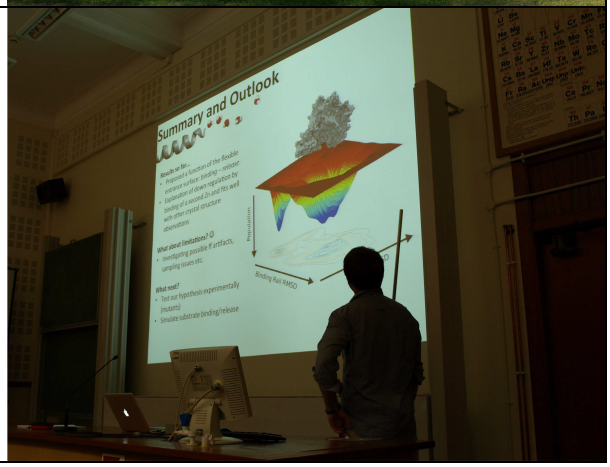
The contributions of the students were complemented by a **Poster Session**, which featured a wide range of research activity. In recognition of the high standard of presentations made by the students in both the talks and posters, the organizers made a small award to Mr. Donghuk Suh for best seminar and Patrick O'Toole for best poster.

The School offered a choice of three **advanced courses** to the students: biomolecular simulations, mesoscale simulations and first principles simulations. Each of these courses comprised 4 one-hour lectures and associated practical sessions on the computer. As with the basic course, students were presented with prepared course notes beforehand. The ***Biomolecular Simulation*** course described the nature of biomolecular structures, the force fields Amber, Gromos and Charmm and the methods and programs used to simulate biomolecular systems and analyse the results. The ***Mesoscale Simulation*** course described the current techniques applied in this area: Lattice Gas Automata, Lattice Boltzmann and Dissipative Particle Dynamics. The ***First-principles simulation*** course introduced simulation from first-principles quantum mechanics, covering the electron-ion Hamiltonian, the Schrodinger equation and the impossibility of a direct solution. Various topics from the quantum theory of the solid state were introduced and the major approximate methods of the Hartree, Hartree-Fock and

density-functional theory described including the LDA and GGA approximations to the XC functional. The aim was to equip the students with sufficient practical knowledge to perform correctly converged calculations.

Picture Gallery





Report on feedback from the students (one paragraph at least)

To assess the quality of the School, each student was asked to complete a questionnaire inviting their response to various specific and general aspects of the School. The full analysis is available on request. The assessment of the course (using the criteria on the CECAM website to which the participants did not have access) is as follows: For the **Basic Course** the quality and level of the lectures was rated good to very good. Similarly, the quality and level of the exercises was rated good to very good. Support for the exercises was considered to be good to very good. There were occasional comments about the timing of the exercises with respect to the lectures, but overall this was rated good to very good. These comments will be taken into account in scheduling the practicals in the 2013 School. Similar levels of satisfaction were recorded for the **First Principles** and **Mesoscale** Advanced Courses. There were a couple of comments about the turn-around for jobs on the cluster for the First Principles exercises. Otherwise the level and quality of computer facilities was fine. The **Biomolecular Simulation** course was rated somewhat lower than the rest of the course, but never less than acceptable and usually good. We intend to revise this course for next year in the light of comments received.

Overall, the comments from the students were extremely positive and encourage us in the belief that the course still meets a real need in the simulation community.

Do you have suggestions for new related tutorials?

The 2013 Summer School is already being planned and will be held at the University of Manchester. The local organiser will be Paola Carbone. We have applied for support from CECAM for this event. The format will be similar to the 2012 school, taking into account the comments from the students this year. In particular, we intend to revise the Biomolecular Simulation Advanced Course.

We consider that Summer Schools of this kind, that both expose students to the methods of simulation and enable them to meet and discuss their projects with their peers are a valuable, even essential, part of the education of PhD students. We would commend to CECAM the idea of supporting other Schools in areas within the CECAM remit.