Report on the Methods in Molecular Simulation Summer School 2011

1. Organizers

The Methods in Molecular Simulation Summer School 2011 was held at Queen's University Belfast from 17 - 26 July, at the Atomistic Simulation Centre and the School of Mathematics and Physics. The School was organised by the CCP5 Summer School Working Group, which consisted of J. Harding (Chairman), J. Purton (Secretary), P. Camp, Jamshed Anwar, M. Del Popolo and D. Willock. The local organisation was handled by M. Del Popolo, from the Atomistic Simulation Centre at Queen's University.

2. Location and Facilities

The School was held on the University campus, more precisely at the Elmwood Learning and Teaching Centre (ELTC) and at the Peter Froggatt Centre (PFC). The computer exercises also took place in the ELTC, which had sufficient places for 70 students working independently. The computing equipment consisted of desktop personal computers running Microsoft Windows, augmented by Virtual Box software, which provided a Linux environment for running the programs of the basic course. An additional multiprocessor platform was available for the advanced courses.

3. Participation

We received 97 applications to attend the School and these were screened by the organisers with the intention of giving priority to students in the first year of postgraduate study and whose research required a significant amount of molecular simulation. Students of the disciplines of chemistry, physics, biology, mathematics and computational science were considered acceptable.

67 students attended. Those attending originated from 17 countries: 29 were from the host nation (UK) and 34 were from elsewhere in Europe. 4 students were from outside Europe. A full list of participants and their nationalities is presented in Appendix 1.

4. Support

A registration fee of £200 was charged to the students, which covered the bulk of the costs. Queen's University of Belfast provided the use of the lecture theatres and the computing equipment at nominal cost. The organisers express their sincere appreciation of the support received from the supporting organisations.

5. Accommodation

The residential students and lecturers were accommodated in the halls of residence of in Queen's Elms Village, within 15 minutes walking distance of ELTC and PFC. Plenary Lecturers were located in local hotels, near the university. Breakfast, lunch and evening meals were provided for all the School participants.

6. Programme

The programme of the School consisted of two parts. The basic course in molecular simulation methodology covered the first 5 ½ days. This was followed by an advanced course lasting 2 ½ days, for which there were three options for the students (see below).

The Basic Course

The basic course was designed to introduce students to the fundamentals of molecular simulation. It covered the basic elements of statistical mechanics, the methodologies and applications of Monte Carlo and molecular dynamics simulation, potential energy functions and optimization methods. More advanced aspects of statistical mechanics, the treatment of long ranged (electrostatic) forces, hyperdynamics and the calculation of free energies by simulation methods were also included. All students were required to attend the basic course and were presented with prepared course notes beforehand. The course content was reviewed after the summer school of 2010 and the student responses were taken into account, as far as was practical, in 2011.

The lectures given in the basic course and the speakers presenting them were as follows (numbers in brackets indicate the number of lectures devoted to the subject):

- (1) Potentials. J Harding
- (1) An overview of molecular simulation. S. Parker
- (2) Statistical mechanics. M. Del Popolo.
- (4) Molecular dynamics. D. Willock
- (4) Monte Carlo. P. Camp.
- (1) Long range forces. J. Harding
- (1) Long timescales methods. J. Harding
- (2) Free energy methods. J. Anwar
- (1) Parallel programming. K. Refson

Three (1 hour) lectures were given in the morning of each day, with a coffee break between lectures 2 and 3. The timetable for the School is presented in Appendix 2.

Computing Workshops

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 thus 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' in which students were required to conduct realistic research on the diffusion of methane in a zeolite cage (Willock). The bulk of the material was supplied by the organisers, with additional material from Prof. M.P. Allen at the University of Warwick and Dr. W. Smith at Daresbury laboratory.

As in previous years, the exercises were accessed via a web browser, allowing the students to read instructions online, and then download the necessary software from a website at Queen's

University, or from a backup at the CCP5 website at Daresbury Laboratory. The work was performed entirely on the PCs running a linux operating system via the Virtual Box software with essential C- and Fortran compilers. The gfortran Fortran compiler was the compiler of choice. Also available were CCP5's DL_POLY program and assorted graphics tools such as RasMol, VMD and JMol.

Plenary Lectures

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:

- **Julia Yeomans**, University of Oxford, *Swimming and scattering at low Reynolds numbers.*
- **Rebecca Wade**, Heidelberg Institute for Theoretical Studies*, Modeling protein interactions and dynamics: From single protein to multi-protein systems.*
- **Dominik Marx**, Ruhr Universitat Bochum*, Magnetostructural Dynamics of [2Fe-2S] Protiens from Spin-Projected Two-Determinant Ab Initio Molecular Dyanmics.*
- **David Coker**, University College Dublin*, Quantum Dynamics in Condensed Phases*
- **David Quigley**, University of Warwick*, Busting the myth of classical nucleation theory, molecular simulations of crystal growth.*
- **Paola Carbone**, The University of Manchester*, Combining atomistic and coarse-coarse grained models to simulate soft matter*

A plenary session was also dedicated to short (15 min.) talks given by the students. The four talks selected this year were:

- **Aaron Finney**, University of Warwick, UK. *Applying Belonoshko's Z Method to Molecular Solids*
- **Sarah Khanniche**, University of Savoie, France. *Molecular Modelling of Chemical Sensor Based on Silica Surfaces*
- **Cloé Lanthony**, LAAS-CNRS, France. *Basic Mechanisms of Al/CuO Bilayer Films Formation: a Theoretical Study*
- **Fredrick Robin Devadoss Victor Paul Raj**, University of Konstanz, Germany. *Analysis and Visual Summarization of Molecular Dynamics*

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 Mrs. Cloé Lanthony, for best short seminar, and Mrs. Weina Du, for best poster.

Advanced Courses

The School offered a choice of three advanced courses:

- **Biomolecular simulation** (Xavier Daura, University of Barcelona)
- **Mesoscale simulation** (Ian Halliday, Sheffield Hallam University; Michael Seaton, Daresbury Laboratory)
- **First principles simulation** (Keith Refson, Rutherford Appleton Laboratory)

Each of these courses was comprised of 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 was run by Dr. Xavier Daura of the University of Barcelona. The 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.

Dr. Ian Halliday from Sheffield Hallam University and Dr. Michael Seaton from Daresbury Laboratory, gave the advanced course on Mesoscale Simulation. The course described the current techniques applied in this area: Lattice Gas Automata, Lattice Boltzmann and Dissipative Particle Dynamics.

The advanced course on First-principles simulation was given by Dr. K. Refson (Rutherford Appleton Laboratory).The course introduced simulation from first-principles quantum mechanics, covering the electron-ion Hamiltonian, the Schroedinger equation and the impossibility of a direct solution. Various necessary 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 discussed. Basis sets and SCF solves were described and the computer representation as used in several major codes discussed. The second half of the course concentrated on practical aspects of FP simulation, with a strong emphasis on convergence issues. The aim was to equip the students with sufficient practical knowledge to perform correctly converged calculations. This was reinforced in the practical sessions which gave the students hands-on experience of running *ab initio* lattice dynamics and molecular dynamics calculations.

7. Performance Assessment

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 analysis of the survey was conducted by Prof. J. Harding and is attached to the present document.

8. The Future

The Summer School in 2012 is planned for Cardiff University. CCP5 will provide some funding and additional funding will be requested from CECAM.

9. Gallery

The Summer School 2011 group photograph

Mrs. Cloé Lanthony receiving the award for best student lecturer

Mrs. Weina Du receiving the award for best poster

During a lecture

Appendix 1. Attendance List

Forename	Surname	Country
Amaal	**Albackri**	UK
Alessio	**Atzori**	UK
Irene	**Bessi**	Italy
Lasse	**Bøhling**	Denmark
Sally	**Bridgwater**	UK
Maria Monica	**Castellanos Mantilla**	USA
Christopher	**Cave-Ayland**	UK
Annalaura	**Del Regno**	UK
Nicodemo	**Di Pasquale**	Italy
Weina	**Du**	Netherlands
Jonas	**Fagerberg**	Sweden
Baptiste	**Farbos**	France
Thomas	**Fenech**	UK
Gaëlle	**Filippini**	France
Aaron	**Finney**	UK
Mathieu	**Fosséprés**	Belgium
Hendrik	**Frentrup**	UK
Federico	**Giberti**	Switzerland
Miguel Angel	**Gonzalez**	Spain
Paul	**Gorman**	Ireland
Kyle	**Hart**	USA
Matti	**Hellström**	Sweden
Andres	**Henao Aristizabal**	Spain
Daniel	**Holden**	UK
Wagner	**Homsi Brandeburgo**	Netherlands
Tanveer	**Hussain**	Sweden
Trond	**Ingebrigtsen**	Denmark
Olga	**Ivchenko**	Germany
Joakim	**Jämbeck**	Sweden
Jesse	**Kern**	USA
Sarah	**Khanniche**	France
Cloé	**Lanthony**	France
Mark Andrew	**Lewis**	UK
Olga	**Lobanova**	UK
Jahangir	**Malik**	UK
Simona	**Mariani**	Italy
Francisco José	**Martínez Ruiz**	Spain
Emmet	**McBride**	Northern Ireland
Mykhailo	**Melnykov**	UK
Anthony	**Nash**	UK

Sang Young	**Noh**	UK
Alvarado	**Orozco**	France
Aurelie	**Ortiz**	France
Ferruccio	**Palazzesi**	Switzerland
Konstantinos	**Papachristos**	UK
Ramiro	**Perezzan**	Spain
Emiliano	**Poli**	Italy
Thomas	**Pope**	UK
Edward Oliver	**Pyzer-Knapp**	UK
Ismael	**Rattalino**	Italy
Stepan	**Ruzicka**	UK
Somwang	**Sae-tang**	UK
Rocío	**Semino**	Argentina
Stefano Artin	**Serapian**	UK
Terence	**Sheppard**	Northern Ireland
Mark	**Siddorn**	UK
Sandeep Kumar	**Singh**	Belgium
Andreas	**Stegmueller**	UK
Bing	**Sun**	Sweden
Artur	**Tamm**	Estonia
Hugh Patrick George	**Thompson**	UK
Fredrick Robin Devadoss	**Victor Paul Raj**	Germany
Sophia Rebecca	**Wheeler**	UK
Alexey	**Zatula**	Norway
Yawen	**Zhang**	UK
Zhuo	**Zhang**	UK
Veranika	**Zobnina**	Italy

Appendix 2. The CourseTimetable

Methods in Molecular Simulation 2011

Click on a Lecture or Workshop for details. For information on using the workshop computers click here.

	17 July	18 July	19 July	20 July	21 July	22 July	23 July	24 July	25 July	26 July
09.00		Overview of Molecular Simulation	Statistical Mechanics 2	Monte Carlo 2	Monte Carlo 3	Molecular Dynamics 4	Long Ranged Forces	**Free Time**	Advanced Seminar 3 FPS BIO MESO	Advanced Seminar 4 FPS BIO MESO
10.00		Potentials	Monte Carlo 1	Molecular Dynamics 2	Molecular Dynamics 3	Monte Carlo 4	Parallel Programming		Practical Session FPS BIO MESO	Practical Session FPS BIO MESO
11.00		***Refreshments***							***Refreshments***	
11.30		Statistical Mechanics 1	Molecular Dynamics 1	Optim - -ization Methods	Free Energy Methods 1	Free Energy Methods 2	Long Timescale Methods		Practical Session FPS BIO MESO	Practical Session FPS BIO MESO
12.30		***Lunch***								
14.00	**Arrival**	Practical Workshop 1	Practical Workshop 3	Practical Workshop 5	Practical Workshop 7	Practical Workshop 9	**Free Time**	Advanced Seminar 1 FPS BIO MESO	Practical Session FPS BIO MESO	Practical Session FPS BIO MESO
15.30		***Refreshments***						***Refreshments***		
16.00		Practical Workshop 2	Practical Workshop 4	Practical Workshop 6	Practical Workshop 8	Practical Workshop 10		Advanced Seminar 2 FPS BIO MESO	Practical Session FPS BIO MESO	**Departure**
17.00		Research Seminar R. Wade	Research Seminar J. Yeomans	Student Research Seminars -> Posters	Research Seminar D. Marx	Research Seminar P. Carbone		Research Seminar D. Coker	Research Seminar D. Quigley	

Main lecturers	Advanced Topics	Research Seminars
John Harding (Sheffield)	**Keith Refson (STFC-RAL)**	**R. Wade (HITS)**
Philip Camp (Edinburgh)	**Xavier Daura (A.U. Barcelona)**	**J. Yeomans (Oxford)**
David Willock (Cardiff)	**Ian Halliday (Sheffield Hallam)**	**P. Carbone (Manchester)**
Jamshed Anwar (Bradford)	Local Organiser/Lecturer	**D. Coker (UCD)**
Keith Refson (STFC-RAL)	**Mario del Popolo (Queens University Belfast)**	**D. Quigley (Warwick)**
		D. Marx (Bochum)

John Purton Last modified 8th April 2011