Report on the Methods in Molecular Simulation Summer School 2010

1. Organizers

The Methods in Molecular Simulation Summer School 2010 was held at Queen's University Belfast from 18 -27 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, P.M. Rodger, 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, mostly at the Elmwood Learning and Teaching Centre (ELTC), with some sessions at the Peter Froggatt Centre. 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 XX 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. The numbers were significantly better than in 2009 – suggesting that some of the effects of the Credit Crunch had abated.

69 students attended. Those attending originated from 29 countries: 20 were from the host nation (UK) and 32 were from elsewhere in Europe.17 students were from outside Europe. A full list of participants, their nationalities and home institutions, is presented in Appendix 1.

4. Support

A registration fee of £390 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 the ELTC. 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 2009 and the student responses were taken into account, as far as was practical, in 2010.

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) Optimization methods. J. Harding
- (1) Potentials. J Purton
- (1) An overview of molecular simulation. M. Rodger.
- (2) Statistical mechanics. M. del Popolo.
- (4) Molecular dynamics. D. Willock.
- (1) Non equilibrium molecular dynamics. M. Rodger.
- (4) Monte Carlo. P. Camp.
- (1) Long range forces. J. Purton.
- (1) Hyperdynamics. J. Harding
- (2) Free energy methods. M. Rodger

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:

- **Xavier Periole**, University of Groningen: *Coarse grained molecular dynamics simulations of biomolecular systems.*
- **Emanuele Paci**, University of Leeds: *Protein landscapes and mechanics*.
- **Syma Khalid**, University of Southampton: *Coarse grained molecular dynamics simulations of DNA-lipoplexes.*
- **Christian Holm**, University of Stuttgart: *Simulating charged macromolecules - what are the current challenges?*
- **Graeme Watson**, Trinity College Dublin: *Periodic DFT modelling of defects in solid state materials.*
- **Michiel Sprik**, University of Cambridge: *Design for a computational normal hydrogen electrode.*

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

- **Matthew Bano** , University of Warick, UK: *A molecular simulation study of nano-particles of tricalcium phosphate.*
- **Sebastien Lectez**, IPNO, France: *Uranyl behaviour at the gibbsite-water interface: a Car Parrinello molecular dynamics study.*
- **Anikó Udvarhelyi**, MPI Medical Research, Germany: *Hydrogen bond dynamics in BLUF blue light photoreceptor proteins.*
- **Szilard Pall**, Stockholm University, Sweden: *Optimizing and Automating Parameter Selection for Free Energy Calculations Using Entropy Measures.*

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. Anikó Udvarhelyi (Max-Planck-Institute for Medical Research, Germany) for best short seminar, and Mr. Sela Samin (Ben-Gurion University of the Negev, Israel) 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).
- 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, 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.

8. The Future

The Summer School in 2011 is also planned for Queen's University of Belfast. CCP5 will provide some funding and additional funding will be requested from CECAM.

9. Gallery

The Summer School 2010 group photograph

Award for best student lecturer

Mark Rodger, Lecturer

At the computing workshops

Appendix 1. Attendance List

Mr	Yahia	Chergui	Badji Mokhtar Annaba	Algerian
Ms	Lauren	Abbott	Pennsylvania State University	American
Mrs	Edita	Sarukhanyan	University of Salerno	Armenian
Mr	Aleksandr	Sahakyan	University of Cambridge	Armenian
Mr	Reinhard	Maurer	Karl-Franzens-Universität Graz	Austrian
Mr	Thomas	Lion	University of Edinburgh	British
Mr	Jeffrey	Armstrong	Queens University Belfast	British
Mr	James	Miller	University of Strathclyde	British
Ms	Laura	Leay	University of Manchester	British
Mr	Michael	Doig	University of Edinburgh	British
Mr	Christopher Andrew	Lee	Cardiff University	British
Ms	Selina	Nawaz	University of Manchester	British
Ms	Kate	Meadows	University of Warwick	British
Ms	Bruck	Taddese	University of Essex	British
Mr	Matthew	Bano	University of Warwick	British
Mr	Adam	Rigby	University of Manchester	British
Mr	Charles	Matthews	Edinburgh University	British
Mr	Hlengisizwe	Ndlovu	University of Leeds	British
Mr	James Alexander	Dawson	University of Sheffield	British
Mr	Chris	Pittock	University of Southampton	British
Mr	Luke	Debono	University of Bristol	British
Mr	Oliver	Warr	University of Manchester	British
Ms	Melissa	Cutler	University College London	British
Mr	Michael	Carter	University of Southampton	British
Mr	Jordan	Muscatello	Imperial College London	British
Mr	Wei	Ke	University of Stavanger	Chinese
Mr	Liang	Wu	Imperial College London	Chinese
Mr	Linjiang	Chen	The University of Edinburgh	Chinese
Ms	Lixian	Zhang	University of Basel	Chinese
Mr	Michal	Kolar	Academy of Sciences of the Czech Republic, v.v.i.	Czech
Ms	Rosanne	Zeiler	Universiteit van Amsterdam	Dutch
Mr	Hailu Kebede	Abay	Stavanger University	Ethiopian
Mr	Sébastien	Lectez	IPNO	French
Mr	Bastian	Ohler	University of Greifswald, Institute for Biochemistry	German
Mr	Manolis	Vasileiadis	Imperial College London	Greek
Ms	Maria	Anagnostopoulou	National Kapodistrian University of Athens	Greek
Ms	Anikó	Udvarhelyi	Max-Planck-Institute for Medical Research	Hungarian
Mr	Ramachandra Moorthy	Bhaskara	Indian Institute of Science	Indian
Mr	Rameshwar U.	Kadam	University of Berne	Indian
Mr	Gavin	Melaugh	Queen's University Belfast	Irish
Ms	Caoimhe	de Frein	University College Dublin	Irish
Mr	Sela	Samin	Ben-Gurion University of the Negev	Israeli
Dr	Simone	Sturniolo	University of Pavia	Italian
Mr	Filippo	Marozzelli	Cardiff University	Italian
Mr	Salvatore Mario	Cosseddu	University of Warwick	Italian
Ms	Carla	Jamous	Université d'Evry-Val-d'Essonne	Lebanese
Mr	Mantas	Gabrielaitis	Lancaster University	Lithuanian
Mr	Grisell	Diaz Leines	University of Amstedam	Mexican
Mrs	Katarzyna	Bartus	University of Silesia	Polish
Mr	Szymon	Daraszewicz	University College London (UCL)	Polish
Mr	Miroslaw	Cwiok	University College London	Polish
Mr	Krzysztof	Gorny	University of Silesia	Polish
Ms	Ana Catarina	Mendonça	Université Blaise Pascal	Portuguese
Ms	Mariana	Oliveira	Universidade de Aveiro	Portuguese
Ms	Marta	Batista	University of Aveiro	Portuguese
Mr	Szilard	Pall	Stockholm University	Romanian
Mrs	Uliana	Alekseeva	Forschungszentrum Juelich	Russian
Mr	Dmitriy	Rozhkov	Ural State University	Russian
Mrs	Milica	Lukic	RWTH Aachen University	Serbian
Mr	Stas	Bevc	National Institute of Chemistry	Slovene
Mr	Ausias-March	Calvo Minguillón	Universitat Politecnica de Catalunya	Spanish
Mr	Jordi	Ortiz de Urbina	Universitat Politecnica de Catalunya	Spanish
Mrs	Maria	Aznar Palenzuela	Universidad de Barcelona	Spanish
Ms	Gabriella	Jonasson	Université de Paris-Sud	Swedish
Mr	Kai-Ming	Tu	Academia Sinica	Taiwanese
Mr	Hung-Ru	Chen	University of Sheffield	Taiwanese
Ms	Nina	Ramrattan	Imperial College London	Trinidadian
Mr	Batu	Hunca	Trakya University	Turkish

	18 July	19 July	20 July	21 July	22 July	23 July	24 July	25 July	26 July	27 July
09.00		Overview of Molecular Simulation	Statistical Mechanics 2	Monte Carlo 2	Monte Carlo 3	Molecular Dynamics 4	Molecular Dynamics 5		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	Long Ranged Forces	Free Time	Practical Session FPS BIO MESO	Practical Session FPS BIO MESO
11.00		*Refreshments*							*Refreshments*	
11.30		Statistical Mechanics 1	Molecular Dynamics 1	Optim - -isation Methods	Free Energy Methods 1	Free Energy Methods 2	Hyper - -dynamics Methods		Practical Session FPS BIO MESO	Practical Session FPS BIO MESO
12.30		*Lunch*								
14.00		Practical Workshop 1	Practical Workshop 3	Practical Workshop 5	Practical Workshop 7	Practical Workshop 9		Advanced Seminar 1 FPS BIO MESO	Practical Session FPS BIO MESO	Practical Session FPS BIO MESO
15.30		*Refreshments*						*Refreshments*		
16.00	Arrival	Practical Workshop 2	Practical Workshop 4	Practical Workshop 6	Practical Workshop 8	Practical Workshop 10	Free Time	Advanced Seminar 2 FPS BIO MESO	Practical Session FPS BIO MESO	
17.00		Research Seminar X. Periole	Research Seminar E. Paci	Student Research Seminars -> Posters	Research Seminar S. Khalid	Research Seminar C. Holm		Research Seminar G. Watson	Research Seminar M. Sprik	Departure