Report on the Methods in Molecular Simulation Summer School 2008

1. Organizers

The Methods in Molecular Simulation Summer School 2008 was held at Sheffield University from 6 -15 July, in the Department of Mathematics and Astronomy. The School was organised by the CCP5 Summer School Working Group, which consisted of J. Harding (Chairman), W. Smith (Secretary), I. Halliday, J. Anwar, K. Travis, P. Camp, P.M. Rodger and D. Willock. The local organisation was handled by J. Harding and K. Travis, from the Department of Engineering Materials of Sheffield University and I. Halliday from the Materials and Engineering Research Institute of Sheffield Hallam University.

2. Location and Facilities

The School was held in the Hicks Building of Sheffield University, which is situated near the municipal centre of Sheffield and is close to the organisational centre of Sheffield University. The students were accommodated close by, in the Broomgrove Hall of Residence, which is managed by Sheffield Hallam.

The main lectures of the School took place in the Hicks Building in the Department of Mathematics and Astronomy and the advanced courses were divided between this theatre and two adjacent lecture rooms, all of which offered projection facilities and on-line access. The computer exercises also took place in the Hicks Building, where there were sufficient places for 70 students working independently. The computing equipment consisted of desktop personal computers running linux for the basic course. In addition two multiprocessor platforms: ICEBERG, a 320 processor Opteron which forms the Sheffield node of the White Rose Computing Grid; and a 48 node Clustervision platform that is owned by the Department of Engineering Materials; were available for the advanced courses.

3. Participation

We received 105 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.

70 students were selected. Those attending originated from 31 countries: 47 were from Europe and 23 from elsewhere in the world. Of the European students, 11 were from the host nation (UK), 36 from other European countries. A full list of participants, their nationalities and home institutions, is presented in Appendix 1.

4. Support

A registration fee of £400 was charged to the students, which covered the bulk of the costs. The University of Sheffield Department of Mathematics and Astronomy provided the use of the Hicks Building, lecture theatres and most of the computing equipment at nominal cost,

though additional computing equipment had to be hired. 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 Sheffield Hallam University. The students were located in Broomgrove Hall. The hall was within 15 minutes walking distance of the Hicks Building. 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 2006 and the student responses were taken into account, as far as was practical, in 2008.

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 Harding
- (1) An overview of molecular simulation. M. Rodger.
- (2) Statistical mechanics. M. Rodger.
- (2) Basic molecular dynamics. W. Smith
- (2) Advanced molecular dynamics. D. Willock.
- (1) Non equilibrium molecular dynamics. K. Travis.
- (4) Monte Carlo. P. Camp.
- (1) Long range forces. D. Willock.
- (1) Hyperdynamics. J. Harding
- (2) Free energy methods. J. Anwar

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.

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 the CCP5 website at Daresbury Laboratory. The work was performed entirely on the PCs running a linux operating system 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:

- **Sarah Harris**, University of Leeds: *Biomolecular Dynamics Investigated by Computer Simulation*.
- **Paul Madden**, University of Edinburgh: *From first-principles to the properties of ionic materials, via transferable interaction potentials*.
- **Mark Wilson**, University of Durham: *Models and methods for the simulation of self-organising molecular materials.*
- **Jean-Pierre Hansen**†, University of Cambridge: *Multi-blob representation of polymer solutions and block copolymer self-assembly.*
- **Kurt Binder**, University of Mainz*: Phase Behavior of Fluids, Fluid Mixtures and Polymer Solutions: Can it be Accurately Predicted by Monte Carlo Simulation?*
- **Mario Orsi**, University of Southampton: *Coarse-grain Modelling of Lipid Bilayers*.

† Prof. Hansen was unable to attend at short notice. In the vacant slot J. Harding presented a lecture on the simulation of bio-inorganic materials.

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

- **Neil Bruce**, University of Manchester: *Molecular Dynamics Simulations and Free Energy Analysis of beta-Amyloid Fibrils*.

- **Ulrich Welling**, Philipps-University Marburg: *Collective Dynamics in Molten Alkali Halides.*

- **Mishal Patel**, University of Southampton: *The Development and Application of Coarse Grained Models*.

- **Juan Luis Aragones**, Universidad Complutense, Madrid: *Properties of Ices at 0K: A Test of Water Models.*

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 **Mishal Patel** (University of Southampton), for best short seminar, and **Syamal Tallury** (North Carolina State University), 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 2009 is planned for The University of Sheffield. Sources of funding for the School are being sought.

9. Gallery

The Summer School 2008 group photograph

At the poster session

Mishal Patel receiving the award for best student lecturer

Syamal Tallury receiving the award for best poster

At the computing workshops

Mario Orsi, Plenary Speaker

Appendix 1. Attendance List

Mr	Mohammad	Abdulhadi	University of Strathclyde	Iraqi
Mrs	Fatmawatil	Adam	Leeds University	Malasyian
Mr	Juan Luis	Aragones	Universidad Complutense de Madrid	Spanish

Mr	Aldi	Asmadi	University of Bradford	Indonesian
Ms	Vera Monica de Oliveira	Batista	University of Cambridge	Portuguese
Ms	Anna	Battisti	La Sapienza University	Italian
Mr	Alan	Bizjak	University of Ljubljana	Slovenian
Mr	Ioannis	Bonis	University of Manchester	Greek
Mr	Neil	Bruce	University of Manchester	British
Mr	Juan Manuel	Castillo Sanchez	Pablo de Olavide	Spanish
Ms	Naomi	Cessford	University of Edinburgh	British
Mr	Stuart	Collins	University of Delaware	American
Mr	Aldo Fabrizzio	Combariza	Polytechnic University of Valencia	Colombian
Ms	Maria M.	Conde	Universidad Complutense de Madrid	Spanish
Ms	Valeria	Conti Nibali	University of Messina	Italian
Mr	Asfaw Gezae	Daful	Universitat Rovira i Virjili	Ethiopian
Mr	Giuseppe	De Marco	University of Sussex	Italian
Mr	Debabrata	Deb	Karl-Franzens Universit¨t Graz	Indian
Mr	Alastair	Dunn	University College London	British
Mr	Hugh	English	University of Manchester	British
Mr	Apostolos E. A. S.	Evangelopoulos	University of Edinburgh	Greek
Dr	Angelo	Felline	University of Modena and Reggio Emilia	Italian
Mrs	Nancy Carolina	Forero-Martinez	Queen's University Belfast	Colombian
Dr	Domenico	Fraccalvieri	Università degli Studi di Milano-Bicocca	Italian
Mr	Alberto	Gallardo	Instituto de Química-Física "Rocasolano", CSIC	Spanish
Mrs	Dawn	Geatches	Durham University	British
Dr	Violeta	Georgieva	University of Antwerp	Bulgarian
Mr	Matthew	Groombridge	Imperial College London	British
Mr	Andy	Ilott	Durham University	British
Mr	Julio	Jover	Imperial College London	Spanish
Mr	Aleksandr	Kalinko	University of Latvia	Latvian
Mr	Andrey	Kazantsev	Imperial College London	Russian
Mr	Abdul Waheed	Khan	University of Leeds	British
Mr	Larry	Lan	University of Bolton	Chinese
Mr	Thabo Ezekiel	Letsoalo	University of the Witwatersrand, Johannesburg	South African
Ms	Claudia Cristina	Loyola	University of Chile	Chilean
Ms	Lien	Luu	Institute of Technology Tallaght, Ireland	Irish
Mr	Karim	Madjer	Univeristy of Marne la Vallée	French
Mr	Luis Martín	Mejía-Mendoza	Universidad Nacional Autónoma de México	Mexican
Mr	Gianmarco	Munao'	University of Messina	Italian
Mr	Satoshi	Numazawa	Research Center Dresden-Rossendorf	Japanese
Mr	Onyekwelu Uzodinma	Okeke	University of the Witwatersrand, Johannesburg	Nigerian

Mr	Sudharsan	Pandiyan	University of Savoie	Indian
Mr	Mishal	Patel	University of Southampton	British
Mr	Joaquin Andres	Peralta	University of Chile	Chilean
Ms	Marine	Petrantoni	Laboratoire d'Analyse et d'Architecture des Systèmes (LAAS)	French
Ms	Carolyn	Phillips	University of Michigan	American
Mr	Francesco	Ragone	Università degli Studi di Salerno	Italiana
Mr	Anton	Raskovalov	Institute of High Temperature Electrochemistry of Ural Branch of Russian Academy of Science	Russian
Mr	Angel	Reyes	Universidad Nacional Autónoma de Mexico	Mexican
Ms	Emilye	Rosas Landa Loustau	Universidad Nacional Autónoma de México	Mexican
Mr	Jonas	Sala	Universitat Politecnica de Catalunya	Spanish
Ms	Marieke	Schor	University of Amsterdam	Dutch
Ms	Lynsey	Shepherd	University of Edinburgh	British
Mr	Ferdinando	Spagnolo	University of Modena and Reggio Emilia	Italian
Mr	Heiko	Strübing	Imperial College London	German
Mr	Adam	Swetnam	University of Wawick	British
Mr	Marek	Szczerba	Polish Academy of Siences	Polish
Mr	Syamal Sanmath	Tallury	North Carolina State University	Indian
Ms	Lipi	Thukral	University of Heidelberg	Indian
Mr	Michel	Tsamados	Universite Lyon 1 Claude Bernard	French
Mr	Germain	Vallverdu	Université Paris Sud 11	French
Ms	Ana Sofia A.	Vila Verde	University College London	Portuguese
Mr	Linas	Vilciauskas	Max-Planck-Institut für Festkörperforschung	Lithuanian
Mr	Rasmus	Wedberg	Technical University of Denmark	Swedish
Mr	Ulrich	Welling	Philipps-University Marburg	German
Ms	Suwimol	Wongsakulphasatch	University of Manchester	Thai
Ms	Mai	Zahran	University of Heidelberg	French
Mr	Amin Reza	Zolghadr	Shiraz University	Iranian
Mr	Nicholas	Zonias	University of Southampton	Cypriot

Appendix 2. The CourseTimetable

	6 July	7 July	8 July	9 July	10 July	11 July	12 July	13 July	14 July	15 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 - -ization 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	**Departure**
17.00		Research Seminar S. Harris	Student Research Seminars -> Posters	Research Seminar P. Madden	Research Seminar M. Wilson	Research Seminar J.-P. Hansen		Research Seminar K. Binder	Research Seminar M. Orsi	