Report on the Methods in Molecular Simulation Summer School 2007

1. Organizers

The Methods in Molecular Simulation Summer School 2007 was held at Sheffield University from 8 -17 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, D. Willock and K. Refson. 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 Woodville 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 60 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 162 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. In addition to the academic criteria, selection was also based on nationality, as required by Marie Curie Actions, concerning the numbers of students in the categories of host nation, European and non-European nationality.

60 students were selected. Those attending originated from 26 countries: 47 were from Europe and 13 from elsewhere in the world. Of the European students, 6 were from the host nation (UK), 41 from other EU countries. A full list of participants, their nationalities and home institutions, is presented in Appendix 1.

42 of our 162 applicants (26%) were female. In our final selection 22 were chosen to participate, thus 37% of the students taking part were female.

4. Support

The Summer School received direct support from the UK's Collaborative Computational Project #5 (£7,500). The bulk of the funding came from Marie Curie Actions, which provided a budget of 85,000 Euros. This enabled a full provision of facilities for the students, including accommodation and meals. A registration fee of £75 was charged to the students. 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 Woodville Hall. The hall was within 10 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 2007.

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. K. Travis
- (2) Advanced molecular dynamics. D. Willock.
- (1) Non equilibrium molecular dynamics. K. Travis.
- (4) Monte Carlo. P. Camp.
- (1) Long range forces. W. Smith.

- (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 G95 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:

- **Barbara Montanari**, Rutherford Appleton Laboratory: *Ab initio Studies of Organic Magnetic Systems.*
- **Marek Sierka**, Humboldt University of Berlin: *Combined Quantum Mechanics - Potential Functions Method and its Applications.*
- **Alain Fuchs†**, Ecole Nationale Supérieure de Chimie de Paris: *Does Water Condense in Hydrophobic Pores?*
- **Christian Holm**, J.W. Goethe University of Frankfurt: *Recent Advances in Simulations of Charged Polymeric Systems.*
- **Doros Theodorou**, National Technical University of Athens: *Hierarchical Simulations of Polymers.*

- **Eduardo Hernandez**, Institute of Materials Sciences Barcelona: *Obtaining Phase Coexistence Conditions and Phase Diagrams from Atomistic Simulations: Techniques and Sample Applications.*

† Prof. Fuchs was unable to attend at short notice due to accidental injury. In the vacant slot J. Harding and P. Camp presented a combined 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:

- **Richard Handel**, University of Leicester: *Interfacial Free Energy of the Ice-Water Interface: Direct calculation using Molecular Dynamics.*
- **Halvor Hansen***,* Eidgenössische Technische Hochschule Zürich: *Local elevation as a building tool for optimised umbrella potentials.*
- **P. Pirzadeh**, University of Calgary, Alberta, Canada: *Molecular dynamic simulation of ice crystal growth.*
- **J-H Prinz**, DFG Research Center Matheon, FU Berlin: *Enhanced phase-space sampling using meta-stability.*

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 **Payman Pirzadeh** (University of Calgary), for best short seminar, and **Katie Mitchell Koch** (University of Kansas), 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

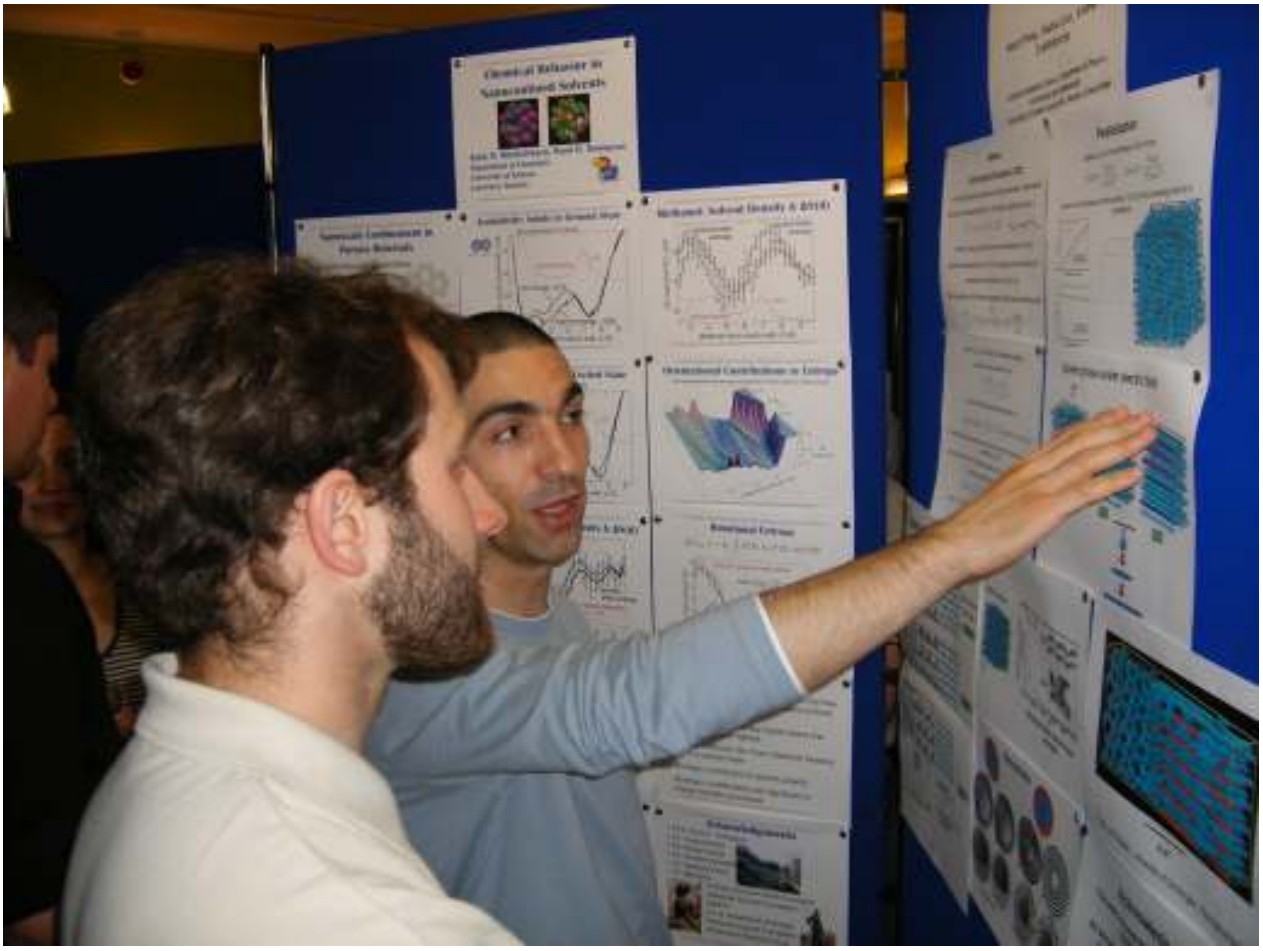
To assess the quality of the School, each student was asked to complete a questionnaire inviting their response to various specific and general aspects of the School. The analysis of the survey was conducted by Prof. J. Harding. The results are summarized in Appendix 3. Students were also directed to the EC website http://webgate.cec.eu.int/sesam to provide a mandatory report on the School.

8. The Future

The Summer School in 2008 is planned for The University of Sheffield. Sources of funding for the School are being sought.

9. Gallery

The Summer School 2007 group photograph

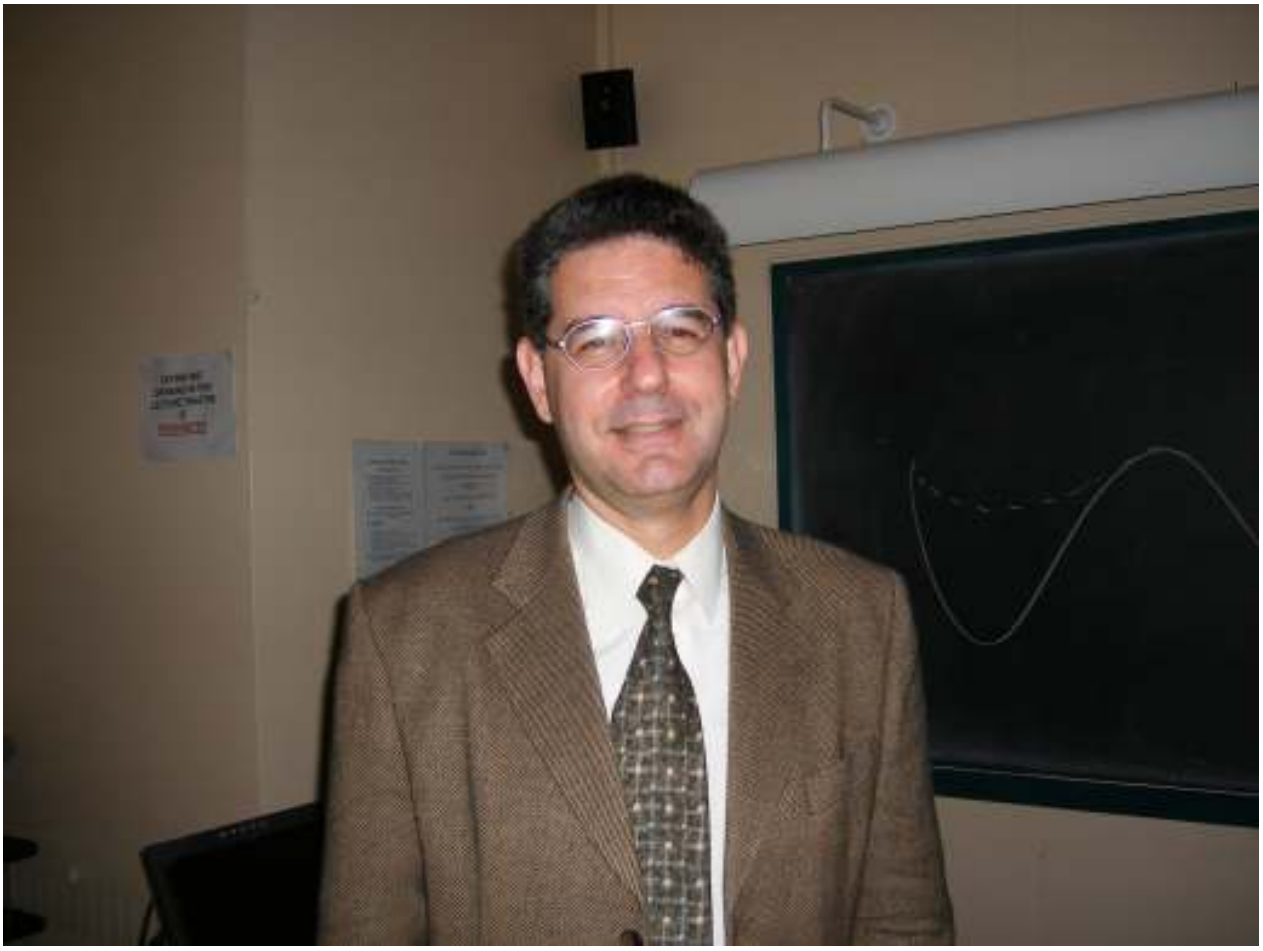


At the poster session

Payman Pirzadeh receiving the award for best student lecturer

Katie Mitchell Koch receiving the award for best poster

At the computing workshops



Prof. Doros Theodorou, Plenary Speaker

Appendix 1. Attendance List

	Forename	Surname	Affiliation	Nationality
	Katie	Mitchell-Koch	University of Kansas	American
	James Edward	Murphy	University of Virginia	American
	Francisco	Vazquez	University of Michigan	American
	Carina Farah	Mugal	Karl-Franzens-University Graz	Austrian
	Patrick	Schopf	University of Southampton	Austrian
	Dieter	Schwanzer	Vienna University of Technology	Austrian
	Clive	Bealing	King's College London	British
	Genevieve	Clapton	University of Southampton	British
	Matthew	Dennison	University of Manchester	British
	Anthony	Devey	University College London	British
	Sheena	Dungey	University College London	British
	Richard James	Handel	University of Leicester	British
	Veluz Maria	Hart Prieto	University of Bath	British
	Kara Louise	Howard	Cardiff University	British
	Kim Elizabeth	Jelfs	Royal Institution	British
	John	McCann	University of Strathclyde	British
	Alexis Michael	Rutherford	University College London	British

	Samantha	Shaw	University of Surrey	British
	Lisa Marie	Simpson	University of Essex	British
	Tom	Stedall	University of Bristol	British
	Gareth	Welch	University College London	British
	David	Wright	University College London	British
	Martin	Gotsev	Bulgarian Academy of Sciences	Bulgarian
	Georgi V.	Pachov	EML Research GmbH	Bulgarian
	Hristina	Popova	Bulgarian Academy of Sciences	Bulgarian
	Julia	Romanova	University of Sofia	Bulgarian
	Philip	Shushkov	University of Sofia	Bulgarian
	Jorge	Saavedra	University of Concepcion	Chilean
	Xiaoyu	Chen	Technical University Darmstadt	Chinese
	Endel	Soolo	Tartu University	Estonian
	Eva	Stjernschantz	Vrije Universiteit Amsterdam	Finnish
	Gregory	Marque	University of Savoie	French
	Cedric	Mastail	LAAS-CNRS	French
	Jan-Hendrik	Prinz	University of Heidelberg	German
	Tim	ten Brink	Univerity of Konstanz	German
	Panagiotis	Grammatikopoulos	University of Liverpool	Greek
	Argyrios	Karatrantos	University of Manchester	Greek
	Nikolaos	Rompotis	King's College London	Greek
	Ioannis	Tanis	Aristotle University of Thessaloniki	Greek
	Raghunadha Reddy	Burri	University of Dortmund	Indian
	Devaprakasam	Deivasagayam	University of Sheffield	Indian
	Gautam	Siddarth	University of Mumbai	Indian
	Mehdi	Davari	Shahid Beheshti University	Iranian
	Payman	Pirzadeh	University of Calgary	Iranian
	Kiamars	Vafayi	Max Planck Institute for Solid State Research	Iranian
	Anthony Martin	Reilly	University of Edinburgh	Irish
	Francesca	Collu	University of Cagliari	Italian
	Emanuela	Giuffre'	Universita' degli Studi di Messina	Italian
	Dario	Marrocchelli	University of Edinburgh	Italian
	Giacomo	Mazzi	University of Edinburgh	Italian
	Manuela	Mura	King's College London	Italian
	Emanuela	Pusceddu	Institute Laue-Langevin 'ILL'	Italian
	Francesco	Raimondi	University of Modena e Reggio Emilia	Italian
	Enrico	Spiga	University of Cagliari	Italian
	Marco	Pinna	University of Central Lancashire	Italy
	Matthew	Borg	University of Strathclyde	Maltese
	Joel	Antúnez García	Universidad Autónoma de Nuevo León	Mexican
	Halvor Schrøder	Hansen	ETH Zürich	Norwegian
	Tomasz	Berezniak	Ruprecht-Karls-University of Heidelberg	Polish
	Wojciech	Gwizdala	University of Silesia	Polish
	Andrzej Jerzy	Rzepiela	University of Groningen	Polish
	Kinga	Sowa	Polish Academy of Sciences	Polish
	Joao	Costa	Imperial College London	Portuguese
	Nicoleta	Hirjaba	Tallaght Institute of Technology	Romanian

	Miha	Luksic	University of Ljubljana	Slovenian
	Elsa	Galbis Fuster	University of Seville	Spanish
	Elisa Isabel	Martín Fernández	University of Seville	Spanish
	Sara	Nuñez	University of Valladolid	Spanish
	Pär	Bjelkmar	Stockholm University	Swedish
	Chen	Peng-Yu	National Tsing Hua University	Taiwan
	Juan Carlos	Araque	Rice University	Venezuelan

Appendix 2. The CourseTimetable

	8 July	9 July	10 July	11 July	12 July	13 July	14 July	15 July	16 July	17 July
09.00		Overview of Molecular Simulation	Molecular Dynamics 1	Molecular Dynamics 2	Molecular Dynamics 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	Monte Carlo 2	Monte Carlo 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	Statistical Mechanics 2	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	
17.00		Research Seminar B Montanari	Student Research Seminars -> Posters	Research Seminar M Sierka	Research Seminar A Fuchs	Research Seminar C Holm		Research Seminar D Theodorou	Research Seminar E Hernandez	**Departure**

Appendix 3: Results of 2007 Course Assessment by Students

Note that for all results marks can vary between +2 (excellent) and (-2) (very poor).

On the main lectures (averaged over the lecturers): 64% overall response	
Were the aims of the lecturer clear?	1.61
Were the lectures clearly presented?	1.37
How good was the use of visual aids	1.18
Were the lectures well organised?	1.44
How interesting were the lectures?	1.27
Was the lecturer prepared to take questions?	1.57
How helpful were the notes?	1.48
Overall score	**1.42**

Workshops (basic course)	
Were the notes clear and helpful?	1.34
Were the demonstrators available and helpful?	1.37
Did the exercises help you understand the course material?	1.13

Averages of these questions for individual days	
9 July	1.29
10 July	1.30
11 July	1.41
12 July	1.27
13 July	1.14
Overall average for exercises	**1.28**

Was there too little (-2) or too much (+2) material	0.95
Were the exercises too easy (-2) or too hard (+2)	0.28

First principles lectures: 20 replies	
Were the aims of the lecturer clear?	1.8
Were the lectures clearly presented?	1.75
How good was the use of visual aids	1.35
Were the lectures well organised?	1.6
How interesting were the lectures?	1.15
Was the lecturer prepared to take questions?	1.85
How helpful were the notes?	1.45
Overall score	**1.56**

First principles workshops	
Were the notes clear and helpful?	0.69
Were the demonstrators available and helpful?	1.18

Did the exercises help you understand the course material?	0.98
Overall average for exercises	**0.95**
Was there too little (-2) or too much (+2) material?	0.37
Were the exercises too easy (-2) or too hard (+2)?	0.27
Mesoscale lectures: 10 replies	
Were the aims of the lecturer clear?	1.60
Were the lectures clearly presented?	1.40
How good was the use of visual aids	1.50
Were the lectures well organised?	1.50
How interesting were the lectures?	1.40
Was the lecturer prepared to take questions?	1.90
How helpful were the notes?	1.2
Overall score	**1.50**
Mesoscale workshops	
Were the notes clear and helpful?	1.47
Were the demonstrators available and helpful?	1.87
Did the exercises help you understand the course material?	1.53
Overall average for exercises	**1.62**
Was there too little (-2) or too much (+2) material?	0.43
Were the exercises too easy (-2) or too hard (+2)?	0.23
Biosimulation lectures: 17 replies	
Were the aims of the lecturer clear?	2.00
Were the lectures clearly presented?	1.88
How good was the use of visual aids	1.47
Were the lectures well organised?	1.71
How interesting were the lectures?	1.94
Was the lecturer prepared to take questions?	1.82
How helpful were the notes?	1.47
Overall score	**1.76**
Biosimulation workshops	
Were the notes clear and helpful?	1.54
Were the demonstrators available and helpful?	1.78
Did the exercises help you understand the course material?	1.31
Overall average for exercises	**1.54**
Was there too little (-2) or too much (+2) material?	1.00
Were the exercises too easy (-2) or too hard (+2)?	0.33

Appendix 4: Student Comments

The students were also invited to make comments on the School. The comments received are presented below.

Basic Course

More proactive help is needed in workshops. The best class was one examining methane adsorption in silicalite – one larger problem is better, relates more to what we really do, therefore more interesting

Great with a lot of material so you can choose the most relevant things yourself and be able to do exercises later

If you had studied the materials mentioned as "preparation before arrival" then none of the theoretical lectures were useful. Instead, I think if the organisers offered the essential parts of a MD or MC code like establishing neighbour list, building initial configuration, evaluating integrals or differential equations, then discuss an algorithm or a sample code in theoretical lectures and then have practical exercises in practical workshops, I think that would be more helpful. In addition, I think if some booklets were given that could elaborate the concepts more explicitly rather than powerpoint slides that might not be easily followed later, it would be more helpful.

The practicals should include more theory of why we perform the simulations and less technical details (how to work on Linux). Better 1 exercise on MD which is completely understood than 6-7 which are unclear. The best would be 15 minutes before the practical the demonstrator to present the physics of the system we will use (equations, quantities to derive).

Very well chosen study material

In the exercises we had to check the code and modify it, it is quite difficult to get into the problem in so little time, so sometimes you have got stuck. The more the links between the theory and the "real" problems we are going to face, the better you can understand everything.

Can you allow more time for questions and discussions? The programme structure was excellent. The accommodation could have been better.

More coordination among the lectures in order to avoid some overlap of the topics.

Maybe it would be better to spend more time on the practical workshops and less on the research seminars, that were too long. Maybe it would be good if you can add evaluation of accommodation, facilities, food etc. Thanks.

No internet access very inconvenient. All other arrangements very good. Computer room too hot.

Philip Camp's lectures were superb. Could there be some group discussion worked into the course, maybe in place of so many exercises? Overall I feel that I have benefited enormously from the course. Thank you!

In my opinion, access to the exercises on the webpage should be secured by password for the exclusive use of CCP5 students.

You should provide people with any kind of wireless connection or some other way to keep active with our own work. The practical sessions should cover less material more effectively.

Nice presentation in Monte Carlo method!

Accommodation was quite poor – unclean and noisy. Courses were very good though

I suggest name tags for everybody in general, since it makes easier to learn the names and talk to people. Plain water during tea times would be nice. The seminars at 1700 are very late since they are interesting but most people find it hard to concentrate after so much thinking

First Principles Calculations

Excellent in my opinion

The approach was quite clear and you didn't use so many equations and a lot of physical meanings to understand the point.

Mr Refson was really worried about us. At the beginning was a little difficult because a program did not install properly. The lectures were very useful to me

Mesoscale Methods

It would be better if a general view of the mesoscale was offered rather than the specific cases, in a way that anybody could grasp the idea of how to implement the algorithm or method in his/her case

Biosimulations

Great course and practical sessions in general, but I wish there were more time to go into the details of the setup for GROMOS