Report on the Methods in Molecular Simulation Summer School 2004

1. Organisers

The Methods in Molecular Simulation Summer School 2004 was held at Cardiff University from 9-17 July, in the Department of Chemistry. The School was organised by the CCP5 Summer School Working Group, which consisted of J. Harding (Chairman), W. Smith (Secretary), J. Anwar, K. Travis, P. Lindan and K. Refson. The local organisation was handled by D.J. Willock, from the Cardiff University Department of Chemistry.

2. Location and Facilities

The School was held in the main building of Cardiff University, which is situated in the attractive municipal centre of Cardiff, which also hosts several of the major civic buildings in Cardiff, including the National Museum of Wales, the Law Courts, The Town Hall and the Welsh Office. Cardiff was chosen ahead of the University of Warwick (the intended location for 2004) for reasons of cost; at that time we did not have the decision regarding the Marie Curie Actions funding proposal. . Cardiff offered excellent facilities and inexpensive accommodation close to the School. All students were residential and paid a small participation fee of £30.
The lectures of the School took place in the Small Lecture Theatre of the Chemistry Department (which conveniently offered projection facilities and on-line access) and the computer exercises took place in the Main Library on the first floor of the Main Building and the computer room of the Department of Geology on the ground floor. There were sufficient places for 60 students working independently. The computing equipment consisted of desktop personal computers for the basic course and a multiprocessor platform (`Helix') with 48 nodes which was ideal for the advanced courses.

3. Participation

We received 89 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 entailed a significant amount of molecular simulation. Additional endorsements were sought from the tutors of the applicants. 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 stipulations laid down by Marie Curie Actions concerning the numbers of students in the categories of host nation, European and non-European nationality. There was inevitably some tension between these selection criteria, leading to slight departures from the ideal required by Marie Curie Actions, for which purpose funds allocated by CCP5 were called into use.

60 students were selected. Those attending came from no fewer than 22 countries: 17 were from the United Kingdom, 25 from mainland Europe and 18 from outside Europe. In all 41 students were citizens of the EC or associated countries and 19 were from third countries. A full list of participants, their nationalities and home institutions, is presented in Appendix 1.

Only 23 of our 89 applicants (26%) were female, which made it impossible to satisfy the 40% female participation suggested by Marie Curie Actions. However the 15 females (25%) attending the School fairly represents the proportion of female applicants.

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 (which in previous years had to be paid for by the students). Hence only a token registration fee of £30 was charged to the students. The host institution provided the use of the main building, lecture theatre and security badges at no cost, though the 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 Cardiff University. The bulk of the students were located in Trevithick Hall (where breakfast and evening meals were provided for all the School participants) and Gordon Hall. Both halls were within 10 minutes walking distance of the Chemistry Department. Plenary Lecturers were located in local hotels, near Tevithick Hall.

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 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 previous summer school (2003) and also took into account the student responses as far as was practical. More time was given to the subjects of statistical mechanics and Monte Carlo methods and an additional seminar was given on optimization methods.

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) A statistical mechanics tutorial. P. Lindan
- (3) Statistical mechanics. K. Travis

- (2) Basic molecular dynamics. W. Smith
- (2) Advanced molecular dynamics. K. Refson.
- (1) Non equilibrium molecular dynamics. K. Travis.
- (4) Monte Carlo. N. Wilding
- (1) Long range forces. W. Smith
- (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 of actual computational work. The bulk of the material was supplied by the organisers, with additional material from Prof. M.P. Allen at the University of Warwick.

At 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, in which the Windows operating system had been augmented by CygWin Unix (from RedHat), which provided a unix-like environment (resembling the Bourne shell) with associated C- and Fortran 77 compilers. A Fortran 90 compiler was supplied free by NAG, to whom we express our gratitude. Also available were CCP5's DL_POLY program and assorted graphics tools such as RasMol, VMD etc and the Java GUI from DL_POLY suite (which students were permitted to take away). A new feature tried out this year was a `Wiki' website, which was used by both students and lecturers as a means for posting questions, announcements and other information.

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 School was inaugurated by a lecture by David Willock (Cardiff University) entitled "Simulation in Catalysis". The other plenary lectures were:

- R. Lynden-Bell (University of Cambridge), "A Close-up View of Molecules in Solution";
- S.C. Parker (University of Bath), "Molecular Simulations of Inorganic Surfaces and Interfaces: Computerised Crystal Gazing";
- N. Quirke (Imperial College, London)"Molecular Dynamics of Transient Flow in Nanopores";
- M. Sansom (University of Oxford), "Molecular Dynamics Simulations of Biological Membranes";
- G. Kneller (University of Orleans), "What is `Complex' in the Dynamics of Complex Systems ?";

• N. Seaton (University of Edinburgh), "Applications of Monte Carlo Simulation to Adsorption Equilibrium in Nanoporous Materials".

It is gratifying to record a high degree of audience interest in these lectures and many probing questions were asked by the students. We are grateful to all the plenary speakers for their enthusiastic support for the School.

For the third year in succession, a plenary session was dedicated to short (15 min.) talks given by the students. The four talks selected this year were:

• T.J. Roussel (University of Marseille), "A Grand Canonical Monte Carlo Simulation of Carbon Nanostructures in Nanoporous Materials ";
• L. Meinhold (University of Heidelberg), "Investigationg Protein Collective Motions Using Molecular Dynamics and X-Ray Diffuse Scattering";
• R. Notman (King's College, London), "Molecular Modelling of the Mechanism of Action of Drug Penetration Enhancers for Drug Delivery through Skin";
• Y. Small (Pennsylvania State University), "A QM/MM Study of an Enzyme Comparing the Wild Type to the Mutant".

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 organisers made a small award to **Lars Meinhold** (University of Heidelberg), for best short seminar, and **Emilia Owczarek** (Technical University of Lodz), for best poster (see Gallery below).

Advanced Courses

The School offered a choice of three advanced courses:
- Biomolecular simulation (Xavier Daura, University of Barcelona)
- Mesoscale simulation (P. Coveney, Queen Mary University of London).
- First principles simulation (P. Lindan, University of Kent, Canterbury).

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. Molecular simulation techniques and computational resources are now sufficiently advanced that we can now investigate molecules of biological significance, such as small proteins in water, using these methods. The simulations can explore the thermodynamic properties, conformational statistics and dynamics of these molecules on the atomistic scale. The course format consisted of a series of tutorial sessions and lectures, and practical sessions using the powerful GROMOS code which comes from the group of Wilfred van Gunsteren at the Laboratory of Physical Chemistry, ETH Hönggerberg, Zurich. This course was rewritten from last year to take better advantage of material presented in the basic course.

Prof. Peter Coveney of Queen Mary and Westfield College, London gave the advanced course on Mesoscale Simulation. This topic is currently of great importance in simulation as it provides methods that bridge between atomistic simulations (such as molecular dynamics) and computational fluid dynamics (Navier-Stokes) that is applied to systems on the industrial scale. It thus offers the potential to unite these distinct disciplines into a coherent toolset for all length and time scales of interest in computer modelling. The potential range of application of these methods is vast; from industrial processes, through biological systems to atmospheric physics, to name but three. The course described the current techniques applied in this area: Lattice Gas Automata, Lattice Boltzmann and Dissipative Particle Dynamics. The foundations of these methods were given and the physical interpretation of the elements of the methods was discussed. The course was backed by computational exercises conducted by Jonathan Chin of Queen Mary and Westfield College.

The advanced course on First-principles simulation was given by Dr. P. Lindan (University of Kent, Canterbury). First-principles simulation is an incisive and powerful tool in the study of matter at the atomic scale. Its key strength is that valence electrons, and therefore chemical bonds, are treated using quantum mechanics, the most fundamental and accurate theory we have. First-principles calculations are truly predictive, and they are highly prized in every field where fundamental atomistic knowledge is the currency: nowadays this means biochemistry and electronics as much as it does condensed-matter physics. However the underpinning theory and the computer codes in which it is implemented are very complicated, and using them is a highly skillful business. Instead of overloading the students with the theory the course concentrated on the practical task of getting started with real calculations. The knowledge this requires is hard to come by in books or papers, but of course the "tricks of the trade" are exactly what a new user needs most. The lectures focused on the idea of taking the new user's point of view, giving the essentials of the theory and its implementation. The hands-on sessions had students running calculations straight away, and gradually introduced the core aspects of how to test and run calculations properly. A popular feature of the course was an open forum in which students could ask any questions relevant to the subject matter and discuss the topic with other students.

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 Dr. J. Harding. The results are summarized in Appendix 3. At the time of the School, the Marie Curie Actions online assessment forms were not available.

8. The Future

The Summer School in 2005 is again planned for The University of Cardiff. Indications are that the event will be only slightly more expensive to run than the 2004 School, but the facilities are expected to be better. CCP5 has a reserved fund £7,500 to sponsor the School and Marie Curie Actions will again provide 85,000 Euros.

During 2003 the Summer School organising committee has been in discussion with Prof. Jonathan Hirst (University of Nottingham) representing the UK's Royal Society of Chemistry Theoretical Chemistry Group. This group is interested in participating in the Summer School, to help promote biomolecular simulation methods. It is probable that some accommodation of this desire within the current framework of the Summer School will be agreed, which will strengthen the advanced course on biosimulation given by X. Daura and provide additional assistance in 2005.

9. Gallery

The Summer School 2004 group photograph

Lars Meinhold receiving the award for best student lecturer

Emilia Owczarek receiving the award for best poster

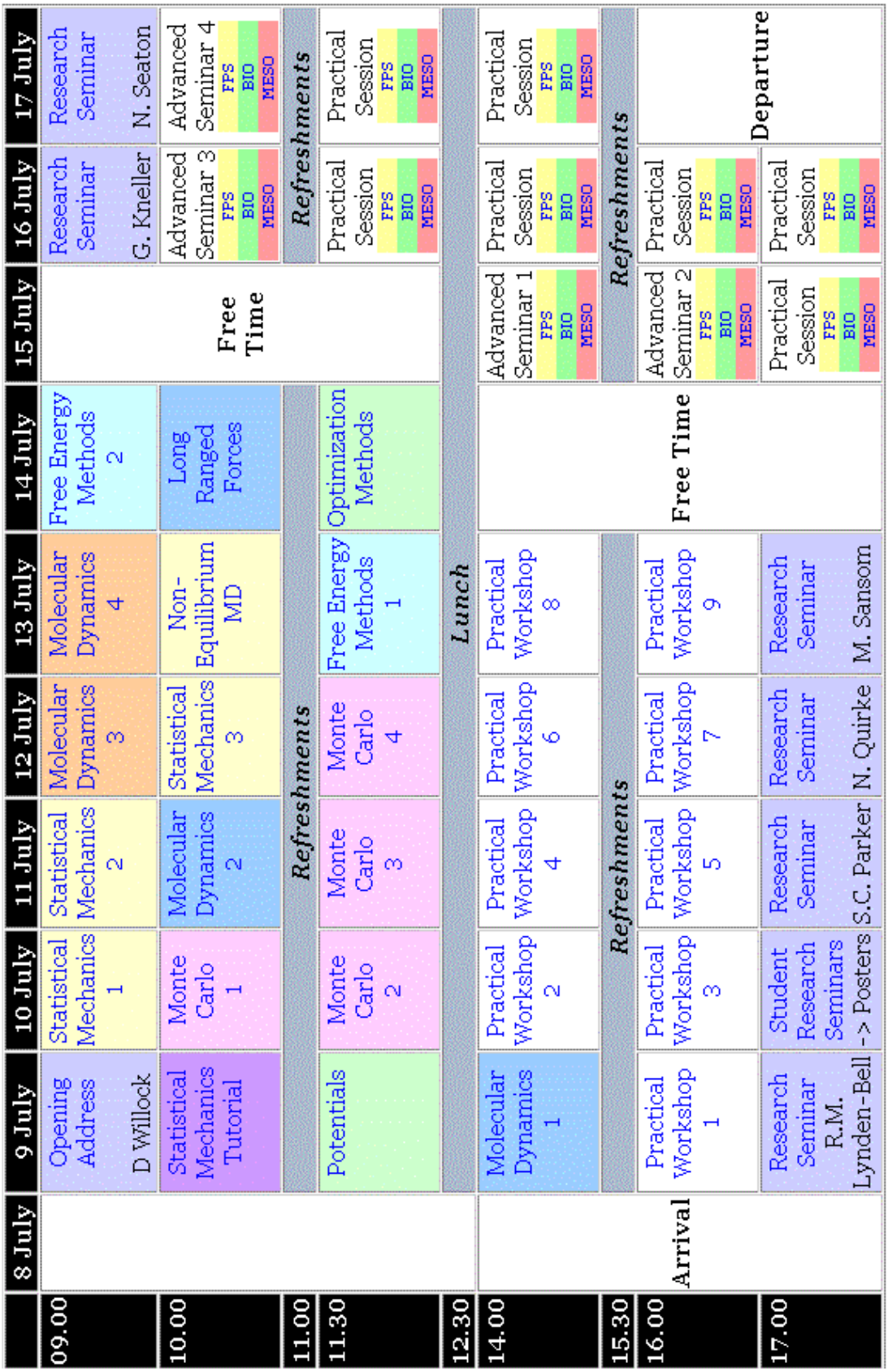
At the Lectures!

Appendix 1: Student Participants

Mr	Jeffery	Ludwig	American	University of Delaware
Ms	Yolanda	Small	American	Penn State University
Ms	Christina	Smith	American	Vanderbilt University
Mr	John	Holyoake	British	University of Oxford
Mr	Graham	McNeil-Watson	British	University of Bath
Mr	Chris	Hobbs	British	Kings College London
Ms	Elizabeth	Wallace	British	University of Leeds
Mr	Daniel	West	British	University of Leeds
Ms	Rebecca	Notman	British	Kings College London
Mr	Simon	Houlding	British	UMIST
Mr	Laurence	Ellison	British	Sheffield Hallam University
Mr	Geoffrey	Costello	British	Heriot-Watt University
Mr	Benjamin	Curley	British	University of Birmingham
Mr	Paul	Martin	British	University of Bath
Mr	Hugh	Docherty	British	Imperial College
Mr	Robert	Hawtin	British	University of Warwick
Mr	Thomas	Trevethan	British	Kings College London
Ms	Sarah	Williams	British	University of Southampton
Mr	Samuel	Edgecombe	British	Lund University
Mr	Kafui	Tay	British	Imperial College
Mr	Shen	Lei	Chinese	Chinese University of Hong Kong
Ms	Qiong	Cai	Chinese	University of Edinburgh
Mr	Fujun	Gou	Chinese	The FOM Institute for Plasma Physics 'Rijnhuizen'
Ms	Ru-Zhen	Li	Chinese	Queen Mary University of London
Mrs	Olga Natalia	Bedoya Martinez	Columbian	CSIC
Mr	Carlos	Pinilla Castellanos	Columbian	Queens University Belfast
Mr	Bart	Vorselaars	Dutch	Eindhoven University of Technology
Mr	Tim	Mulder	Dutch	Eindhoven University of Technology
Ms	Laura	Huijbregts	Dutch	Technical University of Eindhoven
Mr	Thomas	Kaevand	Estonian	Tallinn University of Technology
Ms	Virginie	Hugouvieux	French	Institut Laue-Langevin
Mr	Thomas Julien	Roussel	French	University of Marseille
Mr	Fabien	Fontaine	French	Institut Laue-Langevin
Mr	Lars	Meinhold	German	University of Heidelberg
Mr	Frank	Noé	German	University of Heidelberg
Mr	Abhijit	Chatterjee	Indian	University of Delaware

Mr	Sandip	Paul	Indian	Indian Institute of Technology
Mr	Sanket	Mahajan	Indian	Purdue University
Mr	Yevgeny	Moskovitz	Israel	Israel Institute of Technology
Mr	Antonio	Torrisi	Italian	The Royal Institution of Great Britain
Mr	Alessandro	Patti	Italian	University Rovira i Virgili of Tarragona (URV)
Mr	Sergio	Tosoni	Italian	University of Turin
Mr	Dino	Spagnoli	Italian	University of Bath
Ms	Andrea	Correa	Italian	University of Salerno
Mr	Takayuki	Miyoshi	Japanese	Imperial College
Mr	Sani	Salisu	Nigerian	
Ms	Emilia	Owczarek	Polish	Technical University of Lodz
Mr	Carlos Henrique	Correia Braga	Portuguese	University of Sheffield
Ms	Silvia	Estácio	Portuguese	Universidade de Lisboa
Mr	Nelson	Fonseca	Portuguese	University of Aveiro
Mr	Paulo	Couto	Portuguese	Universidade de Lisboa
Mr	Stanislav	Savvin	Russian	Moscow State University
Mr	Eddie	Rossinsky	Russian	Israel Institute of Technology
Ms	Zuzana	Skrinarova	Slovak	Slovak Academy Of Sciences
Mr	Santiago	Estaban Martin	Spanish	University of Valencia
Mr	Javier	Pérez	Spanish	University Rovira i Virgili of Tarragona (URV)
Mr	Alan Christy	Arokiam	Sri Lankan	University of Liverpool
Mr	Roman	Affentranger	Swiss	Swiss Federal Institute of Technology Zurich (ETH)
Mr	Kanit	Tapasa	Thai	University of Liverpool
Ms	Maria Carolina	Dos Ramos Goncalves	Venezuelan	Universidad de Huelva

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		Opening Address D Willock	Statistical Mechanics 1	Statistical Mechanics 2	Molecular Dynamics 3	Molecular Dynamics 4	Free Energy Methods 2	Free Time	Research Seminar G. Kneller	Research Seminar N. Seaton
10.00		Statistical Mechanics Tutorial	Monte Carlo 1	Molecular Dynamics 2	Statistical Mechanics 3	Non-Equilibrium MD	Long Ranged Forces		Advanced Seminar 3 FPS BIO MESO	Advanced Seminar 4 FPS BIO MESO
11.00		*Refreshments*							*Refreshments*	
11.30		Potentials	Monte Carlo 2	Monte Carlo 3	Monte Carlo 4	Free Energy Methods 1	Optimization Methods		Practical Session FPS BIO MESO	Practical Session FPS BIO MESO
12.30		*Lunch*								
14.00		Molecular Dynamics 1	Practical Workshop 2	Practical Workshop 4	Practical Workshop 6	Practical Workshop 8	Free Time	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 1	Practical Workshop 3	Practical Workshop 5	Practical Workshop 7	Practical Workshop 9		Advanced Seminar 2 FPS BIO MESO	Practical Session FPS BIO MESO	Departure
17.00		Research Seminar R.M. Lynden-Bell	Student Research Seminars -> Posters	Research Seminar S.C. Parker	Research Seminar N. Quirke	Research Seminar M. Sansom		Practical Session FPS BIO MESO	Practical Session FPS BIO MESO	

Appendix 3: Results of 2004Course Assessment by Students

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

On the main lectures (averaged over the lecturers)

Were the aims of the lecturer clear?	1.62	
Were the lectures clearly presented?	1.51	
How good was the use of visual aids	1.28	
Were the lectures well organised?	1.55	
How interesting were the lectures?	1.32	
Was the lecturer prepared to take questions?	1.83	
How helpful were the notes?	1.28	
Overall score	1.48	(43 replies)

Workshops (basic course)

Were the notes clear and helpful?	0.99
Were the demonstrators available and helpful?	1.09
Did the exercises help you understand the course material?	0.75

Averages of these questions for individual days	
9 July	0.61
10 July	0.62
11 July	0.61
12 July	0.62
13 July	0.54

Overall average for exercises	0.94
Was there too little (-2) or too much (+2) material	0.93
Were the exercises too easy (-2) or too hard (+2)	0.55

First principles lectures

Were the aims of the lecturer clear?	1.56	
Were the lectures clearly presented?	1.59	
How good was the use of visual aids	1.31	
Were the lectures well organised?	1.31	
How interesting were the lectures?	1.55	
Was the lecturer prepared to take questions?	1.69	
How helpful were the notes?	0.91	
Overall score	1.42	(16 replies)

First principles workshops

Were the notes clear and helpful?	0.85
Were the demonstrators available and helpful?	1.31
Did the exercises help you understand the course material?	1.24
Overall average for exercises	1.13
Was there too little (-2) or too much (+2) material?	0.75
Were the exercises too easy (-2) or too hard (+2)?	1.44

Mesoscale lectures

Were the aims of the lecturer clear?	0.29
Were the lectures clearly presented?	0.57
How good was the use of visual aids	1.00
Were the lectures well organised?	0.14
How interesting were the lectures?	1.14
Was the lecturer prepared to take questions?	1.00
How helpful were the notes?	0.07
Overall score	0.62 (7 replies)

Mesoscale workshops

Were the notes clear and helpful?	0.57
Were the demonstrators available and helpful?	1.61
Did the exercises help you understand the course material?	1.14
Overall average for exercises	1.11
Was there too little (-2) or too much (+2) material?	0.10
Were the exercises too easy (-2) or too hard (+2)?	0.76

Biosimulations lectures

Were the aims of the lecturer clear?	2.00
Were the lectures clearly presented?	1.50
How good was the use of visual aids ?	0.75
Were the lectures well organised?	1.75
How interesting were the lectures?	2.00
Was the lecturer prepared to take questions?	1.75
How helpful were the notes?	1.50
Overall score	1.61 (4 replies)

Biosimulations workshops

Were the notes clear and helpful?	1.22
Were the demonstrators available and helpful?	1.11
Did the exercises help you understand the course material?	0.75
Overall average for exercises	1.03
Was there too little (-2) or too much (+2) material?	0.00

Were the exercises too easy (-2) or too hard (+2)? 0.00

Student Comments

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

1. Basic Course

- Overall a very informative, stimulating and enjoyable course. Its great strength is that it is very up-to-date and points out the areas that you need to be clued up on to make progress with PhD projects. However I think that it could be improved upon in two aspects: (i) Many of the lectures were just too heavy on equations and it was very easy to lose the thread - more use of pictures and simpler verbal explanations would have been useful. (ii) In the computer exercises it would have been useful if the procedures for getting set up were spelled out more clearly and had been tested before the course began. I would add that the organisers were helpful and patient in dealing with our problems with the exercises. Thanks very much and good luck with future summer schools.
- It is very difficult to follow derivations on slides and listen to the explanation at the same time. We could always go and read a book. I'd prefer to have examples at simulation using the particular theory or equations. It would have been beneficial for us to listen to the advantages of using particular methods in real life and also it'd be good to listen to what is wrong thngs to do.
- I liked the workshop - there was a flavour of different aspects of molecular simulation. So many of these were new for me and the workshop gave me a chance top get exposed to these aspects.
- Great course! Page numbering in the lecture notes would help a lot when referencing.
- The content of the talks was excellent. Some times should be better if the number of equations per slide could be reduced. And I think some extra exercise for home about the mathematical part will be useful.
- A good course.
- Add more practical examples. The less theory, the better.
- I'd prefer some lectures to concentrate on concepts than the full set of equations. Overall a nice summer school. Thanks.
- Some lectures too many equations!! It's more important to get across the ideas; some people got totally lost in the introductory lectures because of all the equations.
- Slow network made editing in CygWin difficult. Too much to do in workshops. One targetted exercise spanning two hours would be better.
- The book given for notes would be better with page numbers.
- It would be helpful if, when questions are posed in regards to practical session material, an answer or reference to an answer also be provided. At the very least provide hints to what conclusions should be reasonably drawn.
- Practical bugs, network slow, small frustrating problems.
- Overall I found the lectures enjoyable. the practicals however I thought were not well set up at all. It would have been nice if the exercises had been worked through by the organisers first. There were serious problems with windows/linux compatibility of software. Also, on the entry form for the summer school it said fortran and c languages would be catered for - the only c I saw was at Cardiff Bay.
- I don't like being a guinea pig!!!
- It would have been helpful if the computers were set up properly before the practical workshops. However overall the course has been useful.
- The exercise time was not long enough to finish all the practicals. If the free time can be in the middle of the summer school, let's say one day earlier, it will be wonderful. It will be nice if a list of all the students' e-mail addresses, subjects etc can be provided. Besides all the above, the summer school is really good and fruitful. I do enjoy it very much! Thank you very much!!
- For someone who has never used Monte Carlo I felt that the lecturer introduced it very well and made it a very approachable part of the course. Cardiff is a very good place to hold this type of course.

- Computer facilities were a big problem. Consider using Exceed/X-term to a real UNIX machine in future. General experience was very good.
- Very good job. I just wonder if lectures devoted to very formal algebras are really useful! Food was really not bad and this is outstanding for the UK. In my opinion, workshops which ask to deeply modify the existing codes are hardly doable.
- Too many informations in too few time both in the lectures and in the practical workshop. Almost all of the lectures gave good general ideas about the problems and the purposes but more visual aids and explanation of Physical meanings could give clearer ideas. Impossible to follow and understand the majority of the equations in such short time. Only the essential equations would be better.
- There are too many equations and formulae during the lectures.
- The exercises were really interesting and helpful. Despite being sometimes tricky, they have covered all the topics presented during the lectures. They made me change my point of view on many things in the field of molecular simulations. Very exciting school, thank you!

2. Mesoscopic Simulation

- I got the impression that the lecturer didn't want me to be at CCP5.
- It would be nice to have lecture notes (at least the electronic version) available for the other advanced courses. The lectures (seminars) for the advanced courses shouldn't be held at the same time so that people have the option to opt for going to more than one advanced seminar rather than to one kind of seminar and its practical sessions.

3. Biosimulation

- I thought that the entire course (beg. and adv.) was very good. I would request for the future a "pitfalls" seminar or practical to be included to provide examples of real (student submitted) cases of error and how they were worked out. Well done the organisers at the conference! One more suggestion is to have lectures with a lot of equations done on the board, handwritten.

4. First Principles Simulation

- It was very informative, both for people without any knowledge on the subject and for those with some experience.
- The open discussion was very useful as it allowed us to gain further information that was of interest, as well as clarifying our understanding of the material.
- More details in the notes (of the lectures), maybe.
- I think the discussion in the last lecture was very useful in allowing students to clear up questions regarding the material. I would have liked to have another lecture in the place of a practical session on the 16^{th}, however.
- No comments. I think the topic was clear but sometimes should better know some topics about of unix use before the course started.
- CASTEP is a little advanced, why not use GAUSSIAN for illustrative purposes.
- The lecturer was good. I liked his approach to go from the basics.
- The open questionnaire (session?) on the last day was useful.
- The open session was a great idea. Why not preparing some more pre-organised tutorials with CASTEP (on MD, for instance)?