Report on the Methods in Molecular Simulation Summer School 2006

1. Organizers

The Methods in Molecular Simulation Summer School 2006 was held at Cardiff University from 17-25 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. Camp, P.M. Rodger 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 also the host for the 2004 and 2005 Schools and the facilities there were found to be excellent. Cardiff also offered inexpensive accommodation close to the School. All students were residential and paid a participation fee of £75.

The main lectures of the School took place in the main Chemistry Lecture Theatre of the Chemistry Department and the advanced courses were divided between this theatre and two smaller lecture rooms, all of which offered projection facilities and on-line access. The computer exercises took place in the Main Library on the first floor of the Main Building, where there were sufficient places for 40 students working independently and the nearby computer laboratory of the Geology Department, which had room for 20 more. The computing equipment consisted of desktop personal computers for the basic course and a multiprocessor platform (`Helix'), which was available for the advanced courses.

3. Participation

We received 127 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 25 countries: 47 were from Europe and 13 from elsewhere in the world. Of the European students, 7 were from the host nation (UK), 35 from other EU countries, 3 from EU candidate countries and 2 from non-EU countries. A full list of participants, their nationalities and home institutions, is presented in Appendix 1.

33 of our 127 applicants (26%) were female. In our final selection 27 were chosen to participate, thus 45% 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 (which in previous years had to be paid for by the students). A registration fee of £75 was charged to the students. The host institution provided the use of the main building, lecture theatres and most of the computing equipment at no 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 Cardiff University. The students were located in Senghennydd Hall. The hall was within 5 minutes walking distance of the Chemistry Department. 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 2005 and the student responses were taken into account, as far as was practical, in 2006.

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. D. Willock
- (2) Statistical mechanics. W. Smith
- (2) Basic molecular dynamics. K. Travis
- (2) Advanced molecular dynamics. M.P. Rodger.
- (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.

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 the CygWin unix emulator (from RedHat), which provided a unix-like environment (resembling the Bourne shell) with associated C- and Fortran 77 compilers. The G95 Fortran compiler from GNU was the compiler of choice. 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.

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:

- **J. Elliott** (University of Cambridge): *Applications of DL_POLY and discrete particle dynamics methods to mesoscale systems.*

- **Ross Brown** (University of Pau): *Investigation of "matrix" effects on molecular electronic transitions with classical molecular dynamics.*

- **A. Laaksonen** (University of Stockholm): *Solvating, manipulating, damaging and repairing DNA in a computer.*

- **P.L.A. Popelier** (University of Manchester): *Quantum chemical topology: A new shot at the design of potential energy functions.*

- **E.S. Marcos** (University of Seville): *Computer simulations of transition metal ions in solution.*

- **D. Duffy** (University of London): Including the effects of electronic losses in molecular dynamics.

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

- **Daniele Coslovich** (University of Trieste): *Dynamical heterogeneities and localized saddles in supercooled Lennard-Jones mixtures.*

- **David de Sancho** (University of Madrid): *A study of protein folding potentials with genetic algorithms.*

- **Matthew Farrow** (University of York): *Shock Wave Simulations using Molecular Dynamics.*

- **Taslima Akter** (University College Dublin): *Kinetic Monte Carlo simulation of the nano-layer deposition of amorphous silica films on a flat substrate.*

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 **Danielle Coslovich** (University of Trieste), for best short seminar, and **Veera Krasnenko** (University of Tartu), 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 (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

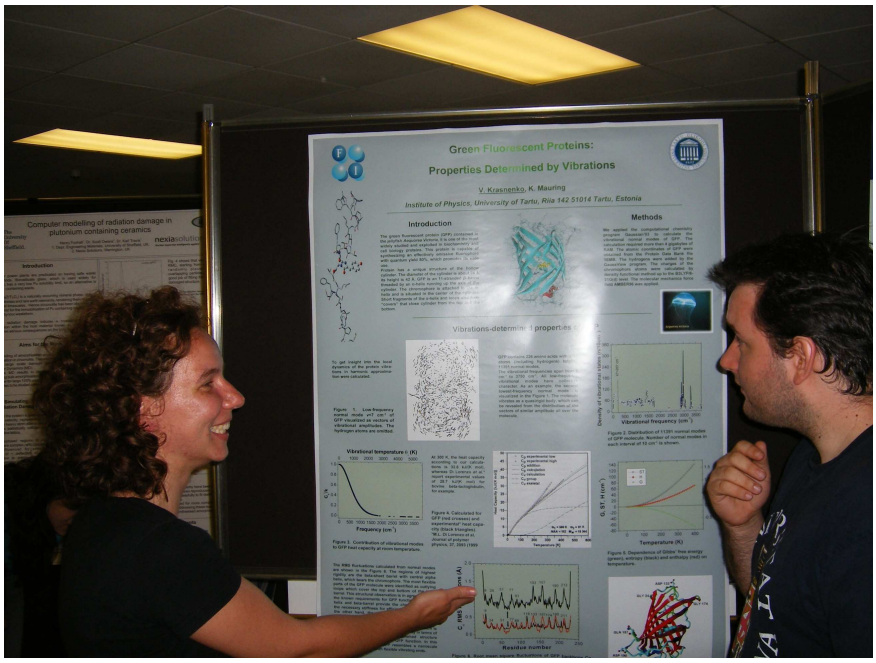
To assess the quality of the School, each student was asked to complete a questionnaire inviting their response to various specific and general aspects of the School. The analysis of the survey was conducted by Dr. J. Harding. The results are summarized in Appendix 3. Students were also directed to the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

8. The Future

The Summer School in 2007 is planned for The University of Sheffield. CCP5 has a reserved fund £7,500 to sponsor the School and Marie Curie Actions will again provide 85,000 Euros.

9. Gallery

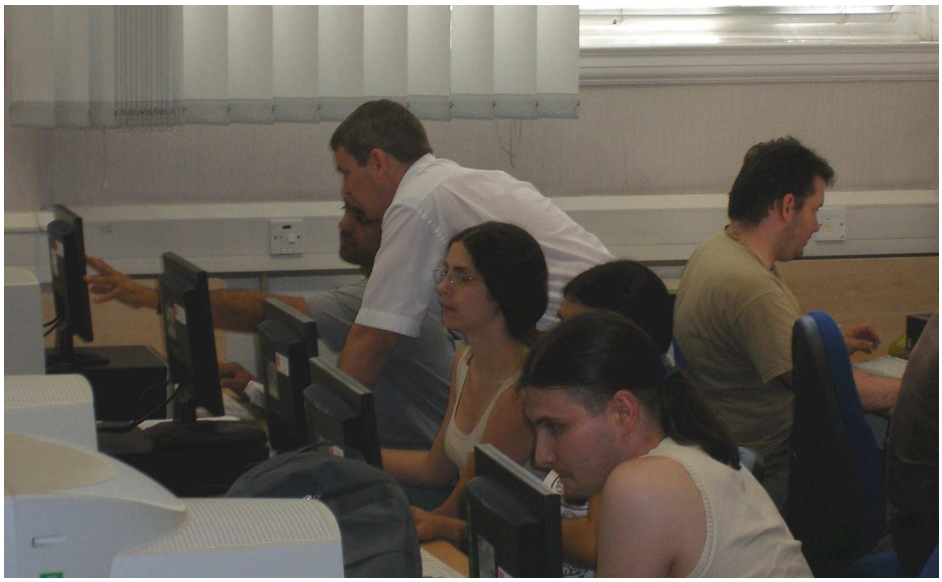
The Summer School 2006 group photograph



At the poster session

Danielle Coslovich receiving the award for best student lecturer

Veera Krasnenko receiving the award for best poster



At the computing workshop

Prof. A. Laaksonen, Plenary Speaker

Appendix 1. Attendance List

Title	Forename	Surname	University	Nationality
Mr	Moritz	Winger	Informatikgestützte Chemie (IGC)	Austrian
Ms	Taslima	Akter	University College Dublin	Bangladeshi
Mr	Mikhail	Yakutovich	Sheffield Hallam University	Belarus
Mr	Giovanni	Bonny	Ghent University	Belgian
Ms	Daniela F.	Botelho	UFSCar (Federal University of São Carlos, Brazil)	Brazilian
Ms	Luana	Pedroza	Universida de São Paulo	Brazilian
Ms	Jennifer	Brookes	University College London	British
Mr	Colin Stewart	Browne	University of Reading	British
Mr	Malek	Deifallah	The Royal Institution of Great Britain	British
Ms	Clare-Louise	Evans	University of Nottingham	British
Mr	Matthew	Farrow	University of York	British
Mr	Henry Robert	Foxhall	University Of Sheffield	British
Mr	Thomas Fraser	Headen	University College London	British
Mr	Christopher	Howard	University of Reading	British
Mr	James	Landon	Cardiff University	British
Ms	Emily Margaret	Michie	Imperial College London	British
Ms	Felicity	Mitchell	University of Manchester	British
Mr	Paul	O'Brien	University of Warwick	British
Ms	Amanda	Page	University of Surrey	British
Mr	Michael	Pounds	University of Edinburgh	British
Mr	Kashif	Sadiq	University College London	British
Ms	Mary-Ann	Thyveettil	University College London	British
Ms	Nadia	Vahdati	University of Southampton	British

Mr	Bibo	Jiang	University of Warwick	Chinese
Ms	Hui	Lei	Queen Mary, University of London	Chinese
Mr	Qiantao	Wang	University of Manchester	Chinese
Mrs	Zrinka	Gattin	Informatikgestützte Chemie (IGC)	Croatian
Ms	Lovorka	Peric	Informatikgestützte Chemie (IGC)	Croatian
Ms	Larisa	Zoranic	University Pierre and Marie Curie	Croatian
Mr	Marc	van Dijk	Utrecht University	Dutch
Mr	Aleksei	Kuznetsov	University of Tartu	Estonian
Ms	Veera	Krasnenko	University of Tartu	Estonian
Ms	Magali	Duvail	Université d'Evry	French
Mr	Mickael Nicolas	Krzeminski	University of Utrecht	French
Mr	Benoit	Mangili	Cranfield University	French
Mr	Gregory	Marque	University of Savoie (France)	French
Mr	Najib	Ouja	University of Warwick	French
Mr	Thomas	Vilmin	Ecole Superieure de Physique et de Chimie Industrielles	French
Mr	Georg	Ganzenmueller	University of Edinburgh	German
Mr	Serdal	Karakurt	University of York	German
Ms	Maria Magdalena	Reif	Swiss Federal Institute of Technology Zurich	German
Ms	Sarah	Ricker	Technical University of Kaiserslautern	German
Mr	Thomas	Splettstoesser	University of Heidelberg	German
Mr	Giorgos	Kritikos	University of Patras	Greek
Ms	Emmanouil	Symianakis	University of Patras	Greek
Mr	Sanket Avinash	Deshmukh	University College Dublin	Indian
Mr	Yashodhan	Gokhale	Otto-von-Guericke-Universität Magdeburg, Germany	Indian
Mr	Amit	Kumar	University of Heidelberg	Indian
Ms	Elisabeth Catherina	Widjajakusuma	Johann Wolfgang Goethe University	Indonesian
Ms	Yasman	Moghaddam	University of Reading	Iranian
Mr	Martin	Burke	Imperial College London	Irish
Mr	Greg	Gannon	Tyndall National Institute	Irish
Mr	John	Moloney	University College Dublin	Irish
Mr	Paolo	Calligari	Institut Laue Langevin	Italian
Ms	Marta	Corno	Universita di Torino	Italian
Ms	Daniele	Coslovich	University of Trieste	Italian
Mr	Paolo	Elvati	ETH Zurich	Italian
Ms	Simona	Giudice	University of Salerno	Italian
Mr	Julius	Ojwang	Technical University of Eindhoven	Kenyan
Mr	Igor	Stepanov	University of Nottingham	Latvian
Mr	Pedro	Fong	University of Manchester	Portuguese
Ms	Alexandra	Marques	Faculdade de Ciências da Universidade do Porto	Portuguese
Ms	Irina	Moreira	Faculdade de Ciências da Universidade do Porto	Portuguese
Ms	Emilia	Tang	University College London	Portuguese
Mr	David	De Sancho		Spanish
Mr	Aitor	Elizondo	Technical University Kaiserslautern	Spanish
Mr	Francisco	Rodriguez Ropero	Universitat Politècnica de Catalunya	Spanish
Mr	Thomas Jakob	Mueller	Technical University Darmstadt	Swiss
Ms	Ozlem	Altunordu	Zonguldak Karaelmas University	Turkish
Mr	Dmitry	Lupyan	Mount Sinai School of Medicine	USA

Appendix 2. The CourseTimetable

	16 July	17 July	18 July	19 July	20 July	21 July	22 July	23 July	24 July	25 July
09.00		Statistical Mechanics Tutorial	Molecular Dynamics 1	Molecular Dynamics 2	Molecular Dynamics 3	Molecular Dynamics 4	Molecular Dynamics 5		Research Seminar ES Marcos	Research Seminar D Duffy
10.00		Potentials	Monte Carlo 1	Monte Carlo 2	Monte Carlo 3	Monte Carlo 4	Long Ranged Forces	**Free Time**	Advanced Seminar 3 FPS BIO MESO	Advanced Seminar 4 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 J Elliott	Student Research Seminars -> Posters	Research Seminar R Brown	Research Seminar A Laaksonen	Research Seminar PLA Popelier		Practical Session FPS BIO MESO	Practical Session FPS BIO MESO	**Departure**

Appendix 3: Results of 2006 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): 78% overall response	
Were the aims of the lecturer clear?	1.29
Were the lectures clearly presented?	1.11
How good was the use of visual aids	1.08
Were the lectures well organised?	1.18
How interesting were the lectures?	1.14
Was the lecturer prepared to take questions?	1.42
How helpful were the notes?	0.93
Overall score	**1.16**
Workshops (basic course)	
Were the notes clear and helpful?	1.25
Were the demonstrators available and helpful?	1.27
Did the exercises help you understand the course material?	0.91
Averages of these questions for individual days	
17 July	1.25
18 July	1.15
19 July	1.30
20 July	1.07
21 July	0.96
Overall average for exercises	**1.14**
Was there too little (-2) or too much (+2) material	1.03
Were the exercises too easy (-2) or too hard (+2)	0.36
First principles lectures: 11 replies	
Were the aims of the lecturer clear?	1.45
Were the lectures clearly presented?	1.72
How good was the use of visual aids	0.54
Were the lectures well organised?	1.09
How interesting were the lectures?	0.82
Was the lecturer prepared to take questions?	1.63
How helpful were the notes?	0.55
Overall score	**1.11**
First principles workshops	
Were the notes clear and helpful?	-0.12
Were the demonstrators available and helpful?	1.06

Did the exercises help you understand the course material?	0.18
Overall average for exercises	**0.37**
Was there too little (-2) or too much (+2) material?	0.61
Were the exercises too easy (-2) or too hard (+2)?	0.21
Mesoscale lectures: 5 replies	
Were the aims of the lecturer clear?	1.60
Were the lectures clearly presented?	1.20
How good was the use of visual aids	1.60
Were the lectures well organised?	1.20
How interesting were the lectures?	1.00
Was the lecturer prepared to take questions?	2.00
How helpful were the notes?	1.2
Overall score	**1.40**
Mesoscale workshops	
Were the notes clear and helpful?	0.73
Were the demonstrators available and helpful?	1.07
Did the exercises help you understand the course material?	0.67
Overall average for exercises	**0.82**
Was there too little (-2) or too much (+2) material?	0.33
Were the exercises too easy (-2) or too hard (+2)?	0.47
Biosimulation lectures: 20 replies	
Were the aims of the lecturer clear?	1.80
Were the lectures clearly presented?	1.45
How good was the use of visual aids	1.25
Were the lectures well organised?	1.40
How interesting were the lectures?	1.30
Was the lecturer prepared to take questions?	1.50
How helpful were the notes?	1.30
Overall score	**1.43**
Biosimulation workshops	
Were the notes clear and helpful?	1.45
Were the demonstrators available and helpful?	1.45
Did the exercises help you understand the course material?	0.90
Overall average for exercises	**1.27**
Was there too little (-2) or too much (+2) material?	0.53
Were the exercises too easy (-2) or too hard (+2)?	0.13

Appendix 4: Student Comments

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

Basic Course

- Overall worshop arrangement is nice
- Good organised, and I enjoyed all these days very much! Thanks!
- Excellent, I enjoy it very much. Well organised. Thanks.
- Lectures are nice and helpful but need little bit more introduction to get familiar with the topics
- Most lecturers tried to fit in far too much material in the time slot. In some lectures no time to digest information, passed very quickly over complex information e.g. equations with no explanation of terms. Voice projection tools could have been used for lecturers with quieter voice (eg Prof Smith)
- Very interesting and nice Summer School. Lectures were quite clear. However, too much based on physics (not enough biology or chemistry). Practical works were very long (Time to integrate new notions and exercises), but very useful. Thank you
- In general I'm very pleased with the course both the information and content. However, I was missing a sort of general introduction lecture on the first day that defines the framework (gives an overview) of the course to get everyone on the same starting level. Or gives an overview ov molecular simulation.
- A common mistake of the majority of the lecturers was trying to fit too much into the lectures. Also the computer practicals contained too much work. It would be more helpful and efficient if there was less "Less is More". Also more free time is needed to relax and absorb
- Less is more. Karl Travis convered too much material. Scrap Saturday, Sunday,. move to the following week. Mark Rodger could have produced and handed out notes that related to his lecture. I felt that the practicals were too ambitious so I had a sense of failure at the end of most of them. The group is large and diverse., maybe too much to lecture to them efficiently. Nothing was done to remedy the hot and humid conditions in the main lecture room.
- There should be greater emphasis on the physical problem during the lectures and less to the explanation of the equation that leads to its solution.
- I think it would be better to have practicals the day after the lectures they're related to… just to let students "prepare" the background.
- Helpful to start lecture with short repetition/summary of the previous lecture. Notes of Prof. Anwar very helpful. Often too much practical exercises.
- This summer school was good in the sense that lot of information was given. The practical sessions contained too much work for a given session
- I think in general that there was too much to do in the practicals. This induced a mechanical progression through the exercises and as there was significant copying and pasting and compiling etc, most time was spent in these aspects. This could be improved by fewer tasks and less copying everything in the tasks and more concentration on analysis.
- Exercises were mere executing a series of orders (hard work) than thinking about what I was doing. To go through the exercises in a given time you had to hurry. All the statements "look at the code and understand what it is doing" were skipped for the sake of time. Should force people to think by hiding the unfinished code.
- I think that the practicals could benefit from being a little more "hands on" (actually writing code rather than just running it)

- The course was good and useful but first lectures were more theoretical than practical. Lectures should cover more than just particle simulations (for example using MD or Monte Carlo for molecular structure prediction (proteins and polymers) or diffusion of large molecules in solution. The targets of exercises should be made clearer. Even so, they were useful for understanding the lectures. All lecturers were good. Thankyou
- I didn't have enough tome even to start Thursday's and Friday's exercises. I think that it would be a good idea to provide the students with a CD with the website html code, in order to comfortably finish the exercises back home. Besides, everything has been perfectly taken care of. Thanks very much for that.
- The best lecturers were undoubtedly those that regularly reviewed what they were doing or had done and repeated new concepts/ideas that they introduced.
- A really great course in general. It may be slightly masochistic, but it would probably be better to cover statistical mechanics completely before dealing with MD and MC.
- I think the contents of the workshop should be organised in a different way. Perhaps it would be better if you started with a lecture covering the basic aspects of molecular simulation, making reference to the more "difficult" topics that would be covered in the next lectures. So I suggest that, instead of starting with statistical mechanics perhaps you should start with the methods. The importance of a starting lecture covering basic aspects is because it could make a link between the different topics. Although I have given an overall negative rating to Bill Smith I think he is very nice and should continue. But he should speak more loudly and be more dynamic so people can understand statistical mechanics better. Congratulations, I think the workshop is really very good.
- The dinner at Tallybont seemed a bit pointless. What I mean to say is that we walked 20-25 minutes away from the city centre to eat food very similar to Trevithick. In relation to the course I believe it was well organised and the content was at an appropriate level (and then some… which was good) and I have taken a lot from it. I like the fact that Philip Camp provided solutions to his exercises. These should be provided for them all. Well done chaps, Thanks.
- Food could be better

Advanced course: Mesoscale modelling

- I think that the advanced courses were better if they have been given another day, because getting through the lectures was like "being in a hurry"
- Advanced course should be at least 4 days. Ian Halliday is very nice person and lecturer
- Too short, another day would be beneficial
- Possibly having codes in both FORTRAN and C would allow for faster progress in practical sessions, one could then choose. Course was a bit too short. Four hours isn't long to teach a technique.

Advanced course: First Principles Simulations.

- I'd have preferred more of the advanced course as it was the most relevant to my current studies. It would also have been nice to get a copy of the seminar slides. Thanks to David [Willock] for organising everything so smoothly
- I think that the structure of the course in general was not ideal. There is a difference between working all day and learning all day. The vast majority of us burned out too soon, The advanced course should be longer as hands on relevant to the project of the student work is far more valuable.

- Not enough time to cover theory in detail (An extra day would be v. useful). Workshop notes were not clear for a beginner or someone new to CASTEP. Also, there were problems with some of the parameters. The lecturer was most helpful during the tutorial however.
- Could have more lectures (theoretical) of the advanced courses.
- Too short
- Advanced Course would benefit from an extra day or two.
- The workshop notes are too unclear. The workshop would be more useful if the notes were rewritten to clarify what to do.
- One extra day would be OL (more time for practical sessions!!) About workshops: written notes are not enough. In my opinion, demonstrators should speak a bit about the goals and contents of the practical session at least at the start. One-to-one communication is not enough – need collective ones.

Advanced course: Biosimulations.

- In general, the length of the course is about right. But, as my work is centred around the simulation of biomolecules I would not mind another day spending more attention to this subject.
- It would have been good to have had the chance to discuss ones own research problems and discover solutions. A presentation on ensembles is needed. Printouts of seminar slides would be good. An extra day for the advanced course is a good idea.
- Another day for the course would be good
- I'm very happy with this advanced course. Great lecture and practical work. The teachers are very helpful
- One more day is needed in my opinion for understanding the advanced course
- I think that some more time is needed for the advanced course – mainly for the lectures. Maybe the scope of the lectures did not give a comprehensive view of the approaches that can be used for biomolecules. There's much more than MD that can be done
- 3 days of advanced courses was OK (Not more!) It was very nice to have the broad overview in the basic courses. It would be useful to zip the trajectory files separately so that they can be unpacked while doing the first part of the exercise.