Report on the Methods in Molecular Simulation Summer School 2005

1. Organizers

The Methods in Molecular Simulation Summer School 2005 was held at Cardiff University from 11-19 July, in the Department of Biology. 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 also the host for the 2004 School 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 £70.

The main lectures of the School took place in the Wallace Lecture Theatre of the Biology Department and the advanced courses were divided between Wallace 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 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 102 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. 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.

60 students were selected. Those not successful were directed to a course run by the Royal Society of Chemistry on biological simulation. Their names were also supplied to Prof. Berend Smit, director of our supporting Marie Curie project for possible reallocation to related schools. Those attending originated from 26 countries: 15 were from the United Kingdom, 29 from other parts of the EC, 3 from EC candidate countries and 13 from outside Europe. In all 44 students were citizens of the EC and 16 were from third countries. A full list of participants, their nationalities and home institutions, is presented in Appendix 1.

Only 21 of our 102 applicants (21%) were female, which made it impossible to satisfy the 40% female participation suggested by Marie Curie Actions. However the 12 females (20%) 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). A registration fee of £70 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 students were located in Column Hall (where breakfast and evening meals were provided for all the School participants). The hall was within 5 minutes walking distance of the Chemistry Department. Plenary Lecturers were located in local hotels, near the university. Lunch was provided for all participants in the main building.

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 previous summer school (2004) and also we took into account the student responses as far as was practical.

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
- (2) 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
- (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 of actual computational work. In a departure from previous years, two afternoons were devoted to `mini-projects' in which students were required to conduct realistic research on chosen topics. The two areas of work were: the diffusion of methane in a zeolite cage (Willock); and the internal dynamics of double walled nanotubes (Smith). 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. The G95 Fortran compiler from GNU was ported by K. Refson. 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. A new feature tried out this year was a `BlackBoardi' website, which was used by 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 plenary lectures were:

- D Brown , Université de Savoie, "Molecular Modelling of Polymer Based Systems".
- M. Wilson, University of London, "Construction and Application of 'Extended' Ionic Models".
- A. Alavi, University of Cambridge, "Adventures with Fermion Quantum Monte Carlo".
- P.V. Coveney, University of London, "Scientific Grid Computing".
- M. Sprik, University of Cambridge, "Car-Parrinello Simulation of Redox Reactions in Solution".
- J.D. Hirst, University of Nottingham, "Biomolecular Simulation: from Folding to Function".

Students responded with a high degree of interest in these lectures and asked many questions of the speakers. It is also pleasing to report the strong support given by plenary speakers to the continued functioning of the School.

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

- Tomohiro Sato, Kansai University, "Molecular Dynamics Observation of Phase Transformation in Ni-Ti Alloy".
- Ioannis Skarmoutsos, University of Athens, "MD Simulation of cis-trans N-Methylformamide (NMF) liquid mixture. Structure and Dynamics".
- Gareth Tribello, The Royal Institution, "A Potential Model for Ice".
- Subramanian Arun Kumar, University of Reading, "Simulation Studies of the Interaction of Bisintercalator Drug Molecules in Higher Order Quadruplex DNA".

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 **Gareth Tribello** (Royal Institution), for best short seminar, and **Emad Noorizadeh** (University of Leicester), 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 (R. Qin, Daresbury Laboratory).
- First principles simulation (K. 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. This year the course was opened to admit participants from the Royal Society of Chemistry's School on biological simulation methods (also being held at Cardiff), which was organized by J. Hirst from Nottingham, thus the two courses shared resources in a spirit of cooperation, raising the total number of participants to 37. 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. R. Qin from Daresbury Laboratory, the appointed CCP5 postdoctoral researcher on mesoscale methods, gave the advanced course on Mesoscale Simulation. The course described the current techniques applied in this area: Lattice Gas Automata, Lattice Boltzmann, Dissipative Particle Dynamics and Smoothed Particle Hydrodynamics. It also introduced the students to CCP5's DL_MESO program which is designed for mesoscale simulation research and incorporates the above mentioned methodologies.

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 2006 is again planned for The University of Cardiff. 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 2005 group photograph

Gareth Tribello receiving the award for best student lecturer

Emad Noorizadeh receiving the award for best poster

Computing Workshop

Appendix 1. Attendance List

Title	Name	Surname	Affiliation	Nationality
Mr	Ivan	Scivetti	Queen's University of Belfast	Argentina
Mr	Florian	Dorfbauer	Vienna University of Technology	Austria
Mr	Christophe	Vandekerckhove	Katholieke Universiteit Leuven	Belgian
Mr	Pieter	Van Leemput	Katholieke Universiteit Leuven	Belgian
Mr	Nicolas	Staelens	Facultés Universitaires Notre-Dame de la Paix	Belgian
Mr	John	Grime	University of Warwick	British
Mr	Graham	Macpherson	University of Strathclyde	British
Mr	Martin	Walker	University of Edinburgh	British
Mr	Edward	Jeffery	University of Cardiff	British
Mr	Stephen	O'Toole	University of Manchester	British
Mr	Jeremy	Rabone	Birkbeck College, London	British
Mr	James	Bowe	Birkbeck College, London	British
Mr	Ben	Sattelle	University of Leicester	British
Mr	Gareth	Tribello	The Royal Institution	British
Mr	Benjamin	Cossins	University of Southampton	British
Ms	Helen	Gibson	University of Bath	British
Mr	Andrew	Connelly	University of Sheffield	British
Ms	Kirsty	MacInnes	University of Southampton	British
Mr	Adam	Herring	University of Leeds	British
Mr	Phil	McCaffrey	The University of Edinburgh	British
Mr	Svetoslav	Ivanov	Bulgarian Academy of Science	Bulgarian
Ms	Shanfeng	Jiang	Delft University of Technology	Chinese
Mr	Yue	Han	University of Cambridge	Chinese
Ms	Monica Sonne	Larsen	University of Copenhagen	Danish
Mr	Jelan	Kuhn	Delft University of Technology	Dutch
Mr	Nicolas	Jardillier	Ecole Nationale Superieure de Chimie de Montpellier	French
Mr	Jérémy	Chabe	CEA Grenoble	French
Mr	François	Faure	Université de Paris Sud	French
Ms	Candy	Anquetil	Sheffield Hallam University	French
Ms	Claudia	Prosenjak	University of Edinburgh	German
Mr	Dieter	Krachtus	University of Heidelberg	German
Mr	Andreas	Biternas	University of Bristol	Greek
Mr	Alexandros	Chremos	University of Edinburgh	Greek
Mr	Ioannis	Skarmoutsos	University of Athens	Greek

Title	Name	Surname	Affiliation	Nationality
Mr	István	Kövesi	Semmelweis University	Hungarian
Ms	Sangeeta	Saini	Indian Institute of Science	Indian
Mr	Subramanian Arun	Kumar	University of Reading	Indian
Mr	Emad	Noorizadeh	University of Leicester	Iranian
Mr	Mario	Orsi	University of Southampton	Italian
Mrs	Angela	Di Lella	Université de Paris Sud	Italian
Mr	Leonardo	Lenoci	University of Edinburgh	Italian
Mr	Tomohiro	Sato	Kansai University	Japanese
Mr	David Manuel Silva	Martins	University of Edinburgh	Luso-Canadian
Mr	Gabriel Oscar	Ibañez Garcia	University of Bristol	Mexican
Mr	Nuno Manuel Ferreira de Sousa de Azevedo	Cerqueira	Universidade Porto	Portuguese
Mr	Sorin	Nita	Queen's University	Romanian
Ms	Rodica	Ghenea	Queen's University	Romanian
Mr	Urban	Borstnik	National Institute of Chemistry Slovenia	Slovenian
Mr	Pau	Cervera i Badia	Universitat de Barcelona	Spanish
Ms	Patricia María	Losada Pérez	Universidade de Vigo	Spanish
Mr	Hector	Martinez-Seara Monne	University of Barcelona	Spanish
Mrs	Isabel	Corominas i Santaulària	Universitat de Barcelona	Spanish
Mr	Vicente	Bitrián	Technical University of Catalonia	Spanish
Ms	Angeles	Pulido	Universidad Politécnica de Valencia	Spanish
Mr	Niklas	Källrot	Lund University	Swedish
Mr	David	Raymand	University of Uppsala	Swedish
Mr	Jen-Chang	Chen	National Taiwan University	Taiwanese
Mr	Chien-Cheng	Huang	Université libre de Bruxelles	Taiwanese
Mr	Aurelio José	Olivet	Institut de Ciència de Materials de Barcelona	Venezuelan

Appendix 2. The CourseTimetable

	10 July	11 July	12 July	13 July	14 July	15 July	16 July	17 July	18 July	19 July
09.00		Statistical Mechanics Tutorial	Monte Carlo 1	Monte Carlo 2	Molecular Dynamics 3	Molecular Dynamics 4	Optim - -ization Methods		Research Seminar M Sprik	Research Seminar J.D. Hirst
10.00		Potentials	Molecular Dynamics 1	Molecular Dynamics 2	Free Energy Methods 1	Non-Equilibrium MD	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	Monte Carlo 3	Monte Carlo 4	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 D Brown	Student Research Seminars -> Posters	Research Seminar M. Wilson	Research Seminar A Alavi	Research Seminar PV Coveney		Practical Session FPS BIO MESO	Practical Session FPS BIO MESO	

Appendix 3: Results of 2005 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): 38 replies

Were the aims of the lecturer clear?	1.51
Were the lectures clearly presented?	1.38
How good was the use of visual aids	1.24
Were the lectures well organised?	1.26
How interesting were the lectures?	1.25
Was the lecturer prepared to take questions?	1.67
How helpful were the notes?	1.39
Overall score	**1.38**

Workshops (basic course)

Were the notes clear and helpful?	1.15
Were the demonstrators available and helpful?	1.42
Did the exercises help you understand the course material?	0.83

Averages of these questions for individual days	
11 July	1.24
12 July	1.11
13 July	1.10
14 July	1.23
15 July	1.09
Overall average for exercises	**1.15**

Was there too little (-2) or too much (+2) material	0.79
Were the exercises too easy (-2) or too hard (+2)	0.12

First principles lectures: 15 replies

Were the aims of the lecturer clear?	1.53
Were the lectures clearly presented?	1.40
How good was the use of visual aids	1.00
Were the lectures well organised?	1.40
How interesting were the lectures?	1.47
Was the lecturer prepared to take questions?	1.53
How helpful were the notes?	1.40
Overall score	**1.39**

First principles workshops

Were the notes clear and helpful?	0.91
Were the demonstrators available and helpful?	1.29
Did the exercises help you understand the course material?	0.64
Overall average for exercises	**0.95**
Was there too little (-2) or too much (+2) material?	0.07
Were the exercises too easy (-2) or too hard (+2)?	-0.02

Mesoscale lectures: 5 replies

Were the aims of the lecturer clear?	1.20
Were the lectures clearly presented?	0.0
How good was the use of visual aids	0.80
Were the lectures well organised?	0.80
How interesting were the lectures?	1.20
Was the lecturer prepared to take questions?	1.40
How helpful were the notes?	0.0
Overall score	**0.77**

Mesoscale workshops

Were the notes clear and helpful?	0.87
Were the demonstrators available and helpful?	1.27
Did the exercises help you understand the course material?	0.67
Overall average for exercises	**0.93**
Was there too little (-2) or too much (+2) material?	-1.87
Were the exercises too easy (-2) or too hard (+2)?	-1.27

Biosimulation lectures: 16 replies

Were the aims of the lecturer clear?	1.12
Were the lectures clearly presented?	1.31
How good was the use of visual aids	1.31
Were the lectures well organised?	1.43
How interesting were the lectures?	1.25
Was the lecturer prepared to take questions?	1.81
How helpful were the notes?	1.50
Overall score	**1.39**

Biosimulation workshops

Were the notes clear and helpful?	1.06
Were the demonstrators available and helpful?	1.35

Did the exercises help you understand the course material?	0.71
Overall average for exercises	**1.04**

Was there too little (-2) or too much (+2) material?	-0.02
Were the exercises too easy (-2) or too hard (+2)?	-0.21

Student Comments

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

1. Basic Course

- Nice week! Thank you. But the pubs shouldn't close at 11.00 p.m.
- The summer school isorganised very well. Thank you very much.
- The lectures were good but would have benefitted from being more than "reading" through the notes in some cases (i.e. more abstract background and thought processes than explaining the equations). The exercises tended to require little thought into the theory and more into the practicalities of running the programs. Some of the exercises were, however, good illustrations of the lecture material.
- Potential fitting and hyperdynamics should provide a practical workshop.
  I felt bored and didn't catch the main points very well on the MD3, MD4, NEMD and free energy. They are very important and I'd like to learn them. Sorry! Frankly speaking I think teachers should state the physical meanings rather than the equations and should say in a simple and clear way. I enjoyed Dr Lindan's talk very much.
  I enjoy research very much. Thank you very much for hosting the school.
- I would recommend to keep all the original presentation slides in web. It will be a great work if all the lectures were video-captured and kept in the CCP5 website in MPEG or WAV format files. So that people from all over the world (including the ones who were not selected for attending the workshop) will be benefitted. Also it will be easy to refer back to the lectures or slides whenever one wants to. This strategy was proven very helpful in the "B star" bioinformatics web course. It is obvious that one can't master everything 100% in 10 days. Still I have given 100% score because I strongly feel it as the best possible work in the given situation, timescale and heterogeneous background of participants.
- The practical workshops are truly useful. I've learnt much from them that theory alone can't give me. I most enjoyed lectures with a systematic approach (JA. NW). I found KT's lectures difficult to follow (but informative) because I felt the formulas presented were not explained adequately.
- There should be a break between the first two lectures. It would be better to have a whole day off instead of two halves and maybe it should not be on a weekend?
- Very well done after all!.
- Overall the course was excellent. However, the practical workshops were frustrating and not focused. I think (my perspective) that it would be more useful for the workshops to focus on how to translate physics into code (either FORTRAN or JAVA)
- The exercises were not that helpful. Students have very different backgrounds and I would prefer to have longer exercises that you work on for linger and where I understand what I'm doing. Just changing values in a program like on the 12th doesn't help to understand. Also it would be good to have more exercises to choose from that I can more concentrate on programs that I am interested in.
- Overall the standard of teaching and organisation has been excellent. It would have helped to know in advance that FORTRAN would be the preferred language so I could have picked up the basics beforehand.
- There could have been a break between the first and second lecture especially later on in the course when the lectures got harder. I liked JH's jokes. The NEMD and free energy methods lectures were the only ones which I felt were impenetrable. The tasks on Tuesday, Wednesday and Friday: there was far too

much to try and do. Furthermore, I felt that stuff like DEMOCRITOS was too easy. It might have been worth introducing the tasks and giving suggestions as to what might be worthwhile exercises for people at different ability levels.

- The exercises were good but explanations sometimes a bit complex to follow
- School was very well organised; lecturers were very helpful. Food was good. The combination of lectures and practical sessions excellent in principle. However some motivations of some practical sessions weren't too clear to me, especially some of the DL_POLY stuff. A break between the two lectures in the morning would be good. "Information density" of this school generally too high (for me)

2. First Principles Simulation

- The lectures were very good. However, they were let down by the practical course. Often the point of what we were trying to do was not clear and it was really annoying that we had to keep resubmitting the jobs because the scripts on the Helix cluster were incorrect.
- I guess it is not possible to "teach FPS in three days, however I got a rough idea what FPS is about. At least I know how some programs [work] and [have] some refs where I can look some details up, if I was going to get more familiar with FPS.
- The practicals were too much like a CASTEP tutorial. I don't need to know how to construct an input file – it doesn't help me know about FPS. Lectures excellent on the other hand.

3. Mesoscopic Simulation

- The lecturer really tried, but unfortunately his English is rather poor. Nice guy but perhaps not fitted to teach at a summer school.
- I think that the exercises are good, but I feel that the exercises are too little. The explanations and guidelines of the practical workshop are too little. The handouts (manual) are too little and without clear explanations.

4. Biosimulations

- A very good course. Absolutely enjoyable. The theory was well linked with the practical aspects of methods discussed. Thank you very much
- As an introduction to MD, GROMOS, as was said by Xavier Daura himself, is not a straightforward program to use. Obviously the code was written for bio-simulations but a more effective program could have been used. Introductions to script writing for different purposes and using different MD programs could have been helpful.
- The workshops were too code-specific. If using other software, then they were of little use. Although they did outline the procedure well. It seems somewhat wasteful though to have 30 people all running the same jobs. But I really cannot think of any way to get around the problems.
- All good
- I hope that the blackboard and all associated web pages and work will be available after the summer school.
- I can give an "excellent" score for the overall performance. Also I take this as my personal opportunity to thank everyone behind the making of the summer school. {Whether] I understood 100% or not, I gained 100% inspiration and obtained self-development ideas to dwell deeply into computational chemistry. Thanks.
- Would have been useful to have more written notes on initial system setup. Exercises would have been much easier if I had been familiar with GROMOS. In general, the course was a good introduction to MD and some of its potential applications. It was helpful.