Report on the Methods in Molecular Simulation Summer School 2003

1. Organisers

The Methods in Molecular Simulation Summer School 2003 was held at King's College London from 7-15 July, in the Department of Pharmacy and was organised by the CCP5 Summer School Working Group, which consisted of J. Harding (Chairman), W. Smith (Secretary), J. Anwar (local organiser), K. Travis, P. Lindan and K. Refson.

2. Location

As for the 2002 School, the School was held in the Franklin-Wilkins Building in Stamford Street, close to Waterloo Station. This is a location conveniently close to some of London's most historic landmarks, including the National Theatre, St. Paul's Cathedral, the Tate Gallery, the Globe (Shakespeare) Theatre, Tower Bridge and the Tower of London. The School made full use of the facilities at the Franklin-Wilkins Building, namely the lecture rooms (with projection facilities) and the computer training room, which had places for 60 people.

3. Participation

89 applications to attend the School were received and were screened by the organisers with the purpose of giving priority to students in the first year of postdoctoral study and whose research entailed a significant amount of molecular simulation. Students were accepted from the disciplines of chemistry, physics, biology and mathematics. 60 were selected (though this was reduced to 58 by late cancellations). Those attending came from no fewer than 17 countries: 24 from the United Kingdom, 5 from the Netherlands, 3 from each of Switzerland, France, Sweden and South Africa, 2 from the USA and Japan and the remainder from other countries of Europe. A full list of participants, the nationalities of their home institutions, and their eligibility for SIMU support is presented in Appendix 1. It should be noted that many students possessed nationalities differing from that of their home institution. Residential students paid a participation fee of £370, while non-residential students paid £170.

4. Support

The Summer School received direct support from the UK's Collaborative Computational Project #5 (£7,500). The ESF Programme SIMU provided 15,000 euros as bursaries for students from member Laboratories of SIMU. The organisers express their appreciation of the support received from these organisations. There was no support or concession from the host institution, for which this was purely a contractual arrangement. All facilities used were paid for. The impact of this on services provided to the students was significant, in particular meals were not provided, though in this area of London there were many places to obtain meals at reasonable prices.

5. Accommodation

The residential students and lecturers were accommodated at the Union Jack Club, Waterloo, which is a United Kingdom Services hotel, only 5 minutes' walk from the Franklin Wilkins Building. This offered good quality accommodation at a reasonable price, with the advantage of a good location.

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 optimisation 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. Students were presented with prepared course notes beforehand. All students attended the basic course.

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) Optimisation methods. J. Harding
- (1) Potentials. J Harding
- (4) Statistical mechanics. K. Travis
- (2) Molecular dynamics. W. Smith
- (2) Advanced molecular dynamics. K. Refson.
- (3) Monte Carlo. N. Wilding
- (1) Long range forces. W. Smith
- (2) Free energy methods. J. Anwar
- (1) Programming and program design. 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 morning lectures, the afternoons were devoted to computational workshops, in which the students were required to complete exercises highlighting and sometimes extending the topics covered in the basic course. These exercises follow the

pattern of previous Schools and we are grateful to Prof. Mike Allen for allowing us to make use of some of the previous exercises. The bulk of the material was supplied by J. Harding, K. Refson and W. Smith.

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. 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 some Java programs from the DL_POLY suite (which students were permitted to take away). The use of computer graphical user interfaces and graphical methods to process data were a strong feature of the exercises.

Plenary Lectures

The plenary lectures are a traditional feature of the School and are intended to show students what may be accomplished by molecular simulation methods. This year the School was inaugurated by a lecture from Prof. C.R.A. Catlow (UC London and Royal Institution) on "What We Can Learn from Simulation". The other plenary lectures were:

- D. Sayle (Cranfield University), "Simulated Amorphisation and Recrystallisation";
- A. J. Mulholland (University of Bristol), "Modelling Enzyme Catalysed Reaction Mechanisms with Combined Quantum mechanics/Molecular Mechanics (QM/MM)";
- B. Leimkhuler (University of Leicester), "Constant and Inconstant Temperature Molecular Dynamics: New Schemes for Enhanced sampling";
- N.M. Harrision (Imperial College and Daresbury Laboratory), "Progress in Density Functional Calculations of Real Systems: Band gaps, Thermodynamics and Kinetics".
- D.W. Lewis (UC London), "Right Model, Right Method, Right Answer!"
- D.J. Tildesley (Unilever), "Industrial Applications of Molecular Simulation".

The talk by Prof. Tildesley was unfortunately cancelled on the day.

Once again this year, a plenary session was given over to short (15 min.) talks given by the students. The four talks selected this year were:

- K. Finch (University of Manchester), "Oilfield Barite Scale Formation and Inhibition";
- T. Gibbs (UC London), "Effect of Hydration Levels and Pressure on Zeolite Structure";
- S. Rahatekar (University of Cambridge), "Conductivity of Polymer Nanotube Composite Materials";
- A-J. van Dijk (University of Utrecht), "Dynamics of Amino Acid Side Chains in Proteins: Comparing with NMR Data".

The contributions of the students were complemented by a **Poster Session**, which featured a wide range of research activity.

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 (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. 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.

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. K. Refson (Rutherford Appleton Laboratory). 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 knowlege is the currency: nowadays this means biochemistry and electronics as much as

it does condensed-matter physics. The catch is that 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. In the lectures, the lecturers stuck to the idea of taking the new user's point of view, giving the essentials of the theory and its implementation. The hands-on practicals had students running calculations straight away, and gradually introduced the core aspects of how to test and run calculations properly. The approach appeared to work very well, making for an uncluttered starter course that let students see what is possible in their research field.

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.

8. The Future

The Summer School in 2004 is planned for The University of Warwick. The location is such that students will not have such easy access to food sources as was possible at King's College London, and therefore the meals will need to be included. Indications are that this will make the event more expensive to students than the King's College Schools. CCP5 has agreed to sponsor the School at £7,500, but other sources of funding are uncertain. The organising committee has joined a bid with colleagues on the continent for funding of the Schools through a Marie Curie award.

9. Gallery

The Summer School 2003 group photograph

Resident lecturer Dr Keith Refson in action

Plenary lecturer Prof. Nic Harrison

Student seminar speakers: A-J. van Dijk, S. Rahatekar, K. Finch and T. Gibbs:

Happy students working in the practical sessions

Appendix 1. The Student Participants

First Name	Surname	Country	SIMU
Lai Kwan	Lui	UK	
Katie	Finch	UK	
Christina	Forster	Austria	
Cem	Sevik	Turkey	
Ana Rita	Alves	Portugal	
Katrina	Austen	UK	
Caterina	Barillari	UK	
Brian	Barnes	USA	
Jean-Paul	Becker	France	✓
Mark	Broome	UK	
Bouke	Bunnik	Netherlands	✓
Francois	Chiaruttini	France	✓
John	Coe	UK	
Miguel Dias	Costa	Portugal	✓
Jones	de Andrade	UK	✓
Peter David	Duncan	UK	
Sebastien	Foucher	UK	
Tanya	Gibbs	UK	
Richard	Gilham	UK	
Marja-Leena	Hannila	Finland	
Tim	Heinz	Switzerland	
Carmelo	Herdes	Spain	✓
Chrétien	Hermse	The Netherlands	✓
Carl-Johan	Högberg	Sweden	✓
Zhidong	Jia	UK	✓
Peter	Kindt	Netherlands	✓
Outi	Lampela	Finland	
Jean-Marc	Leyssale	France	✓
Muhammad Sanusi	Liman	Japan	
Georgia - Evangelia	Logotheti	Greece	✓
David Joel	Michel	UK	✓
Julien	Michel	UK	
Yamato	Okano	Japan	
Pooja	Panchmatia	UK	
Evangelia	Pantatosaki	Greece	✓
Christina	Pereira	Switzerland	
Bernardino	Pereira Lo	UK	✓
Sameer	Rahatekar	UK	✓
Duncan	Riley	UK	✓

Esteban	Rodriguez Regueras	Spain	✓
Henrik	Rundgren	Sweden	✓
Misbah	Sarwar	UK	
Patric	Schyman	Sweden	✓
Gregory	Sutcliffe	UK	✓
Judy	To	UK	
Daniel	Trzesniak	Switzerland	✓
Albert	Van den Noort	Netherlands	✓
Aalt-Jan	van Dijk	Netherlands	
Pete	Watkins	UK	
Jing	Xu	Norway	✓
Konrad	Piwowarczyk	Poland	✓
Maje Jacob	Phasha	South Africa	
Regina	Maphanga	South Africa	
Richard	Chauke	South Africa	
Jan	Fischer	Germany	✓
Nawaf	Aldiwan	UK	
Carolyn	Koh	UK	
Matome	Ramusi	South Africa	

Appendix 2. The Course Timetable

	6 July	7 July	8 July	9 July	10 July	11 July	12 July	13 July	14 July	15 July
09.00		Opening Address C.R.A. Catlow	Molecular Dynamics 1	Monte Carlo 1	Advanced Monte Carlo	Molecular Dynamics 3	Molecular Dynamics 4		Research Seminar NM Harrison	Research Seminar DW Lewis
10.00		Optimisation Methods	Statistical Mechanics 1	Monte Carlo 2	Long Ranged Forces	Statistical Mechanics 3	Potentials	**Free Time**	Advanced Seminar 3 FPS BIO MESO	Advanced Seminar 4 FPS BIO MESO
11.00		***Refreshments***							***Refreshments***	
11.30		Basic Statistical Mechanics	Molecular Dynamics 2	Statistical Mechanics 2	Free Energy Methods 1	Free Energy Methods 2	Programming & Program Design		Practical Session FPS BIO MESO	Practical Session FPS BIO MESO
12.30		***Lunch***								
14.00		Practical Workshop 1	Practical Workshop 2	Practical Workshop 4	Practical Workshop 6	Practical Workshop 8		Advanced Seminar 1 FPS BIO MESO	Practical Session FPS BIO MESO	Practical Session FPS BIO MESO
15.30		***Refreshments***						***Refreshments***		
16.00	**Arrival**	Poster Session	Practical Workshop 3	Practical Workshop 5	Practical Workshop 7	Practical Workshop 9	**Free Time**	Advanced Seminar 2 FPS BIO MESO	Practical Session FPS BIO MESO	
17.00		Research Seminar D Sayle	Student Research Seminars	Research Seminar AJ Mulholland	Research Seminar B Leimkuhler	Research Seminar D Tildesley		Practical Session FPS BIO MESO	Practical Session FPS BIO MESO	**Departure**

Appendix 3: Results of 2003 Course 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?	1.29
Were the lectures clearly presented?	1.07
How good was the use of visual aids	0.92
Were the lectures well organised?	1.01
How interesting were the lectures?	1.06
Was the lecturer prepared to take questions?	1.42
How helpful were the notes?	1.84
Overall score	1.08 (51 replies)

Workshops (basic course)

Were the notes clear and helpful?	0.84
Were the demonstrators available and helpful?	1.04
Did the exercises help you understand the course material?	0.53

Averages of these questions for individual days	
Monday	0.87
Tuesday	0.83
Wednesday	0.61
Thursday	0.85
Friday	0.89

Overall average for exercises	0.81
Was there too little (-2) or too much (+2) material	1.05
Were the exercises too easy (-2) or too hard (+2)	0.08

First principles lectures

Were the aims of the lecturer clear?	1.64
Were the lectures clearly presented?	1.57
How good was the use of visual aids	1.29
Were the lectures well organised?	1.36
How interesting were the lectures?	1.75
Was the lecturer prepared to take questions?	1.79
How helpful were the notes?	1.50
Overall score	1.56 (14 replies)

First principles workshops

Were the notes clear and helpful?	1.00
Were the demonstrators available and helpful?	1.50
Did the exercises help you understand the course material?	1.25
Overall average for exercises	1.25
Was there too little (-2) or too much (+2) material?	-0.14
Were the exercises too easy (-2) or too hard (+2)?	0.04

Mesoscale lectures

Were the aims of the lecturer clear?	1.60
Were the lectures clearly presented?	1.60
How good was the use of visual aids	1.00
Were the lectures well organised?	1.40
How interesting were the lectures?	1.60
Was the lecturer prepared to take questions?	1.30
How helpful were the notes?	1.30
Overall score	1.10 (10 replies)

Mesoscale workshops

Were the notes clear and helpful?	1.00
Were the demonstrators available and helpful?	0.70
Did the exercises help you understand the course material?	0.60
Overall average for exercises	0.77
Was there too little (-2) or too much (+2) material?	0.30
Were the exercises too easy (-2) or too hard (+2)?	0.20

Biosimulations lectures

Were the aims of the lecturer clear?	1.42
Were the lectures clearly presented?	1.25
How good was the use of visual aids ?	0.83
Were the lectures well organised?	1.25
How interesting were the lectures?	0.58
Was the lecturer prepared to take questions?	1.50
How helpful were the notes?	1.17
Overall score	1.14 (12 replies)

Biosimulations workshops)

Were the notes clear and helpful?	1.13
Were the demonstrators available and helpful?	1.25
Did the exercises help you understand the course material?	0.54

Overall average for exercises	0.97
Was there too little (-2) or too much (+2) material?	0.33
Were the exercises too easy (-2) or too hard (+2)?	-0.13

Student Comments

The students were also invited to make comments on the School. Several themes emerged from these, which we summarise below.

- Some students felt the level of statistical mechanics was too high.
- There was a general feeling that there was too much material in the workshops attached to the main courses. Also there may be slightly too much in the advanced courses.
- There were problems with the computer hardware, which impacted on the practical sessions.
- The students want more emphasis on how to write algorithms rather than just running programs.
- The workshops and lectures still need to be better co-ordinated.