ESF Science Meeting

MolSim 2009

Organizers: E.J. Meijer, B. Ensing, D. Frenkel

(Activity: SimBioMa; Molecular Simulations in Biosystems and Materials Science)

Summary

MolSim2009 has been held in Amsterdam (The Netherlands) as a two-week (January 5-16, 2009) school in the field of molecular simulation. It was organized by the Amsterdam Center for Multiscale Modeling (ACMM), with administrative support form the HRSMC and CECAM, and financial support from the ESF-SimBioMa and CECAM. The school was attended by 62 participants and involved 7 lecturers, 10 lab-course assistants, and one administrative organizer.

MolSim2009 focused on numerical techniques for study of properties of many-particle systems to be applied in studies in materials science, biomolecular science, and other fields in physics, chemistry or biology. The school was arranged as an integrated program of lectures and lab courses with hands-on exercises. The lectures and lab course involving researchers from the ACMM and invited guests, including world class scientists. The program also involved a poster session and social events.

The opinion of the participants, assessed by a a questionnaire, was very positive on all aspects of the school. From the perspective of the lecturers, teaching assistants and administrative organizer, the participants group was considered outstanding: qualified, motivated and with an exemplary working attitude.

The large number of qualified and motivated participants, and the positive overall assessment provides confidence that the MolSim school fullfils a need in the computational science community and has a very attractive and balanced setup. This makes the organizers believe that they should continue the school in the present setup.

Scientific Content and Discussion

MolSim2009 was a two-week school in the field of molecular simulation targeting PhD students, but also open to advanced MSc students and postdoctoral researchers. The school took place January 5 - 16, 2009 in Amsterdam and was organized by the Amsterdam Center for Multiscale Modeling (ACMM), with support from the HRSMC[1], and CECAM[2]. The ACMM (www.acmm.nl) is a scientific center composed of researchers from the University of Amsterdam, the Free University Amsterdam, and the FOM institute AMOLF.

The MolSim-2009 school focused on numerical techniques for study of properties of many-particle systems to be applied in studies in materials science, biomolecular science, and other fields in physics, chemistry or biology. The course offered a recap of the statistical mechanics relevant for molecular simulation and covered basic and advanced simulation techniques including Monte Carlo, molecular dynamics, free energy calculations, rare events, coarse-graining. All techniques will were illustrated by illustrative examples of present day research. No previous knowledge in molecular simulations was required, though elementary knowledge in thermodynamics and statistical thermodynamics was assumed.

The school was arranged as an integrated program of lectures and lab courses with hands-on exercises. The lectures were given by active scientist in the field, all of them having an excellent scientific reputation, and some regarded as world class in the field. The book "Understanding Molecular Simulation" by Frenkel and Smit provided the basis of the lectures. Each of the participants was provided a copy of the book. This was supplemented by handouts and copies of the lecture slides.[3] During the lectures a low treshold for direct interaction with the lecturers was maintained: the participants were encouraged to ask questions during the lectures, and after the lecturers were available for further questions and discussion after the lectures and (sometimes) during the lab course hours.

The hands-on computer exercises were an essential part of the school and allowed the participants to apply the theory of the lectures in practice, using specially designed examples. For this purpose a 55-page lab course book in combination with pre-installed computer code was used. The pre-installed computer code was provided both in FORTRAN as in C as to facilitate participants as much as possible. The lab courses were tutored by experienced PhD students, postdoctoral researchers, and staff researchers.

A poster session was organized to provide the participants the opportunity to present their research. It consisted of flash presentations in a morning lecture session, and a poster display session at the end of the subsequent afternoon session. The poster display session was held in an informal setting and accompanied by food and drinks.

Lectures rooms, dedicated computer-class rooms, computer system administration, and catering were provided by the University of Amsterdam.

[1] The HRSMC (Holland Research School of Molecular Chemistry, www.hrsmc.nl) is a cooperation between research groups of the van 't Hoff Institute for Molecular Sciences (HIMS) of the Universiteit van Amsterdam (UvA), the Leiden Institute of Chemistry (LIC)), Leiden Observatory (LO) and the Leiden Institute of Physics (LION) of the Universiteit Leiden (UL), and the Institute for Electrons and Molecular Structure (EMS) of the department of chemistry of the Vrije Universiteit (VU).

[2] CECAM (Centre Europeen de Calcul Atomique et Moleculaire, www.cecam.org) is a European organization devoted to the promotion of fundamental research on advanced computational methods and to their application to important problems in frontier areas of science and technology, and based in Lausanne (CH).

[3] A copy of the lecture slides can be downloaded from http://molsim.chem.uva.nl/molsim2009/index.html. These could not be appended to this report due to size considerations.

The full program of the school is available via internet:
http://molsim.chem.uva.nl/molsim2009/index.html . The program is also listed in the appendix. All teaching material (lecture slides, hand outs, lab course book, exercises software) was (and is) available via this website The web site also shows a vivid group picture of the school.

Assessment and Future Directions

The school was widely publicized through various channels. It was announced on the websites of CECAM (www.cecam.fr), ACMM (www.accm.nl), and the HRSMC (www.hrscm.nl). Publicity was also generated by posting an announcement of the school on mailing lists, including the CPMD list (cpmd-list@cpmd.org) and the computational chemistry list (ccl.net). Personal contacts of lecturers also provided an important channel for publicity within the community of computational science.

Registration for the course was organized online via the CECAM website. The school administrator provided assistance in organizing travel and accomodation for foreign participants. This included providing directions for travel and guiding through visa procedures. The accomodation was arranged via a "large volume" contract with a walking-distance hotel, allowing for sharply discounted rates. Most participant used this opportunity. During the school all information was provided via the MolSim2009 website.

The school has been attended by 62 participants. Most of them were PhD student, but there were also advanced MSc students, postdoctoral, and industrial researchers among the participants. The teaching involved 7 lecturers (including the coordinator of the lab course), 10 teaching assistants, and a school administrator.

Extensive experience from organizing earllier editions of the MolSim school in previous years ensured that the program ran in a smooth and efficiently manner.

The overall impression of the people involved in running the school (lecturers, assistants, and secretariat) was that the participants had a very positive opinion about all aspects of the school. From the perspective of the lecturers, teaching assistants and school administrator the participants group was considered outstanding. The were very motivated and had an exemplary working attitude, with many students working through the lab course exercises into the evening hours.

The attendance of the lectures and lab courses was excellent. In the rare cases a student did not attend a lecture or lab course, almost always a valid reason was given beforehand. The assessment of the participants was quantified by a questionnaire provided at the end of the school. About half of the participants send in a completed questionnaire. The response confirmed the above mentioned positive opinion. It also contained useful suggestions for improvement and critical remarks that provided us useful input for keeping the school at the highest level. Remarks included *"Good lectures and excellent exercises"*, *"So far, the best tutorial I ever attended"*, *"Great organization. First class accommodation relative to the price to be paid ..."*, *"... please give more comment on source code and point out algorithms behind it in more detail ..."*, *"... the student should be encouraged to do a final research project"*. All suggestions for improvement and critical remarks will be carefully considered and used to further improve possible future editions of the MolSim school. A summary of the response provided by the returned questionnaires is provided as an appendix.

All participants were provided a certificate of attendance. (An example is provided in the appendix).

The present edition of MolSim clearly indicates that there is a continuing need for a PhD level school in the field of molecular simulations. The present edition of MolSim continued the tradition of attracting large numbers of motivated and qualified participants seen in previous editions of the school. The positive overall assessment provides confidence that the MolSim school fullfils a need in the computational science community and has has a very attractive and balanced setup. This convinces the organizers they should continue the school in its present setup.

Appendix
MolSim2009 - Final Program

Day	Time	Lecturer	Topic
Sunday			Arrival
Monday	08:00-09:00		Registration
	09:00-09:15	Meijer	Welcome
	09.00-12:30	Smit	Intro Statistical Thermodynamics (Part I & Part II)
	13:00-19:00	Ensing & Charbonneau	Lab Course
Tuesday	09.00-12:30	Smit	Monte Carlo: Basic Techniques
	13:00-19:00		Lab Course
Wednesday	09:00-12:30		Lab Course
	13:00-16:30	Smit	Intro Molecular Dynamics
Thursday	09:00-12:00	Bolhuis	Ensembles I
	12:00-12:30		Flash Presentation Posters
	13:00-16:00		Lab Course
	16:30-19:00		Poster Session
Friday	09:00-12:30	Bolhuis	Ensembles II
	13:00-19:00		Lab Course
Weekend		Social Event	Amsterdam Canal Cruise
Monday	09.00-12:30	Meijer	Free Energy and Phase Equilibria
	13:00-19:00		Lab Course
Tuesday	09.00-12:30	Vlugt	Configurational-bias Monte Carlo
	13:00-19:00		Lab Course
Wednesday	09:00-12:30		Lab Course
	13:00-17:00	Meijer	Advanced MC and MD Techniques
Thursday	09:00-12:30	Frenkel	Rare Events
	13:00-19:00		Lab Course
Friday	09:00-12:30	Frenkel	Advanced Topics
	13:00-19:00		Lab Course

Note: Lecture slides can be downloaded by following the link under the description of the topic.

Appendix
MolSim2009 - Organizers, Lecturers, and Teaching Assistants

Organizers
Ineke Weijer (Administrative organizer), University of Amsterdam (NL)
Dr. Bernd Ensing, University of Amsterdam (NL)
Dr. Evert Jan Meijer, University of Amsterdam (NL)
Prof. Daan Frenkel, Cambridge University (UK) and University of Amsterdam (NL)

Lecturers
Prof. Berend Smit, University of California, Berkeley (US)
Prof. P. G. Bolhuis, University of Amsterdam (NL)
Dr. B. Ensing, University of Amsterdam (NL)
Prof. Daan Frenkel, Cambridge University (UK) and University of Amsterdam (NL)
Dr. Evert Jan Meijer, University of Amsterdam (NL)
Dr. T.J.H. Vlugt, Delft University of Technology (NL)

Teaching Assistants
Dr. Patrick Charbonneau, Duke University (US)
MSc. Francesco Colonna , University of Amsterdam (NL)
MSc. Lizhe Zhu, University of Amsterdam (NL)
MSc. Marieke Schor, University of Amsterdam (NL)
Dr. Jutta Rogal, University of Amsterdam (NL)
Dr. Jocelyne Vreede, University of Amsterdam (NL)
MSc. Grisell Diaz Leines, University of Amsterdam (NL)
MSc. Koos van Meel, FOM Institute AMOLF (NL)
Dr. Ana Vila Verde, FOM Institute AMOLF (NL)
MSc. Sanne Abeln, FOM Institute AMOLF (NL)

APPENDIX: MolSim2009 Participants

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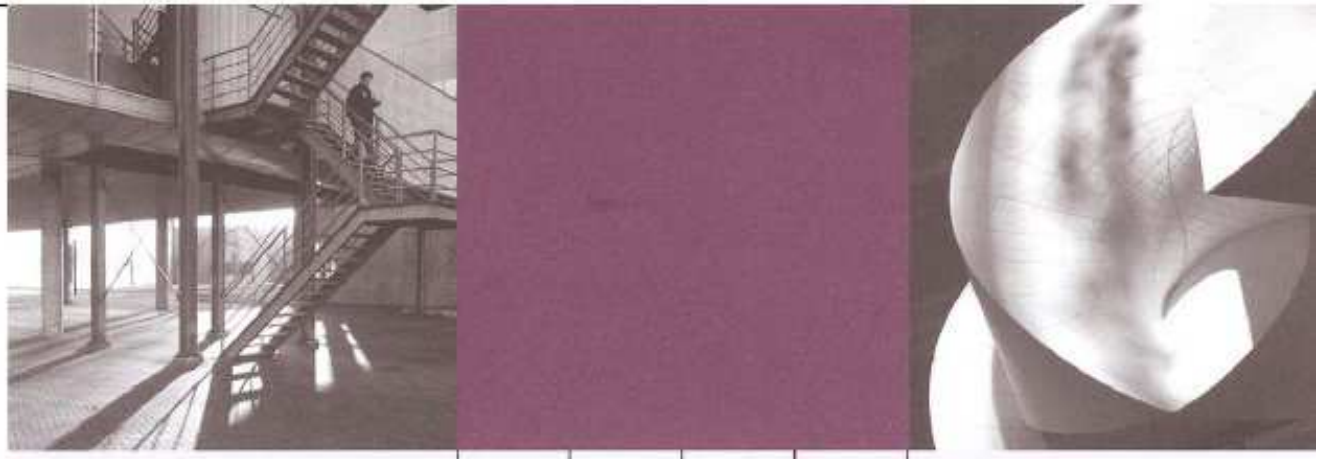
Appendix: MolSim-2009 Certificate (example)



2009

FACULTEIT DER NATUURWETENSCHAPPEN, WISKUNDE EN INFORMATICA
Van 't Hoff Institute for Molecular Sciences (HIMS)

has fulfilled the requirements for the course

"Understanding Molecular Simulations"

Thaught at the University of Amsterdam

January 5-16, 2009

Lecturers:
Prof. dr B. Smit, Prof. dr D. Frenkel, Dr E.J. Meijer, Dr B. Ensing, Prof. dr P. Bolhuis,, Dr T.J.H. Vlugt

Amsterdam, January 16, 2009

D. Frenkel *E.J. Meijer* *B. Ensing* *P. Bolhuis*
Organizers

UvA UNIVERSITEIT VAN AMSTERDAM