ESF Science Meeting

MolSim 2011

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

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

Summary

MolSim2011 has been held in Amsterdam (The Netherlands) as a two-week (January 3-14, 2011) school covering 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 **76** participants and involved **8** lecturers, **13** lab-course assistants, and one school manager.

MolSim2011 focused on numerical techniques for study of properties of many-particle systems that can be applied to study topics 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 that included world class scientists. The program also involved a poster session and social events.

The opinion of the participants was assessed by a questionnaire that could be handed in anonymously. On basis of the response we concluded that the the school was considered very positive. This positive impression that was obtained through direct contact during the meeting and post-school email contact confirmed the picture provided by the response on the questionnaire. From the perspective of the lecturers, teaching assistants and administrative organizer, the participants group was considered excellent: qualified, motivated and with an exemplary working attitude.

The large number of applications and the final selection of qualified and motivated participants, combined with the positive overall assessment confirms the confidence that the MolSim school fulfills a need in the computational science community and has an attractive and balanced setup. This makes the organizers believe that they should continue the school in the present setup, incorporating the suggestions for improvement that are provided.

Training and Scientific Content

MolSim2011 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 3 - 14, 2011 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-2011 school focused on numerical techniques for study of properties of many-particle systems to be applied to study topics 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 threshold 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 57-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 (lunch, coffee) were provided by the University of Amsterdam.

The full program of the school is available via internet:
http://molsim.chem.uva.nl/molsim2011/index.html . The program is also listed in the appendix.

[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 University

[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/molsim2011/index.html These could not be appended to this report due to size considerations.

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.

Participation, 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). An extensive list of personal contacts of the organizers also provided an important channel for publicity within the community of computational science.

Registration for the course was arranged online via the CECAM website. The school administrator provided assistance in organizing travel and accommodation for foreign participants. This included providing directions for travel and guiding through visa procedures. The accommodation was arranged via a "large volume" contract with hotel in the city allowing for sharply discounted rates. A small number of participants were housed at a second hotel. There was a frequent and fast public transport connection between the hotels and lecture facilities. Most participant used this opportunity. During the school all information was provided via the MolSim2011 website.

In total there were over 100 applications, a number that exceeded the capacity of the school. The participants were selected on basis of scientific quality, background, area of interest, and letters of support. The school has been attended by **76** participants. Most of them were PhD student, but there were also advanced MSc students, postdoctoral, and industrial researchers among the participants. The teaching involved **8** lecturers (including the coordinator of the lab course), **13** teaching assistants. The organization was supported by a managing assistant and the financial administration.

Extensive experience from organizing earlier 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 excellent. 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 outstanding. The assessment of the participants was assessed through direct contacts during the school and from post-school email contact. 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. These included the suggestion to include a poster mini-presentation session, and a better scheduling of the poster session. There were also some remarks on the a couple of the hotel rooms that appeared to be cleaned less frequently. All suggestions for improvement and critical remarks will be carefully considered and used to further improve possible future editions of the MolSim school.

All participants were provided a certificate of attendance and a copy of the group picture, similar to that show at the top of this report.

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 fulfills 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 A
MolSim2011 - Final Program

Day	Time	Lecturer	Topic
Sunday 02-Jan			Arrival
Monday	09:00-09:05	Evert Jan Meijer	Welcome
	09:05-12:30	Daan Frenkel	Intro Statistical Thermodynamics
	13:30-17:00		Lab Course
	17:00		Welcome Drinks
Tuesday	09:00-12:30	Peter Bolhuis	Intro Monte Carlo
	13:30-18:00		Lab Course
Wednesday	09:00-12:30	Peter Bolhuis	Intro Molecular Dynamics
	13:30-18:00		Lab Course
Thursday	09:00-12:30	Berend Smit	MC: Ensembles I
	13:30-18:00	Bernd Ensing et al	Lab Course
Friday	09:00-12:30	Berend Smit	MC: Ensembles II
	13:30-18:00		Lab Course
Weekend			Social event: Canal Tour and Dinner
Monday	09:00-12:30	Berend Smit	Free Energies and Phase Equilibria
	13:30-18:00		Lab Course
Tuesday	09:00-10:30	Evert Jan Meijer	MD: Advanced Methods
	11:00-12:30	Sanne Abeln	MC: Lattice Methods
	13:30-16:30		Lab Course
	17:00-18:00		Poster Session & Drinks
Wednesday	09:00-12:30	Thijs Vlugt	Configurational Bias MC
	13:30-18:00		Lab Course
Thursday	09:00-12:30	Evert Jan Meijer	Rare Events
	13:30-18:00		Lab Course
Friday	09:00-12:30	Christopher Lowe	Coarse Grained models
	12:00-12:05	Evert Jan Meijer	Closing

* All Lab Courses were supervised by Ensing and Dubbeldam.

Appendix B
MolSim2011 - Organizers, Lecturers, and Teaching Assistants

Organizers

Ineke Weijer (Managing assistant), 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

Dr. Sanne Abeln, Free University of Amsterdam (NL)
Prof. Peter G. Bolhuis, University of Amsterdam (NL)
Dr. David Dubbeldam, University of Amsterdam (NL)
Dr. Bernd Ensing, University of Amsterdam (NL)
Prof. Daan Frenkel, Cambridge University (UK) and University of Amsterdam (NL)
Dr. Evert Jan Meijer, University of Amsterdam (NL)
Prof. Berend Smit, University of California, Berkeley (US)
Dr. Thijs J.H. Vlugt, Delft University of Technology (NL)

Teaching Assistants

Dr. Ana Vila Verde, FOM Institute AMOLF (NL)
MSc. Murat Kilic, University of Amsterdam (NL)
MSc. Anna Pavlova, University of Amsterdam (NL)
MSc. Marieke Schor, University of Amsterdam (NL)
Dr. Jocelyne Vreede, University of Amsterdam (NL)
MSc. Rosanne Zeiler, University of Amsterdam (NL)
MSc. Lizhe Zhu, University of Amsterdam (NL)
MSc. Wagner Homsi Brandeburgo, University of Amsterdam (NL)
MSc. Grisell Diaz Leines, University of Amsterdam (NL)
MSc. Weina Du, University of Amsterdam (NL)
MSc. Jurriaan Luiken, University of Amsterdam (NL)
MSc. René Pool, Free University Amsterdamm (NL)
MSc. Kushagra Singhal, University of Amsterdam (NL)