SoftSimu2002 - Novel Methods in Soft Matter Simulations

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The summer school SoftSimu2002 - Novel Methods in Soft Matter Simulations - was organized in early June 2002 at the Helsinki University of Technology in Finland. The school was targeted to graduate students and young researchers working in computational and theoretical soft condensed matter sciences. Although the school was originally planned for 50 participants, it aroused so much interest that the limit had to be stretched to allow a total of 79 participants from 42 different laboratories in 14 countries to attend the meeting.

The meeting centred on the concept of coarse graining, where the aim is to simplify complicated molecular level systems in such a way that only the essential degrees of freedom are systematically taken into account. This seemingly simple idea is bothered by the fact that there is no unique way to do it, and yet coarse graining is essential for studies of soft matter systems over large length and time scales.

The idea to concentrate on the computational aspects in soft matter systems surfaced during the "Physics meets biology" meeting in Helsinki in August 2001. The discussions during this cross-disciplinary meeting made it very clear that even though a number of new simulation techniques and methodologies have emerged during the past 10 years, no review articles or even summer schools have tried to cover them. SoftSimu2002 aimed to fill this gap and to bring together people who have developed and actively used those methods in their current research. Due to the inter-disciplinary nature of the school, and the different backgrounds of the attendees, the school was designed to provide the participants with a concise theoretical description of each method as well as a broad overview of their applicability and limitations in soft matter simulations. The lectures were further complemented by hands-on computer exercises that focused on a few computational techniques. In total, the school comprised the expertise of 12 invited lecturers who presented three hours of lectures each.

On the analytical and methodological side, Pep Espanol gave an excellent set of lectures describing the statistical mechanics behind coarse-grained models, and provided an overview of how the problem of coarse-graining can be approached through a systematic theoretical framework. Christopher Lowe went further along the same themes and addressed the problem of achieving real quantitative mesoscopic simulations using dissipative particle dynamics as a specific example. The topics of non-Hamiltonian dynamics and constrained systems were treated in great detail in Giovanni Ciccotti's set of lectures, giving the participants a good example of the importance of proper analytical and algorithmic treatment underlying computer simulations. These issues are of fundamental importance, for example, in non-equilibrium molecular dynamics simulations of complex systems.

Description of different time and length scales is essential to be able to describe the dynamics of complex liquids such as suspensions of colloids, proteins, or surfactants. The basic difficulty lies in the fact that the time and length scales associated with the solute and the solvent can differ by orders of magnitude. Raymond Kapral presented a set of lectures concentrating on the so-called Malevanets-Kapral method that couples a mesoscopic description for the solvent and a microscopic description for the solute. An older but related method, the lattice-Boltzmann approach, was discussed by Ignacio Pagonabarraga. Both methods have the advantage that they can be applied to flow problems at both high and low Reynolds numbers. Alternative methods were discussed by Eirik Flekkoy, who talked about coupling continuum and particle descriptions as the system is described in varying detail in different parts of the system. A Voronoi tessellation-based technique for colloidal systems provided but one of the examples discussed.

Whereas the above methods are based on coupling schemes between different levels of description, coarse-graining over microscopic degrees of freedom and replacing them by continuum fields is the essence of the so-called phase-field model. This method, its theoretical foundations, and applications to interface dynamics of liquids was the topic of Tapio Ala-Nissila's lectures. Alexander Lyubartsev in turn concentrated on the so called inverse problem, where the idea is to consider a system whose pair correlations are known, and then ask whether it is possible to extract the interactions from the known information for the pair correlation functions. The inverse Monte Carlo method has many similarities to the various methods used in polymeric systems as discussed by Florian Mueller-

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Plathe. This type of coarse-graining can yield, among others, effective potentials between different pairs of particles that can then be used in higher level simulations.

In addition to the time and length scales, long-range Coulombic interactions are a timely problem in all molecular simulations. In his lectures, Andre Moreira concentrated on the situation where this is particularly true, namely in systems containing surfaces and interfaces where the standard Ewald summation techniques cannot be used. Finally, a great variety of applications from polymeric systems and non-equilibrium methods for calculating transport coefficients to the mesophase formation of block copolymers, and the interaction of biological membranes with surfactants were described by Florian Mueller-Plathe, Robert Groot, and Aatto Laaksonen.

Although the school faced stiff competition from the great weather and seaside, participation in all the lectures, poster sessions, and organised events was exceptionally active, and the lectures were followed by long and lively discussions. Due to the enthusiastic response from the participants, a follow-up to SoftSimu2002 is being planned for 2004. Further information of the summer school and related material for the proceedings and computer software is available at www.softsimu.org/softsimu2002.

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