5th MATCOR summer school of the Graduate School MAINZ

“Simulation of macromolecules on different scales”

August 31-September 5, 2008 in Hall/ Tirol

Computer Simulations play a crucial role for the understanding of material properties. They are applied on different scales, ranging from atomistic level to various coarse grained simulations. The main aim of this summer school was the understanding of simulations on different scales using techniques such as Molecular Dynamics and Monte Carlo simulation. The scientific program has been organized by T. Gruhn. Invited speakers, who are professors or research group leaders in the field, and PhD students, have come to attend the school from more than five countries.

One of the first methods, which were developed in the early fifties of the last century, was the Monte Carlo simulation technique. The basic aspects of the method were presented by K. Binder, using models of polymers as examples. He gave an overview on the most important results of last century and recent investigations in this field. Examples included the dynamics of polymer melts, the translocation dynamics of polymers through membranes, and the demixing of symmetric binary polymer mixtures, as well as asymmetric polymer solutions. Three advanced Monte Carlo methods for the simulation of lattice polymer models were discussed in the lecture of W. Paul. Applications of the Lattice-Boltzmann simulation technique on polymer solutions and on the hydrodynamic screening of polymers were the main topic in the talk of B. Dünweg.

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Another important method which is used worldwide was presented by M. Wilson. In his lecture he introduced molecular dynamics (MD) simulations and presented recent results on atomistic and coarse-grained simulations of a chromonic and thermotropic liquid crystal as well as amphiphilic polymers. The following lecture by D. Sebastiani was dedicated to recent results and basics of the Car-Parrinello technique, an ab initio molecular dynamics simulation method. In his talk, he illustrated the potential of first-principles calculations for the determination of the microscopic structure of a variety of extended systems, ranging from molecular crystals over covalently and hydrogen-bonded nanostructures to liquids and solvated molecules.

Furthermore, the density-functional-based bridging-scale approach was presented as a method for simulations of large molecules near metal surfaces (L. delle Site). Much attention was sparked on multiscale molecular simulations. Atomistic and coarse-grained force field simulations of polymers were discussed by N. van der Vegt. Further examples of mesoscale simulations were the multiple collision dynamics (MPC) algorithm (R. Winkler), coarse-grained membrane hydrodynamics (G. Gompper), and dissipative particle dynamics (DPD) simulations with recent results for fluid lipid bilayer membranes, vesicles and quasi-rigid nanoparticles (J. Shillcock). A summary of the aspects of quantum mechanical and classical force-field-based methods was given by T. E. Exner. The theory and methodology of the transition path sampling method, which is based on the statistical mechanics of trajectories, was presented in the lecture of C. Dellago. This method can be applied to study rare but important transitions between long-lived stable states.

One particularly important session during the school was the poster session, which contained the presentation of 18 posters, followed by exciting discussions about investigations of all the participants. Afterwards, four PhD students gave oral presentations about their current research topics.

The intensive scientific program would have been hard to follow without the accompanying social activities, such as a hiking tour in the Alps, an excursion to the silver mine in Schwaz, a very interesting guided sightseeing tour in Innsbruck and a nice dinner in the “Stiftskeller” in Innsbruck.

In conclusion, this motivating summer school covered a good deal of the current simulation techniques of statistical physics. Moreover, most of the participants showed great interest in the talks and, according to a questionnaire made after the school, learned a lot about the most powerful methods in computer simulations. (L. Spirin)