CECAM Tutorial: Atomistic Monte Carlo Simulations of Bio-Molecular Systems

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The CECAM tutorial "Atomistic Monte Carlo Simulations of Bio-molecular Systems" took place at Forschungszentrum Jülich from September 15 to 19, 2014 and was attended by scientists from seven countries. The five days of the tutorial featured a range of lessons and hands-on practical sessions to provide scientists with everything necessary to apply this technique to their own research topics.

After the initial presentation by Prof. Anders Irback (Lund University) on the first afternoon that summarized the theory of Monte Carlo (MC) simulation and its application to biological macromolecules, the participants were introduced to the open source Monte Carlo simulation package ProFASi that served as the basis for the hands-on parts of the tutorial. ProFaSi is under active development by the organizers from the Simulation Laboratory Biology at JSC. It is a powerful alternative to molecular dynamics (MD), in particular for cases where the underlying process is too slow to be simulated by classical MD, such as in protein folding and peptide aggregation.

Two introductory sessions enabled the participants to set up, monitor, and analyze MC simulations of protein folding, peptide aggregation with ProFASi on the HPC resources of JSC. The following sessions addressed several advanced features including advanced error analysis and visualization. Wouter Boomsma (Univ. Copenhagen) demonstrated the use of different constraints obtained from predictions and experiments in connection with MC simulations. Finally, the programming interface of ProFASi was introduced that allows for rapid development of new algorithms and simulation strategies using atomistic Monte Carlo.

The CECAM tutorial concluded with some recent research highlights using atomistic MC simulations, and a lively discussion of best practices and future developments with the participants.

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