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Sano Computational Medicine Seminars

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Join us via Zoom: https://seminar.sano.science/

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www.fz-juelich.de/ias/jsc/EN/AboutUs/Organisation/ComputationalScience/Simlabs/slbio/_node.html

All-atom Markov Chain Monte Carlo simulation of protein folding and other large scale conformational changes

Abstract

Many biologically relevant processes are characterized by major conformational changes of the involved biomolecules. While recent advances in experimental methods have improved our ability to observe proteins and other biomolecules these experiments do not give us a full account of the microscopic changes from which the observable conformational changes arise. For a more complete and thereby also more causal understanding of such structure formation and transition processes all-atom molecular simulations have become the method of choice.

This talk will discuss processes such as protein folding and peptide aggregation which involve large scale conformational changes and happen on time scales that are difficult to reach by all-atom molecular dynamics simulations. As a potential efficient alternative for such applications all-atom Markov Chain Monte Carlo (MCMC) simulation methods will be introduced. The talk will focus on the High Performance MCMC software ProFASi which has been developed at the Simulation and Data Laboratory Biology of the Jülich Supercomputing Centre. Several large scale exmples, ongoing developments including links to machine learning and proteomics, as well as remaining challenges will be discussed.

Dr. Olav Zimmermann – has organised since 2008 the Simulation Laboratory Biology a dedicated research and support unit at the Jülich Supercomputing Centre (JSC), that helps life scientists to employ the supercomputers in Jülich for their research. As a biologist with a background in experimental molecular genetics Olav changed to structural bioinformatics for his PhD on FFT docking at the University of Cologne. At the same time he cofounded the bioinformatics startup science-factory. During a PostDoc at the Center of Excellence in Bioinformatics at SUNY Buffalo he started to use Supercomputers for his work and in 2005 returned to Germany where he is now a staff scientist at JSC. Olav's main interests are high performance methods at the interface of machine learning and physics based simulation for applications in structural bioinformatics.

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