CECAM Tutorial - Atomistic Monte Carlo Simulation

An efficient Tool for studying large Scale conformational Changes of Biomolecules

Molecular simulation has become an indispensable tool to study the molecular mechanisms that underlie biological function. For fast processes, such as ligand binding, molecular dynamics (MD) is a popular and effective tool. In contrast, processes that involve large conformational changes like protein folding and peptide aggregation are typically much slower, acting on time scales between milliseconds and seconds. Such time scales are difficult to sample in MD simulations, and alternative techniques circumventing these difficulties should be integrated into scientific workflows to derive the necessary biophysical insights. Atomistic Markov chain Monte Carlo (MC) has been recently demonstrated to be a computationally efficient alternative to MD simulations [1] for such problems. While excellent training courses for atomistic molecular dynamics simulations already exist, students rarely get a useful exposure to Monte Carlo techniques. To fill this gap, a five-day tutorial "Atomistic Monte Carlo Simulations of Biomolecular Systems" funded by CECAM (Centre Européen de Calcul Atomique et Moléculaire) will take place at the Jülich Supercomputing Centre (JSC), September 19-23, 2016.

The goal of the tutorial, organized for the second time by the SimLab Biology of the JSC, is to introduce atomistic Monte Carlo simulations in sufficient detail, that researchers can apply it productively to their own research tasks. As a demonstration tool for the highly transferable MC techniques, the open source protein folding and aggregation package ProFASi, developed at the SimLab Biology, will by used. For realistic tests of advanced parallel simulation techniques like replica exchange MC or Wang-Landau, participants will have access to JURECA, Jülich's recently installed 2 PetaFlop Supercomputer.

Interested researchers can apply and obtain detailed information on the tutorial contents on the web page for the CECAM school:

http://www.cecam.org/workshop-1339.html

References

[1] Mohanty, S., Meinke, J.H., Zimmermann, O.,
Folding of Top7 in unbiased all-atom Monte Carlo simulations. Proteins 81:1446–1456, 2013

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