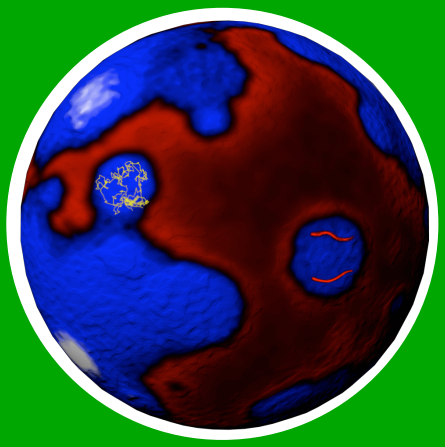

Sächsische Forschergruppe
"From Local Constraints to Macroscopic Transport"

June 24th 2011, 15:30

Theoretical Lecture Hall

Faculty of Physics and Earth Science
University of Leipzig
Linnéstrasse 5, Leipzig

Simulation of biological molecules

Handan Arkin-Olgar
Ankara University/University of Leipzig

The protein folding problem has been attracting the attention of scientists from various disciplines for several decades. Although the physical principles are known, the complex energy profile of proteins and peptides makes the analysis of realistic proteins extremely difficult. Generalized ensemble simulations overcome this difficulty by performing a random walk in energy space and sample a much wider phase space than conventional methods.Such a goal can be achieved within the multicanonical approach [1]. In this talk, a brief discussion of the powerful multicanonical simulation method will be given. The intermediate steps of the simulation method starting from a given sequence as the input leading to the folded three- dimensional structure will be shown for a AB model [2,3] to all-atom simulations [4,5]. The determination of the topografic structure of the energy landscape will be discussed. After that, simulation results for a special example, elastin-like polypeptides, are presented [6,7].

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