Studying nucleic acid and peptide dynamics using advanced sampling simulations

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Molecular dynamics-replica exchange (REMD) simulations that allow exchanges between MD simulations at different temperatures are frequently used to study peptides and proteins. However, a drawback of standard REMDs is the rapid increase of the number of replicas with system size for a desired temperature range. To limit the number of replicas we have developed new Hamiltonian-REMD methods that employ various biasing potential levels associated with soft degrees of freedom for each replica run. One approach is designed to enhance conformational sampling by applying a backbone biasing potential. It lowers the barrier for backbone dihedral transitions and promotes frequent transitions along the replicas. Efforts to employ biasing potentials along other soft degrees during REMDs will also be discussed. The biasing potential (BP)-REMD methods require only a very modest number of replicas and were successfully tested on several systems. Applications of the methods to study conformational dynamics of proteins and nucleic acids will be presented.

Thursday, May 20th

16:00 Institute for Computational Physics, Allmandring 3

Room 1.079