

LECTURE I:

Enhanced Conformational Sampling using Monte Carlo and Molecular Dynamics Simulations of Classical Systems in the Tsallis Ensemble

Ioan Andricioaei

Chemistry & Bioinformatics, University of Michigan, Ann Arbor

Abstract:

As one of the possible ways to alter the sampling distribution in configuration space in a manner that is conducive to enhanced sampling, we present a strategy based on probability distributions that arise in the generalization of statistical mechanics proposed by Tsallis.

We introduce the method for classical Metropolis Monte Carlo and present applications to simulations of Lennard-Jones clusters and to peptides.

The definition of a Tsallis effective potential enables one to also conceive a constant-temperature molecular dynamics method (instead of Monte Carlo) to generate the Tsallis distributions. Given this effective potential, it is possible to define a constant temperature molecular dynamics algorithm such that the Tsallis distribution is sampled in the trajectory.