

Adaptively Biased Molecular Dynamics

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Over the past few years several methods targeting the computation of the free energy surface of a reaction coordinate using non-equilibrium dynamics have become popular. The methods in this category use the history of the sampling process to bias the simulation thus forcing it to explore as of yet unexplored values of the reaction coordinate. In context of molecular dynamics, the idea was first introduced by the local elevation method by Huber, Torda and van Gunsteren (the Wang-Landau algorithm employs similar ideas in context of Monte Carlo simulations). More recent approaches include the adaptive-force bias method, and the non-equilibrium metadynamics. The adaptively biased molecular dynamics is a variation on the same theme that benefits from a smoother biasing potential and replica exchange mechanism. I am going to present the method and illustrate its workings via a study of the folding of the Ace-GGPGGG-Nme peptide in a gaseous and solvated environment.