ID de Contribution: **10** Type: **Non spécifié**

Dynamically-accurate biasing using Accelerated Molecular Dynamics

lundi 11 septembre 2023 11:30 (1 heure)

Modifying or biasing the dynamics of atomistic systems can result in faster mixing and convergence of thermodynamic observables, but it generally yields non-physical kinetics. I will introduce a family of so called "Accelerated Molecular Dynamics" methods that are specifically designed to produce statistically accurate "state-to-state" dynamics for metastable systems at a much reduced computational cost compared to brute force molecular dynamics. I will discuss the basics of the methodology, as well as implementation on parallel computers.

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Classification de Session: Challenge and Perspective