

Extracting Dynamical Quantities from Parallel Tempering Simulations Using Reweighting Techniques

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Abstract

Parallel tempering or replica-exchange molecular dynamics, an easy-to-implement multicanonical simulation algorithm able to broadly explore configuration space, has previously found use solely for the calculation of equilibrium quantities. Here, we demonstrate that dynamical quantities can be extracted from these simulations, and provide examples for computing transition rates and time-correlation functions at arbitrary temperatures from the simulation data using reweighting techniques.