

New Ensembles and Integrators for Accelerated Sampling

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Abstract

In recent years there has been a great deal of interest in MD simulation in various statistical mechanical ensembles (constant temperature, constant temperature and pressure, grand canonical, etc.). While these classical ensembles are of obvious fundamental interest, they all exhibit similar serious difficulties in the sampling of complex potential landscapes. After work by Tsallis, Straub and others and related to ideas of Voter, it is interesting to study methods that sample (using molecular dynamics) a much broader class of ensembles. The underlying mechanism used here is an adaptation of Nose's dynamical thermostat; it is interesting that the Nose framework also admits substantial generalization.