

An efficient method to reconstruct multidimensional free energy surfaces by molecular dynamics

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Abstract

We introduce a novel molecular dynamics method for exploring the properties of the multidimensional free energy surfaces of complex many-body systems. The method is based on the construction of a coarse-grained non-Markovian dynamics in the space defined by a few collective coordinates. The dynamics is biased by a history-dependent potential term that, in time, fills the minima in the free energy surface, allowing the efficient exploration and accurate determination of the free energy surface. We discuss the usefulness of this approach for simulating chemical reactions, solid-solid phase transitions in material science and conformational transitions in biopolymers.