CROSSING THE POTENTIAL BARRIERS

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ABSTRACT

Free energy calculations are important for our understanding of physical, chemical, and biological processes on an atomic scale. Provides information on the various mechanisms; computational methods to find interactions and reactions in such systems are very helpful. However, they are limited to timescales typically much shorter than in nature. In particular, the time scales of reactions depend on the high of the free energy barrier between the states, typically are far from the feasible time scales of atomistic simulations. Even coarse graining of the systems and application of semi-classical force fields cannot help to follow reactions of the machines.

In principle, finding the free-energy landscape is straightforward from the probability distribution of the states of the system. The problem is that to find the barriers, we need to calculate the free energy at points in the phase space that are usually very unlikely to be visited by the system during the simulation time.

Over the years, many computational methods have been developed to calculate free energy barriers by forcing the system to meet rare events. Jarzynski's equality enables free energy calculations for both experimental and computational works as a bridge between equilibrium statistical mechanics and non-equilibrium systems [1]. Instead, it could be more accurate to calculate the equilibrium free energy with an equilibrated method, such as umbrella sampling [2]. However, the presence of non-conservative forces in the out-of-equilibrium method and the need of considering environmental dependencies of the force fields during transitions (in both non-equilibrium and equilibrium ones) could affect the efficiency as well as the accuracy of the methods. Here we will propose some simple modification to solve these problems without increasing the computational cost very drastically [3] [4].

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