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(POS-10) Extending the Mean First-Passage Time Formalism to the Reconstruction of High Free Energy Barriers

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Rare events like crystal nucleation in mildly supercooled liquids occur infrequently but proceed rapidly, resulting in the waiting time for their occurrence being much longer than the timescale of the microscopic dynamics. Activated processes are analyzed through free energy landscapes defined on one or more appropriate reaction coordinates, where transitions between states require overcoming a barrier. In the single reaction coordinate case, the mean first-passage time (MFPT) formalism [J. Wedekind and D. Reguera, J. Phys. Chem. B, 112, 11060 (2008)] enables estimation of transition rates and free energy landscapes using data from unbiased molecular dynamics (MD) simulation, which is useful when the energy barrier is not too high. For a sufficiently large barrier, spontaneous barrier crossings become rare and difficult to observe within feasible simulation times, making the now-conventional MFPT approach impractical. We extend the MFPT-based reconstruction method to overcome the large barrier problem by starting MD trajectories near the transition state. To validate our approach, we apply it to random walk models on a one-dimensional potential energy landscape and compare our results with solutions from transfer matrices and numerical integrals. We further test our method on crystal nucleation in the Lennard-Jones liquid, comparing our results against the umbrella sampling Monte Carlo method.

Keyword-1

computational method

Keyword-2

molecular dynamics

Keyword-3

nucleation and rare events

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