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Investigating rare events with modified Monte Carlo method based on fluctuation theorem

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The Monte Carlo (MC) method is a useful tool to solve a broad range of problems numerically; random numbers are used to decide whether a process is accepted resulting in a desired equilibrium distribution. In certain complex problems where transitions to some states are rare, however, this method dramatically consumes more resources and spends a long time trying to find the equilibrium states. To improve upon the conventional MC, we apply a fluctuation theorem (FT) to MC which provides a relative weight of a backward trajectory with respect to the forward one. Interestingly, not only does FT double information but also assists a probability of system to converge to equilibrium more rapidly. We apply the algorithm to solve a test problem where the energy barrier to a certain state is comparatively high. The result of the simulation is consistent with the analytic solution, but with significant speed gain compared to that from the conventional method.

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