Action−derived molecular dynamics in the study of rare events

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We present a practical method to generate classical trajectories with fixed initial and final boundary conditions. Our method is based on the minimization of a suitably defined discretized action. The method finds its most natural application in the study of rare events. Its capabilities are illustrated by non−trivial examples. The algorithm lends itself to straightforward parallelization, and when combined with *ab initio* molecular dynamics it promises to offer a powerful tool for the study of chemical reactions.

Research of D.P. at MPI has been sponsored by the Alexander von Humboldt foundation

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