Metadynamics of paths

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Many physical phenomena like crystallization, chemical reactions or protein folding take place on a time scale that cannot be reached using standard atomistic simulation methods. This could severely limit the scope of a most invaluable scientific tool. In order to address this problem a plethora of enhanced sampling methods have been suggested. Such methods enhance sampling but distort the dynamics that can only be recovered by appropriately engineered runs. In order to combine enhanced sampling with the calculation of dynamical properties we change our focus and rather than sampling individual configurations we sample path segments. This is done by using a discretized version of the Onsager-Machlup action. In order to remove kinetic bottlenecks, we sample the action with the help of metadynamics. We show that this approach is highly effective in the study of static and dynamics properties. In view of the next generation highly parallel exascale machine our algorithm has the appealing feature of being highly parallel.