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Enhanced sampling methods to mitigate topological freezing

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In lattice field theories with topological sectors, such as QCD and four-dimensional SU(N) gauge theories with periodic boundary conditions, conventional update algorithms struggle to sample the whole configuration space due to large action barriers separating distinct topological sectors. This manifests itself in the form of long autocorrelation times that diverge in the continuum limit and can compromise the correctness of simulations.

Here, we demonstrate that with suitably constructed bias potentials, Metadynamics and related enhanced sampling methods can mitigate this problem and significantly reduce the integrated autocorrelation times of the topological charge and associated observables. In addition, we show how combining a biased and an unbiased simulation stream in a parallel tempering setup allows us to obtain unbiased expectation values without the need to perform any reweighting.

Special requests

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