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Accelerating Metadynamics to overcome action barriers in 4D-SU(3) gauge theory with an eye on full QCD

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MCMC simulations of topologically non-trivial gauge theories such as QCD are plagued by long autocorrelation times, due to systems spending exponentially longer time stuck in a single topological sector at finer lattice spacings, which are necessary for high precision studies. This phenomenon is known as topological freezing, and several algorithms have been suggested to amend it throughout the years.

A relatively novel algorithm, Metadynamics (MetaD), introduces a so-called bias potential dependent on a collective variable (CV) to the theory and has been shown to improve this behavior. One drawback is a required reweighting procedure, which can significantly reduce the effective sample size. We combine MetaD with parallel tempering (PT-MetaD) to eliminate this cost altogether, with only a single additional parallel simulation stream. In this way, the algorithm shows significantly better scaling than conventional algorithms in 2-dimensional U(1) gauge theory and is shown to work in 4-dimensional SU(3) gauge theory as well, with no apparent hurdles for full QCD.

Apart from the smearing necessary to define a suitable CV for non-Abelian theories in 4 dimensions, the only other, albeit more up-front, cost is the computational time required to build or thermalize the bias potential. In this talk, we discuss some strategies that are employed to reduce the overhead, potentially making the application of the algorithm reasonable within the scope of full QCD.

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