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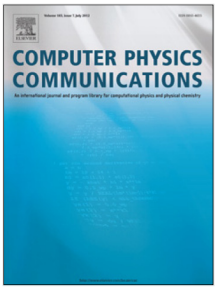

Tuning the hybrid Monte Carlo algorithm using molecular dynamics forces' variances

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Tuning the Hybrid Monte Carlo algorithm using molecular dynamics forces' variances

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Abstract

Within the HMC algorithm, we discuss how, by using the shadow Hamiltonian and the Poisson brackets, one can achieve a simple factorization in the dependence of the Hamiltonian violations upon either the algorithmic parameters or the parameters specifying the integrator. We consider the simplest case of a second order (nested) Omelyan integrator and one level of Hasenbusch splitting of the determinant for the simulations of a QCD-like theory (with gauge group SU(2)). Given the specific choice of the integrator, the Poisson brackets reduce to the variances of the molecular dynamics forces. We show how the factorization can be used to optimize in a very economical and simple way both the algorithmic and the integrator parameters with good accuracy.

Keywords: Lattice Gauge Theory, Hybrid Monte Carlo, Shadow Hamiltonian
PACS: 11.15.Ha, 12.38.Gc

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