ILDG Algorithm Glossary for `qcdsfAcceleratedHMC`: Accelerated Hybrid Monte Carlo Algorithm

Dirk Pleiter (QCDSF Collaboration)

18 December 2005

The simulations of QCD with $N_{\rm f} = 2$ flavours of degenerate, non-peturbatively improved Wilson-fermions have been realised using an accelerated Hybrid Monte Carlo algorithm [1].

The standard action is modified in the following way by introducing additional auxiliary pseudo-fermion fields:

$$S_1[U,\phi^\dagger,\phi] = S_G[U] + S_{det}[U] + \phi^\dagger W (Q^\dagger Q)^{-1} W^\dagger \phi + \chi^\dagger (W^\dagger W)^{-1} \chi, \tag{1}$$

where

$$W = Q + \rho. \tag{2}$$

The special case $\rho = 0$ corresponds to the unmodified action.

Two different time-scales are used for different segments of the action:

$$V_M(\tau) = V_{IR}\left(\frac{\tau}{2}\right) \cdot \left[V_{UV}\left(\frac{\tau}{2M}\right) V_Q\left(\frac{\tau}{M}\right) V_{UV}\left(\frac{\tau}{2M}\right)\right]^M \cdot V_{IR}\left(\frac{\tau}{2}\right) \tag{3}$$

Evolution takes place at two different time scales τ and τ_1. The ratio between both time scales is $M = \tau/\tau_1$, where M is an integer. The special case $M = 1$ corresponds to the ordinary leap-frog integrator.

The following splitting of the action is used:

$$\begin{aligned} S_{\rm UV} &= S_G[U] + S_{det}[U] + \chi^\dagger (W^\dagger W)^{-1} \chi, \\ S_{\rm IR} &= \phi^\dagger W (Q^\dagger Q)^{-1} W^\dagger \phi \end{aligned} \tag{4}$$

To solve equations of type $M \cdot \chi = \phi$ the Conjugate Gradient algorithm is used. The algorithm is iterated until the residuum vector $r = M \cdot \chi - \phi$ fulfils the condition $|r| < R$, where R is the target residuum.

The algorithm is controlled by the following parameters:

Parameter	XML Tag	Comment
τ	`<stepSize>`	Step size
N_τ	`<numberSteps>`	Number of steps per trajectory
M	`<timeScaleRatio>`	Time scale ratio
ρ	`<rho>`	Auxiliary pseudo-fermion parameter
R	`<solverResiduum>`	Solver residuum

References

[1] A. Ali Kahn et al. (QCDSF collaboration), "Accelerating the Hybrid Monte Carlo algorithm," Phys.Lett. B564 (2003) 235-240.