RHMC Code Documentation

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1 Introduction

A simple RHMC code to simulate $n_f + n_f$ QCD with isospin chemical potential, using unimproved staggered fermions and the Wilson SU(3) gauge action.

2 QCD formulation

2.1 Gauge Action

Wilson SU(3) plaquette lattice gauge action,

$$S_g[U] = -\frac{\beta}{3}\sum_x \sum_{\mu<\nu} Re\mathrm{Tr}\left[U_\mu(x)U_\nu(x+\hat{\mu})U^\dagger_\mu(x+\hat{\nu})U^\dagger_\nu(x)\right] \tag{2.1}$$

where $U_\mu(x)$ is a 3x3 complex matrix at the site x in the direction μ.

Defining the staple

$$A_\mu(x) \equiv \sum_{\mu\neq\nu}\left\{U_\nu(x+\hat{\mu})U^\dagger_\mu(x+\hat{\nu})U^\dagger_\nu(x) + U^\dagger_\nu(x+\hat{\mu}-\hat{\nu})U^\dagger_\mu(x-\hat{\nu})U_\nu(x-\hat{\nu})\right\} \tag{2.2}$$

the terms in the action that depend on a given link $U_\mu(x)$ are then

$$S_g^{local}[U_\mu(x)] = -\frac{\beta}{6}\mathrm{Tr}\left[U_\mu(x)A_\mu(x) + A^\dagger_\mu(x)U^\dagger_\mu(x)\right] \tag{2.3}$$

which is related to the full action by

$$S_g[U] = \frac{1}{12}\sum_x\sum_\mu S_g^{local}[U_\mu(x)] \tag{2.4}$$

2.2 Fermion Action

The fermion action for $4+4$ staggered flavors with isospin chemical potential μ_I and mass m is given by

$$S_f[U] = \phi^\dagger(D(\mu_I,m)[D(\mu_I,m)]^\dagger)^{-1}\phi \tag{2.5}$$

where $D(\mu_I,m)$ is the staggered lattice Dirac operator

$$[D(\mu_I,m)]_{xy} = e^{\mu_I/2}U_0(x)\delta_{n,m-\hat{0}} - e^{-\mu_I/2}U^\dagger_0(x-\hat{0})\delta_{n,m+\hat{0}} \tag{2.6}$$

$$+\sum_{\mu=1}^{3}\eta_\mu(x)\left[U_\mu(x)\delta_{n,m-\hat{\mu}} - U^\dagger_\mu(x-\hat{\mu})\delta_{n,m+\hat{\mu}}\right] \tag{2.7}$$

and $\eta_\mu(x) = -1^{\sum_{\nu<\mu} x_\nu}$ are the space-dependent staggered equivalent of Dirac γ-matrices, i.e.

$$\eta_0(x) = 1 \tag{2.8}$$
$$\eta_1(x) = -1^{x_0} \tag{2.9}$$
$$\eta_2(x) = -1^{x_0+x_1} \tag{2.10}$$
$$\eta_3(x) = -1^{x_0+x_1+x_2} \tag{2.11}$$
$$\eta_5(x) = -1^{x_0+x_1+x_2+x_3} \tag{2.12}$$

For $\mu_I = 0$ this reduces to the standard $n_f = 8$ staggered action, with the usual staggered γ_5–hermicity property $D^\dagger = \eta_5 D \eta_5 = -D$ for the massless case, which allows us to write the operator in the action in the form $DD^\dagger + m^2$.

However for non–zero μ_I we have instead the relation

$$[D(\mu_I, m)]^\dagger = -D(-\mu_I, -m) \tag{2.13}$$

so that

$$D(\mu_I, m)[D(\mu_I, m)]^\dagger = -D(\mu_I, m)D(-\mu_I, -m) \tag{2.14}$$

To generate a field ϕ according to the distribution $e^{-S_f[U]}$ we can first generate a complex vector χ with distribution $e^{-\chi^\dagger \chi}$, then set $\phi = D(\mu_I, m)\chi$

3 HMC

The hamiltonian for the HMC is

$$S[P, U, \phi] = S_p[P] + S_g[U] + S_f[\phi, U] \tag{3.15}$$

where we need to solve the classical equations of motion

$$\frac{dP_\mu(x)}{dt} = -\frac{\partial}{\partial U_\mu(x)}(S_g[U] + S_f[\phi, U]) = -F_g(x, \mu) - F_f(x, \mu) \tag{3.16}$$
$$\frac{dU_\mu(x)}{dt} = P_\mu(x) \tag{3.17}$$

The steps required to update a gauge configuration U:

- Generate gaussian momenta P
- Generate χ with distribution $e^{-\chi^\dagger \chi}$, then set $\phi = D\chi$
- Integrate the force terms to generate U', P'
- Accept or reject U' with probability $e^{S[P,U,\phi]-S[P',U',\phi]}$

3.1 Momenta

The momenta $P_\mu(x)$ are defined as

$$P_\mu(x) = \sum_{a=1}^{8} p^a_\mu(x) T_a \tag{3.18}$$

where T_a are the generators of SU(3) and $p^a_\mu(x)$ are real numbers. The action is given by

$$S_p[P] = \sum_{x,\mu} \mathrm{Tr}\left\{[P_\mu(x)]^2\right\} = \frac{1}{2}\sum_{x,\mu}\sum_{a=1}^{8}[p^a_\mu(x)]^2 \tag{3.19}$$

so we can generate momenta simply by sampling the numbers p^a from the gaussian distribution $e^{-(p^a)^2/2}$.

The resulting matrices P have $\mathrm{Tr}[P] = 0$ and $\langle \mathrm{Tr}[P^2] \rangle = 4$.

3.2 Gauge Force

The gauge force is given by

$$F_g(x,\mu) = \sum F_g^a(x,\mu) T_a \tag{3.20}$$

where

$$F_g^a(x,\mu) = \frac{\partial S_g[U]}{\partial U_\mu^{(a)}(x)} = \frac{\partial S_g^{local}[U_\mu(x)]}{\partial U_\mu^{(a)}(x)} \tag{3.21}$$

$$= -\frac{\beta}{6}\frac{\partial}{\partial U_\mu^{(a)}(x)} \mathrm{Tr}\left[U_\mu(x)A_\mu(x) + A_\mu^\dagger(x)U_\mu^\dagger(x)\right] \tag{3.22}$$

$$= \frac{i\beta}{6}\mathrm{Tr}\left[T_a\left(U_\mu(x)A_\mu(x) - A_\mu^\dagger(x)U_\mu^\dagger(x)\right)\right] \tag{3.23}$$

But the quantity (...) is traceless and anti-hermitian, i.e. can be written as $\sum_b c_b T_b$, so that using the trace identity $Tr[T_a T_b] = \frac{1}{2}\delta_{ab}$ we find

$$F_g(x,\mu) = \sum_{ab} \frac{i\beta}{6}\mathrm{Tr}\left[T_a c_b T_b\right] T_a = \frac{i\beta}{12}\sum_a c_a T_a \tag{3.24}$$

$$= \frac{i\beta}{12}\left[U_\mu(x)A_\mu(x) - A_\mu^\dagger(x)U_\mu^\dagger(x)\right] \tag{3.25}$$

3.3 Fermion Force

3.4 Force Integration

The integration of the force terms is done by alternating two discrete steps,

3.5 OMF2

4 Inverters

4.1 CG

4.2 CG-Multishift

4.3 CG-Block

A SU(3) Matrix Algebra

A.1 Generators

The generators of SU(3) are the set of traceless 3×3 hermitian matrices T_a, where $a = 1, 2, \ldots, 8$, with the properties

$$\mathrm{Tr}\big[T_a\big] = 0, \quad T_a^\dagger = T_a, \quad \mathrm{Tr}\big[T_a T_b\big] = \tfrac{1}{2}\delta_{ab} \tag{A.26}$$

$$[T_a, T_b] = T_a T_b - T_b T_a = f_{abc} T_c \tag{A.27}$$

where f_{abc} is real and antisymmetric in all indices. An SU(3) matrix U can be written as

$$U = e^{i\omega_a T_a} \tag{A.28}$$

where ω_a are real numbers.

A.2 Differentiation

Differentiation w.r.t an element of the algebra can be defined as

$$\frac{\partial F(U)}{\partial U^{(a)}} \equiv \frac{\partial}{\partial \omega} F(e^{i\omega T_a} U)\Big|_{\omega=0} \tag{A.29}$$

which gives for SU(3) matrices U, V, W,

$$\frac{\partial}{\partial U^{(a)}} (VUW) = iVT_aUW \tag{A.30}$$

$$\frac{\partial}{\partial U^{(a)}} \left(VU^\dagger W\right) = -iVUT_aW \tag{A.31}$$