μRHMC Code Documentation
github.com/lkeegan/muRHMC

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1 Introduction

A simple RHMC code to simulate $n_f + n_f$ QCD with isospin chemical potential $\mu_u = -\mu_d = 2\mu_I$, 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,

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

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

Defining the staple

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

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

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

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 $\mu_u = -\mu_d = 2\mu_I$ and mass m is given by

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

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

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

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

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

$$D(0,m)D^\dagger(0,m) = (D(0,0)+m)(D(0,0)+m)^\dagger = D(0,0)D^\dagger(0,0) + m^2 \tag{2.13}$$

Moreover, if we split the pseudofermion field into even and odd sites we find a block diagonal operator

$$D(0,m)D(0,m)^\dagger\phi = \begin{pmatrix} D(0,0)D^\dagger(0,0)+m^2 & 0 \\ 0 & D(0,0)D^\dagger(0,0)+m^2 \end{pmatrix} \begin{pmatrix} \phi^{even} \\ \phi^{odd} \end{pmatrix} \tag{2.14}$$

so we can find the determinant of just one of these blocks and square it, halving the size of the effective Dirac operator. Equivalently an LU preconditioning of the Dirac operator applied to even and odd sites allows us to compute the inverse of the operator by inverting a hermitian operator applied to only even sites.

However, for non–zero μ_I the γ_5–hermicity property becomes instead $D(\mu_I)^\dagger = \eta_5 D(-\mu_I)\eta_5 = -D(-\mu_I)$. This means that the above matrix is no longer block diagonal, but instead

$$D(\mu_I, m)[D(\mu_I, m)]^\dagger\phi = \begin{pmatrix} D(\mu_I,0)D^\dagger(\mu_I,0)+m^2 & m\hat{D}(\mu_I) \\ m\hat{D}(\mu_I) & D(\mu_I,0)D^\dagger(\mu_I,0)+m^2 \end{pmatrix} \begin{pmatrix} \phi^{even} \\ \phi^{odd} \end{pmatrix} \tag{2.15}$$

where

$$[\hat{D}(\mu_I)]_{xy} = \sinh(\mu_I) \left[U_0(x)\delta_{x,y-\hat{0}} + U_0(x-\hat{0})\delta_{x,y+\hat{0}} \right] \tag{2.16}$$

and the LU preconditioning results in a non-hermitian operator (which is ok but means BiCGstab instead of CG will need to be used for the inversion).

3 HMC

The hamiltonian for the HMC is

$$S[P, U, \phi] = S_p[P] + S_g[U] + S_f[\phi, U] \tag{3.17}$$

where we need to solve the classical equations of motion

$$\frac{dP_\mu(x)}{dt} = -\frac{\partial}{\partial U_\mu(x)} \left(S_g[U] + S_f[\phi, U] \right) = -F_g(x,\mu) - F_f(x,\mu) \tag{3.18}$$

$$\frac{dU_\mu(x)}{dt} = P_\mu(x) \tag{3.19}$$

The following steps are required to update a gauge configuration U:

1. Generate gaussian momenta P
2. Generate χ with distribution $e^{-\chi^\dagger\chi}$, then set $\phi = D\chi$
3. Integrate the force terms to generate U', P'
4. 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

$$P_\mu(x) = \sum_{a=1}^{8} p_\mu^a(x) T_a \tag{3.20}$$

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

$$S_p[P] = \sum_{x,\mu} \mathrm{Tr}\left\{[P_\mu(x)]^2\right\} = \frac{1}{2}\sum_{x,\mu}\sum_{a=1}^{8}[p_\mu^a(x)]^2 \tag{3.21}$$

so we can generate momenta simply by sampling the numbers p^a from the normal 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 Pseudofermions

The pseudofermion fields are 3-component complex vectors defined on each site of the lattice. To generate a field ϕ according to the distribution $e^{-S_f[U]}$ we can first generate a complex vector χ with distribution $e^{-\chi^\dagger\chi}$, i.e. set each of the six real numbers that make up the 3 complex components of χ to a random value r sampled from the normal gaussian distribution $e^{-r^2/2}$.

Then set $\phi = D(\mu_I, m)\chi$.

3.3 Gauge Force

The gauge force is given by

$$F_g(x,\mu) = \sum F_g^a(x,\mu) T_a \tag{3.22}$$

where

$$\begin{aligned}
F_g^a(x,\mu) &= \frac{\partial S_g[U]}{\partial U_\mu^{(a)}(x)} = \frac{\partial S_g^{local}[U_\mu(x)]}{\partial U_\mu^{(a)}(x)} && (3.23)\\
&= -\frac{\beta}{6}\frac{\partial}{\partial U_\mu^{(a)}(x)} \mathrm{Tr}\left[U_\mu(x)A_\mu(x) + A_\mu^\dagger(x)U_\mu^\dagger(x)\right] && (3.24)\\
&= \frac{i\beta}{6}\mathrm{Tr}\left[T_a\left(U_\mu(x)A_\mu(x) - A_\mu^\dagger(x)U_\mu^\dagger(x)\right)\right] && (3.25)
\end{aligned}$$

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 $Tr[T_aT_b] = \frac{1}{2}\delta_{ab}$ we find

$$\begin{aligned}
F_g(x,\mu) &= \sum_{ab}\frac{i\beta}{6}\mathrm{Tr}\left[T_a c_b T_b\right] T_a = \frac{i\beta}{12}\sum_a c_a T_a && (3.26)\\
&= \frac{i\beta}{12}\left[U_\mu(x)A_\mu(x) - A_\mu^\dagger(x)U_\mu^\dagger(x)\right] && (3.27)
\end{aligned}$$

3.4 Fermion Force

3.5 Force Integration

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

$$I_P(P, F, \epsilon) : P \leftarrow P - \epsilon F \tag{3.28}$$

$$I_U(U, P, \epsilon) : U \leftarrow e^{i\epsilon P} U \tag{3.29}$$

which can be combined to form reversible integrators of different orders.

3.6 Leapfrog

The simplest integrator is the leapfrog, where an integration step of size ϵ is given by

- $I_P(\epsilon/2)$
- $I_U(\epsilon)$
- $I_P(\epsilon/2)$

giving a second order integrator with one Dirac operator inversion required per step.

3.7 OMF2

One integration step of size ϵ is given by

- $I_P(\lambda\epsilon)$
- $I_U(\epsilon/2)$
- $I_P((1 - 2\lambda)\epsilon)$
- $I_U(\epsilon/2)$
- $I_P(\lambda\epsilon)$

where λ is a tunable parameter, e.g. $\lambda = 0.193$. This is also a second order integrator, with $\sim 10\times$ smaller errors than leapfrog, but requires two Dirac operator inversions per step.

3.8 OMF4

todo?

4 Inverters

4.1 CG

4.2 BiCGstab

4.3 CG-Multishift

4.4 BiCGstab-Multishift

4.5 BiCGstab-Block

4.6 BiCGstab-Block-Multishift

5 Observables

5.1 Gauge Observables

5.1.1 Plaquette

The plaquette is averaged over the whole lattice and normalised to 1,

$$plaquette[U] = \frac{1}{L^4} \sum_{x} \frac{1}{6} \sum_{\mu<\nu} \frac{1}{3} Re\mathrm{Tr}\left[U_\mu(x) U_\nu(x+\hat{\mu}) U_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x)\right] \tag{5.30}$$

5.1.2 Polyakov Loop

The polyakov loop is the product of links in the time direction, averaged over the spatial voume, normalised to 1,

$$polyakov[U] = \frac{1}{L^3} \sum_{x}^{L^3} \frac{1}{3} Re\mathrm{Tr}\left[\prod_{t=0}^{T-1} U_0(x,t)\right] \tag{5.31}$$

5.2 Fermionic Observables

Fermionic observables generally involve traces of the inverse of the Dirac operator, which can be estimated stochastically by inverting gaussian noise vectors. For this purpose we define here ϕ as a gaussian noise vector with unit norm, $\phi^\dagger.\phi = 1$, which we use as a source vector to find

$$\chi = \left[D(\mu_I, m) D^\dagger(\mu_I, m)\right]^{-1} \phi = -\left[D(\mu_I, m) D(-\mu_I, -m)\right]^{-1} \phi \tag{5.32}$$

and also

$$\psi = -\left[D(\mu_I, m)\right]^{-1} \phi = D(-\mu_I, -m)\chi \tag{5.33}$$

from which we can construct estimators of various fermionic observables.

5.2.1 Quark condensate

$$condensate = -\left\langle \phi^\dagger.\psi \right\rangle \tag{5.34}$$

5.2.2 Pion susceptibility

$$susceptibility = \left\langle \phi^\dagger.\chi \right\rangle \tag{5.35}$$

5.2.3 Isospin density

$$density = 2\Re \left\langle \chi^\dagger . \left(\frac{\partial D(\mu_I, m)}{\partial \mu_I} \psi \right) \right\rangle \tag{5.36}$$

where

$$\left[\frac{\partial D(\mu_I, m)}{\partial \mu_I} \psi \right]_x = \frac{\mu_I}{2} \left[e^{\mu_I} U_0(x) \psi(x + \hat{0}) + e^{-\mu_I} U_0^\dagger(x - \hat{0}) \psi(x - \hat{0}) \right] \tag{5.37}$$

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

$$\mathrm{Tr}\big[T_a\big] = 0, \quad T_a^\dagger = T_a, \quad \mathrm{Tr}\big[T_a T_b\big] = \tfrac{1}{2}\delta_{ab} \tag{A.38}$$

$$[T_a, T_b] = T_a T_b - T_b T_a = f_{abc} T_c \tag{A.39}$$

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

$$U = e^{i\omega_a T_a} \tag{A.40}$$

where ω_a are real numbers.

A.2 Differentiation

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

$$\frac{\partial F(U)}{\partial U^{(a)}} \equiv \frac{\partial}{\partial \omega} F(e^{i\omega T_a} U)\Big|_{\omega=0} \tag{A.41}$$

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

$$\frac{\partial}{\partial U^{(a)}} (VUW) = iVT_a UW \tag{A.42}$$

$$\frac{\partial}{\partial U^{(a)}} \big(VU^\dagger W\big) = -iVUT_a W \tag{A.43}$$