Algorithms for lattice QCD II

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HMC

Momentum Heatbath

Refresh momenta π (Gaussian random numbers)

Molecular Dynamics

Solve numerically MD equations for some MC time τ (trajectory) deriving from Hamiltonian $H = \frac{1}{2}(\pi, \pi) + S[U]$.

Acceptance Step

Correcting for inaccuracies in integration.

Numerical integration

$$\dot{U}_{x,\mu} = \pi_{x,\mu} U_{x,\mu} \qquad\qquad \dot{\pi}_{x,\mu} = -F_{x,\mu}$$

Splitting methods

$$H = \frac{1}{2}(\pi, \pi) + S[U] = T + S$$

- Eom for each part T, S can be solved exactly $\rightarrow$ symplectic
- T defines T_U

$$U_{x,\mu}(\tau) = e^{\pi\tau} U_{x,\mu}(0), \quad \pi(\tau) = \pi(0)$$

- S defines T_p

$$U_{x,\mu}(\tau) = U_{x,\mu}(0), \quad \pi(\tau) = \pi(0) - \tau F$$

Splitting methods

$$T_U = e^{\epsilon\hat{T}}: \qquad U_{x,\mu}(\epsilon) = e^{\pi\epsilon}U_{x,\mu}(0), \qquad \pi(\epsilon) = \pi(0)$$

$$T_p = e^{\epsilon\hat{S}}: \qquad U_{x,\mu}(\epsilon) = U_{x,\mu}(0), \qquad \pi(\epsilon) = \pi(0) - \epsilon F$$

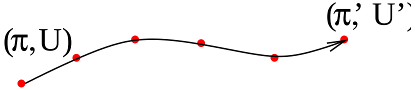
Can be put together in any order.

Legal integrator:
Time steps of T_U and T_p sum up to 1.

Symmetric integrator
→Integration error automatically $O(\epsilon^2)$

Example: leapfrog ($\epsilon = \tau/N$)

$$T = (T_U(\epsilon/2)T_p(\epsilon)T_U(\epsilon/2))^N$$



Omelyan & Co

Leapfrog has been long-time workhorse
Robust, but in general not optimal.

Easy improvement without detailed knowledge of physics system.

Seminal paper `Omelyan, Mrygold, Folk, 2003`

Introduce *reduandant* parameters and optimize

$$T = [T_p(\epsilon\lambda)T_U(\epsilon/2)T_p(\epsilon(1-2\lambda)T_U(\epsilon/2)T_p(\epsilon\lambda)]^{N/2}$$

$\lambda = 0.19$ performs roughly $2\times$ better than leapfrog.

The paper contains O(100) integrators.

Optimizing integrators

Exact time evolution operator

$$e^{\tau \frac{d}{dt}} = e^{\tau \hat{H}} \qquad \text{with} \qquad \hat{H} = -\frac{\delta S}{\delta U}\frac{\partial}{\partial U} - \frac{\delta T}{\delta \pi}\frac{\partial}{\partial \pi} = \hat{S} + \hat{T}$$

with $T(\pi) = (\pi, \pi)$ and $S[U]$ the action.
$\hat{H}$ is the Hamiltonian vector field.

Leap-frog integrator

$$\begin{aligned} & [e^{\epsilon/2\,\hat{S}} e^{\epsilon\,\hat{T}} e^{\epsilon/2\,\hat{S}}]^{\tau/\epsilon} \\ = & \exp\{(\hat{S}+\hat{T})\epsilon - \frac{\epsilon^3}{24}([\hat{S},[\hat{S},\hat{T}]] + 2[\hat{T},[\hat{S},\hat{T}]])\}^{\tau/\epsilon} \\ = & \exp\{(\hat{S}+\hat{T})\tau - \frac{\tau\epsilon^2}{24}([\hat{S},[\hat{S},\hat{T}]] + 2[\hat{T},[\hat{S},\hat{T}]])\} \end{aligned}$$

Baker-Campbell-Hausdorff formula has been used.
see series of paper by Clark and Kennedy

Shadow Hamiltonian

For each symplectic integrator, there is the conserved **shadow Hamiltonian**

Can be constructed by a power series
Commutators $\rightarrow$ Poisson brackets

$$\begin{aligned}\tilde{H} &= H + \epsilon^2(c_1\,\{S,\{S,T\}\} + c_2\{T,\{S,T\}\}) \\ &= H + \epsilon^2(c_1\,\partial_a S \partial_a S - c_2\,\pi_a \pi_b \partial_a \partial_b S)\ldots\end{aligned}$$

Convergence of the series?

c_1 and c_2 depend only on the integrator

For a long time, it has been believed that what matters is the *size* of

$$\delta H = \tilde{H} - H$$

Optimizing integrators

At the beginning of the trajectory

$$H_1 = \frac{1}{2}(\pi_1, \pi_1) + S[U_1] \qquad \tilde{H}_1 = H_1 + \delta H_1 \tag{1}$$

At the end of the trajectory

$$H_2 = \frac{1}{2}(\pi_2, \pi_2) + S[U_2] \qquad \tilde{H}_2 = H_2 + \delta H_2 \tag{2}$$

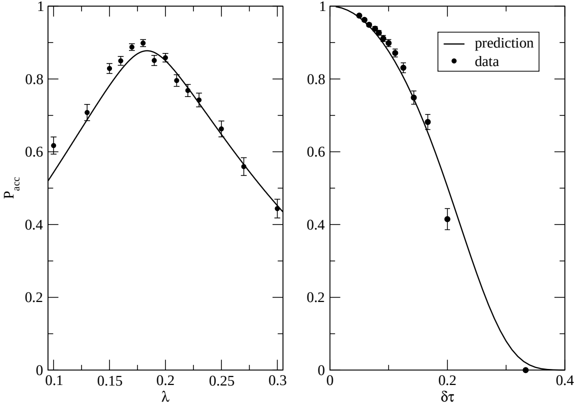
During the trajectory, $\tilde{H}$ is conserved. $\tilde{H}$=$\tilde{H}_1$=$\tilde{H}_2$

$$\Delta H = H_2 - H_1 = (H_2 - \tilde{H}) - (H_2 - \tilde{H}) = \delta H_2 - \delta H_1$$

What matters is the fluctuation of δH.

Example

From Clark, Joo, Kennedy, Silva, 1108.1828



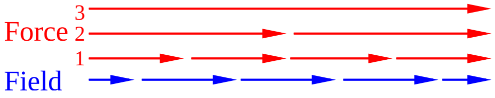
Multiple time scales

In the HMC, different forces have vastly different size.

$$F_g \gg F_{\mathrm{ferm},UV} \gg F_{\mathrm{ferm},IR}$$

This is the oppostite ordering of the cost of their computation.

Multiple time scale integrators have been proposed.



The idea is to integrate “large forces” on a finer time scale — exacter.

Multiple time scales

$$T_\pi(\epsilon/2)T_U(\epsilon)T_\pi(\epsilon/2)$$
$$\to T_{\pi,1}(\epsilon/2)\,[T_{\pi,2}(\epsilon/2m)\,T_U(\epsilon/m)\,T_{\pi,2}(\epsilon/2m)]^m\,T_{\pi,1}(\epsilon/2)$$

Experimental finding: it never works as well as expected.

Can be understood by Shadow Hamiltonian

$$\tilde{H} = H + [c_1(F_1, F_1) + c_2\pi^a\pi^b S_1^{(ab)} + c_2(F_1, F_2) + \frac{1}{m^2}(c_2(F_2, F_2) + c_2\pi^a\pi^b S_2^{(ab)})]$$

Interference term between "large" and "small" force not suppressed by relative times scale m.

Summary: Integrators

Integrators have contributed to improvement in algorithms.

Typical gains are factor two.
No miracles to be expected.

Difficulty separating IR from UV.

Optimization by measurement is possible.

Fermions
Formulation of the theory

Fermions

Textbook verions contains Grassmann fields ψ and $\bar{\psi}$

$$Z = \int \prod_i d\psi_i d\bar{\psi} \prod_{i,\mu} dU_{i,\mu} e^{-S_g - \sum_f \bar{\psi}_f D(m_f) \psi_f}$$

We integrate out the fermions and get the quark determinant

$$Z = \int \prod_{i,\mu} dU_{i,\mu} \prod_f \det D(m_f)\, e^{-S_g}$$

Determinant not usable in large volume situation
$\rightarrow$ too complicated/expensive to compute

Fermions in simulations

Ideally, we would want to use

$$S_{\text{ferm}} = -\sum_{i=1}^{N_f} \text{tr}\,\log D(m_i) = -\sum_{i=1}^{N_f} \log\,\det D(m_i)$$

Unfortunately, the determinant of a $N \times N$ matrix is virtually impossible to compute for large N.

Need $\mathrm{O}(N^2)$ operations.

Large memory requirement.

Is numerically extremely unstable.

$\Rightarrow$
Need algorithm with is based on solutions of linear equations.

Pseudofermions

PETCHER, WEINGARTEN'81

$$\det Q^2 \propto \int [\mathrm{d}\phi][\mathrm{d}\phi^\dagger]\, e^{-(\phi,\, Q^{-2}\phi)}\,, \qquad Q = \gamma_5 D$$

Pseudofermion field ϕ can be easily generated:

- Generate Gaussian complex-valued quark field η

$$P[\eta] \propto e^{-(\eta,\eta)}$$

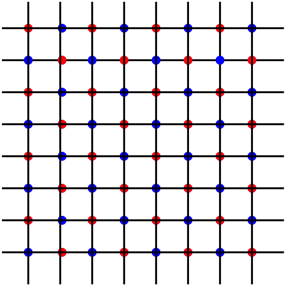
- Multiply with Q

$$\phi = Q\eta$$

Even–odd preconditioning

The Wilson Dirac operator connects only neighboring sites.

Label them “even” and “odd”.



$$D = \begin{pmatrix} D_{ee} & D_{eo} \\ D_{oe} & D_{oo} \end{pmatrix}$$

D_{oo} and D_{ee} are site-diagonal matrices.

Even–odd preconditioning

Matrix identity

$$\begin{pmatrix} D_{ee} & D_{eo} \\ D_{oe} & D_{oo} \end{pmatrix} =$$
$$\begin{pmatrix} 1 & D_{eo}D_{oo}^{-1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} (D_{ee} - D_{eo}D_{oo}^{-1}D_{oe}) & 0 \\ 0 & D_{oo} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ D_{oo}^{-1}D_{oe} & 1 \end{pmatrix}$$

For the determinant this means

$$\det D = \det D_{oo}\, \det(D_{ee} - D_{eo}D_{oo}^{-1}D_{oe}) \equiv \det D_{oo} \det \hat{D}$$

with $\hat{D}$ the Schur complement.

In the following, I will mostly write D or $Q = \gamma_5 D$.
In practice, this frequently means $\hat{D}$ or $\hat{Q}$.

Partition function

Include pseudofermions in path integral.

$$Z = \int [dU][d\pi][d\phi][d\phi^\dagger]\, e^{-\frac{1}{2}(\pi,\pi) - S_g[U] - (\phi, \frac{1}{Q^2}\phi) + 2\log \det Q_{oo}}$$

S_g: gauge action

effective fermion action for $N_f = 2$.

$$S_{f,eff} = (\phi, \frac{1}{\hat{Q}^2}\phi) - 2\log \det Q_{oo}$$

HMC

Momentum and pseudofermion Heatbath

Refresh momenta π
Refresh pseudofermions $\phi \rightarrow$ kept fixed during trajectory

Molecular Dynamics

Solve numerically MD equations for some MC time τ (trajectory) deriving from Hamiltonian $\boldsymbol{H} = \frac{1}{2}(\pi, \pi) + \boldsymbol{S}[\boldsymbol{U}]$.

Acceptance Step

Correcting for inaccuracies in integration.

Problems

Pseudofermions — Petcher, Weingarten'81

$$\det Q^2 \propto \int \mathrm{d}\phi \, e^{-(\phi,\, Q^{-2}\phi)}$$

- Works only for pairs of degenerate flavors
  Solution: take square root $\rightarrow$ PHMC, RHMC
- Force evaluation expensive: 2 solutions of Dirac eq.

$$F_{\mathrm{pf}} = -(\phi,\, Q^{-2}\, \delta Q\, Q^{-1}\, \phi) + \text{h.c.}$$

- Seems somewhat unnatural
  Start with manifestly local action
  $\rightarrow$ quite non-local expression

Berlin Wall

Status 2000 Quarks 16× heavier than in nature.
No perspective even with 2010 computers.

Coarse lattices $a \approx 0.1\text{fm}$
(the typical length scale is 1fm)

Cost of a simulation (Ukawa Lattice 2001)

$$\text{Cost} = C \left[\frac{\#conf}{1000}\right] \cdot \left[\frac{m_q}{16 m_{\text{phys}}}\right]^{-3} \cdot \left[\frac{L}{3\text{fm}}\right]^{5} \cdot \left[\frac{a}{0.1\text{fm}}\right]^{-7}$$

$C \approx 2.8$ Tflops year

Fermions

Pseudofermions — PETCHER, WEINGARTEN'81

$$\det Q^2 \propto \int \mathrm{d}\phi\, e^{-(\phi,\, Q^{-2}\phi)}$$

- **HMC + single pseudofermion action not successful**
- Compare

$$F_{\mathrm{pf}} = \delta(\phi,\, Q^{-2}\phi) \qquad \text{and} \qquad F_{\mathrm{ex}} = -\delta \mathrm{tr}\,\log Q^2$$

- F_{pf} is "stochastic estimate" of F_{ex}
  At beginning of the trajectory $\langle F_{\mathrm{pf}}\rangle_\phi = F_{\mathrm{ex}}$
- Very large fluctuations in F_{pf}

$$|F_{\mathrm{pf}}| \gg |F_{\mathrm{ex}}|$$

Fermions
Modifications

Determinant Splitting

Insight

- Need better estimate of determinant.
- Frequency splitting.

Mass preconditioning

Hasenbusch'01, Hasenbusch,Jansen'03

$$\det Q^2 = \det \frac{Q^2}{Q^2 + \mu^2} \det(Q^2 + \mu^2)$$

- Each determinant represented by pseudo-fermion
- "Pauli-Villars" for fermion force
- more intermediate $\mu \to$ Noise reduction in force.
- success depends on choice of μ. Urbach et al'04

Numerical examples

Action

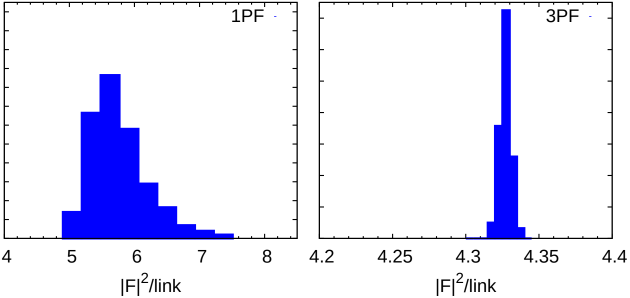
- $N_{\mathrm{f}} = 2 + 1$ NP improved Wilson fermions
- Iwasaki gauge action
- 64×32^3 lattice with $a = 0.09$fm
- studied extensively by PACS-CS — AOKI ET AL'09,'10
- $m_\pi = 200$MeV
- $m_\pi L = 3$

Algorithm — M. LÜSCHER, S.S.'12

- Reweighting to avoid stability problems.
- Generated with public `openQCD` code.
  `http://cern.ch/luscher/openQCD`

Effect of determinant factorization

Forces for light quark, 20 configurations. $\mu_1 = 0.05$, $\mu_2 = 0.5$



- Fluctuations of force not much reduced.
- Fluctuations in **norm** squared of force:
  Spread reduced by more than factor 100.
  (Different scale!)

Understanding the improvement

Framework — Clark, Joo, Kennedy, Silva'11

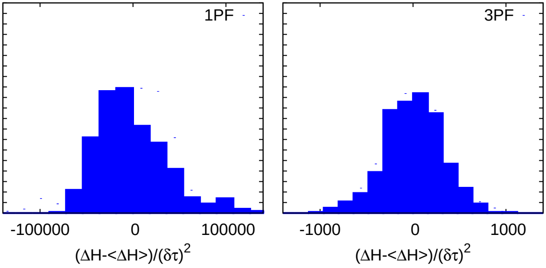
- Shadow Hamiltonian of symplectic integrators

$$\tilde{H} = H + (c_1\, \partial_a S \partial_a S - c_2\, \pi_a \pi_b \partial_a \partial_b S)\delta\tau^2 + \dots$$

- Large cancellation between the two terms
  → **potential for optimization.**

- 2nd order minimum norm integrators:
  minimum of $c_1^2 + c_2^2$ Omelyan, Mrygold, Folk'03
- **Symplectic integrators profit from reduced fluctuations in norm of force.**

Numerical examples



- $\Delta H = \tilde{H} - H$, fermions only.
- Second order min. norm Omelyan integrator.
- Much larger step-size possible.