Simulations in Lattice QCD

Lattice Practice 2024 at The Cyprus Institute - Simulations

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- Basic
  - Markov Chain Monte Carlo
- Intermediate
  - Hybrid Monte Carlo algorithm
- Advance
  - Fermions in simulations and more

this talk is based on Mattia Della Brida's constribution from 2021

Goal: Evaluation of pathintegral

Compute

$$< \square >= \frac{1}{Z} \int D\phi e^{-S(\phi)} \square(\phi) \qquad D\phi = \prod_{i=1}^{M} d\phi_i \quad e.g. \quad \phi = U, \overline{\psi}, \psi$$

- Deterministic integration methods not feasible!

  Current lattice QCD simulations can have M = O(10^9)

- Monte Carlo: evaluates integral by sampling the integrand at points selected with probability under the

  integration measure

Basic idea

1. Generate sequence of field configurations with probability

$$P(\phi^{(t)}) = \frac{1}{Z} e^{-S(\phi^t)}$$

1. Evaluate

$$\overline{O} = \frac{1}{N} \sum_{t=1}^{N} \square(\phi^{(t)})$$

Monte Carlo integration

Consider

$$\langle f \rangle = \int_D dx\ f(x) \qquad x = (x_1, \dots, x_d) \quad D = [0,1]^d$$

Compute

$$\overline{f_N} = \frac{1}{N} \sum_{k=1}^{N} f(x^{(k)}) \qquad x^{(k)} = (x_1^{(k)}, \dots x_d^{(k)})$$

where *x* are random numbers uniformly distributed within [0,1] . This requires a solid random number generator.

Central limit theorem

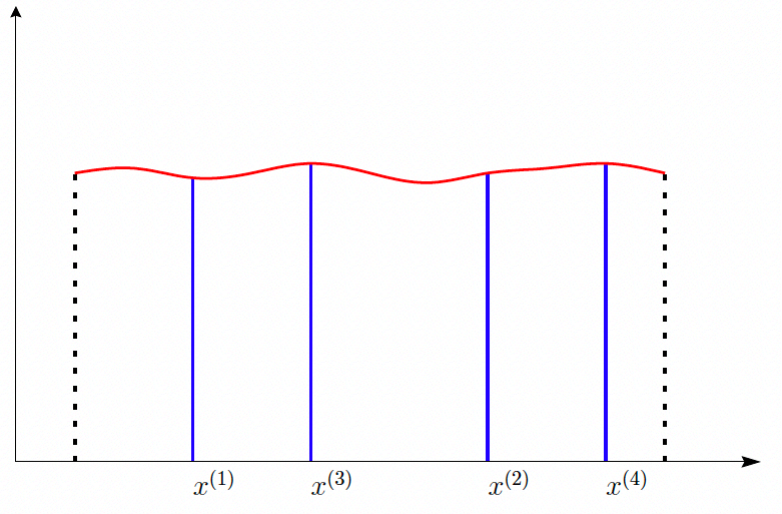
$$P(\overline{f_N}) \overset{N\to\infty}{\propto} \exp\left[-\frac{1}{2}\frac{(\overline{f_N} - \langle f \rangle)^2}{\mathrm{var}(f)/N}\right] \quad \text{with} \quad \mathrm{var}(f) = \langle (f - \langle f \rangle)^2 \rangle$$

with

$$\overline{f_N} - \langle f \rangle = (O)(1/\sqrt{N})$$

- Uncertainty of results are of statistical rather than systematic nature
- Error scales as $1/\sqrt{N}$ independently of the dimension d
- Rate of convergence depends on var(f)

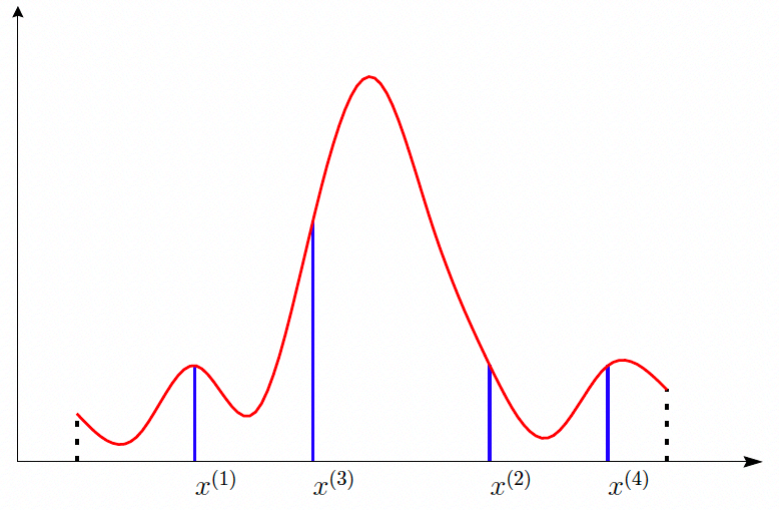
Monte Carlo integration



Uniformly sampling is effective for approximately constant functions;

here:

var(f) is small



in contrast:

Sampling of more complicated functions is more difficult

here

Using uniformly distributed random numbers can easily require large values of N to reach a good precision.

Importance sampling

Consider

$$\langle f \rangle = \int_D dx \; p(x) \left[\frac{f(x)}{p(x)} \right] = \langle g \rangle_p \qquad \text{with} \quad p(x) > 1 \quad \text{and} \quad \int_D dx \; p(x) = 1$$

with

$$g(x) = \frac{f(x)}{p(x)}$$

Compute

$$\overline{g_N} = \frac{1}{N} \sum_{k=1}^{N} g(x(k)) \qquad x^{(k)} = (x_1^{(k)}, \ldots x_d^{(k)})$$

with x random vectors distributed according to p(x)

Importance sampling

Central limit theorem

$$P(\bar{g}_N) \overset{N\to\infty}{\propto} \exp\left[-\frac{1}{2}\frac{(\overline{g_N} - \langle f\rangle)^2}{\mathrm{var}(g)/N}\right] \quad \text{with} \quad \mathrm{var}(f) = \langle (g - \langle f\rangle)^2\rangle_p$$

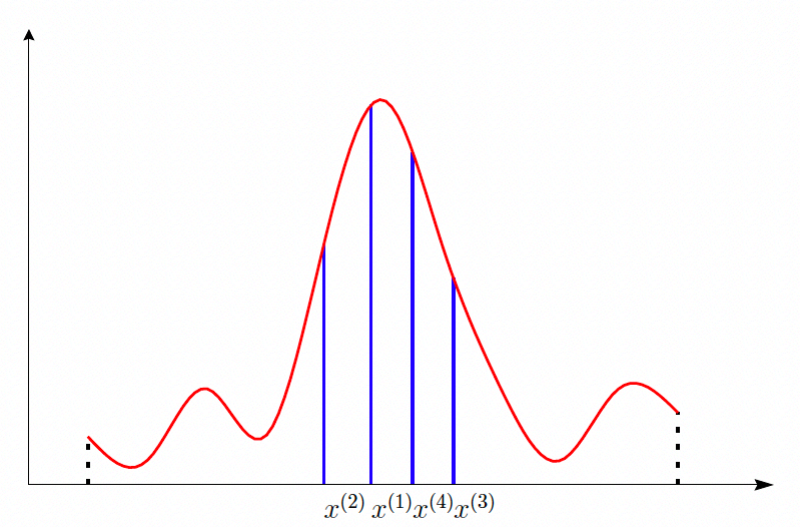
with

$$\langle f\rangle = \overline{g_N} \pm \sigma(\overline{g_N}) \quad \sigma(\overline{g_N}) = \sqrt{\mathrm{var}(g)/N}$$

Choice of p(x) can signicantly affect convergence

- Optimal p(x) but this requires <|f|>
- Only relatively simple distributions p(x) can be directly sampled, e.g. via inverse transform, hit-and-miss, etc.

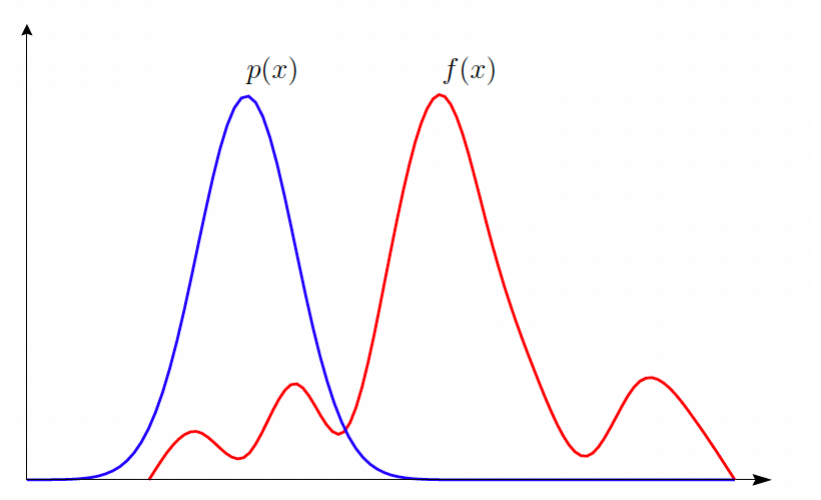
Importance sampling



Effective

A better sampling distribution allows for sampling more frequently the regions that give more contribution to the integral

$\Rightarrow$ faster convergence



However

When the sampling distribution and the function to integrate have little overlap, we say there is an overlap problem

$\Rightarrow$ very ineffective sampling

Importance sampling

Application to lattice field theory:

$$\langle \square \rangle = \int D\phi \, P_S(\phi) \square(\phi) \qquad P_S(\phi) = \frac{1}{Z} e^{-S(\phi)}$$

- Sharply peaked around configurations of minimal action
- Far too **complicated distribution** for a direct sampling
- We need method based on relative probabilities
  - avoids computation of normalization Z
- Convenient, but not necessarily optimal for all O(x)
  - may result in some large variances
- $S(\phi)$ must be real (and bounded)

Markov Chain Monte Carlo

A (discrete) Markov chain is a sequence of random variables

$$\phi^{(0)} \to \phi^{(1)} \to \cdots \to \phi^{(t)} \to \cdots \cdots \to \phi^{(N)} \qquad \phi(t) \in \Omega \leftarrow \text{state space}$$

which probability of extraction is given by a transition probability

$$T(\phi \to \phi')$$

(t is referred to as Markov time)

Properties

1. **Markovian**

$$T(\phi \to \phi') \quad \text{only depends on the current } (\phi) \text{ and future } (\phi') \text{ state}$$

2. **Time-homogeneous**

$$T(\phi \to \phi') \quad \text{is constant along the chain, i.e. t-independent}$$

3. **Probability (density)**

$$\int D\phi' \; T(\phi \to \phi') = 1 \quad \text{and} \quad T(\phi \to \phi') >= 0$$

4. **Ergodic (& irreducible)**

$$T(\phi \to \phi') > 0 \quad \forall \phi, \phi' \in \Omega$$

A chain is completely specified by the starting distribution $P_0(\phi^{(0)})$ and $T(\phi \to \phi')$

Why Markov chains ?

T is a linear map: $T : \square \to \square$, where $\square$ is the linear space of real functions on Ω.

This contains the subset of probability distributions P_Ω . Along a Markov chain

$$P_{n+1}(\phi') = (TP_n)(\phi') = \int D\phi\, P_n(\phi) T(\phi \to \phi')$$

with

$$P^{(n)} \in P_\Omega$$

Equilibrium distribution

Given an ergodic Markov chain with transition probability T, the limit

$$\lim_{t\to\infty} P^{(t)} = \lim_{t\to\infty} T^t P^{(0)} = \Pi \in P_\Omega$$

exits, is unique and independent on $P^{(0)} \in P_\Omega$.

Im particular, Π , is the unique fixed point of the chain, i.e. $(TP) = P \Leftrightarrow P = \Pi$

Remark

This is the consequence that T has a unique eigenvalue $\lambda_0 = 1$ and

$\lambda_0 > |\lambda_1| \geq |\lambda_2| \geq \ldots$, where $T v_n = \lambda_n v_n$ and $v_0 = \Pi$

$$P^{(t)} = \Pi + \sum_{n>0} c_{t,n} (\lambda_n)^n v_n \overset{t\to\infty}{=} \Pi + O(e^{-t/\tau^{exp}}) \quad \tau^{exp} = 1/\ln|\lambda_1|$$

Detailed balance condition

How can we find a T that has the desired distribution Π as equilibrium distribution ?

If T is ergodic, a sufficient (but not necessary) condition is detailed balance

$$\Pi(\phi')T(\phi' \to \phi) = \Pi(\phi)T(\phi \to \phi')$$

Proof:

Integrate both sides over ϕ and use $\int D\phi\, T(\phi' \to \phi) = 1.$

This gives the stability or fix point condition

$$\Pi(\phi') = (T\Pi)(\phi')$$

Since T is ergodic, its fixed point is unique and corresponds to its equilibrium distribution

Remarks

- If T satisfies detailed ballance or stability but is not ergodic, the convergence for large t is not guaranteed
- We can combine transition probabilities:

  $$T = T_1 \circ T_2 \circ \dots,$$

  with Ti not ergodic but satisfies detailed balance and such that T is ergodic. T will automatically satisfy the stability condition and converge to PI.

Metropolis-Hastings algorithm

A simple way to satisfy detailed balance is given by

$$T(\phi \to \phi') = P_C(\phi \to \phi')P_A(\phi \to \phi')$$

- A candidate ϕ' is proposed from ϕ with probability P_C
- ϕ' is accepted as the next step in the chain with probability P_A
- If ϕ' is rejected, ϕ is the next element, i.e. it is repeated in the chain

Acceptance probability

We can ensure detailed balance for any choice of Pc by taking

$$P_A(\phi \to \phi') = \min\left[1, \frac{\Pi(\phi')P_C(\phi' \to \phi)}{\Pi(\phi)P_C(\phi \to \phi')}\right]$$

If $P_C(\phi \to \phi') = P_C(\phi' \to \phi)$ (symmetric proposal)

$$P_A(\phi \to \phi') = \min\left[1, \frac{\Pi(\phi')}{\Pi(\phi)}\right]$$

Other PA are in principle possible but have lower acceptance.

Metropolis-Hastings algorithm

Remarks

- only the relative probabilities $\Pi(\phi')/\Pi(\phi)$ are needed to construct T

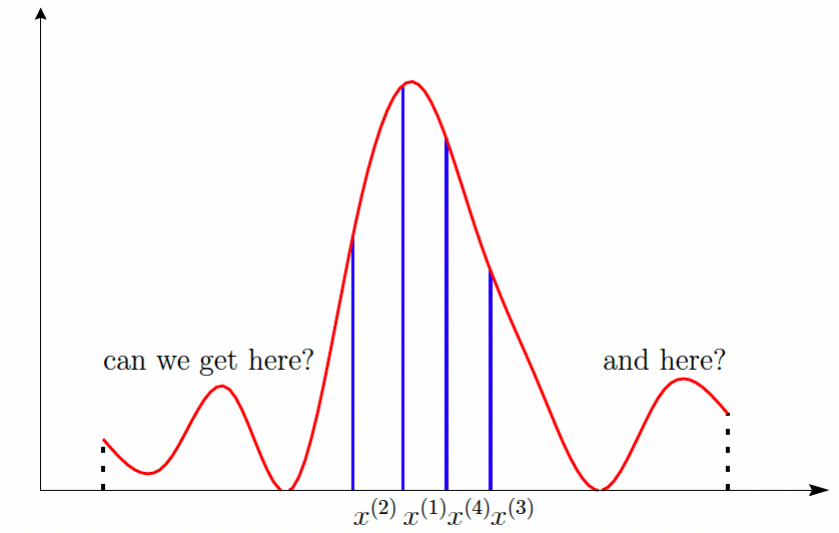
$$\Rightarrow \text{ no need for normalization of } \Pi$$

- We cannot use Markov chains to compute integrals directly, only ratios

$$\langle \square \rangle = \frac{\int D\phi \; \Pi(\phi)\square(\phi)}{\int D\phi \; \Pi(\phi)}$$

In practice there may be challenges in assuring that T is ergodic

-> can lead to improper sampling and biased results



Simulating lattice phi4-theory

Action

$$S = \sum_x \left[\sum_{\mu=0}^{D-1} \frac{1}{2} \left(\frac{\phi(x+\mu\hat{)} - \phi(x)}{a} \right) + \frac{m_0^2}{2}\phi^2(x) + \frac{g_0}{4!}\phi^4(x) \right]$$

Accept-reject step

1. Set $\phi(x) = \phi_0(x)$
2. Propose $[\Delta > 0,\ r \in [0,1)]\ \phi'(x) = \phi(x) + \Delta(r - \frac{1}{2})$
3. Accept ϕ' or keep ϕ according to

$$P_A = \min\left[1, e^{-\delta S}\right] \qquad \delta S = S(\phi') - S(\phi)$$

δS only involves $\phi'(x), \phi(x), \phi(x \pm \hat{\mu})$

1. Repeat 2. & 3. for all points x [sweep]
2. Skip k sweeps (thermalization) so that

$$P(\phi^{(t)}) \propto e^{-S(\phi^{(t)})} \qquad \Rightarrow \overline{\square} = \frac{1}{N} \sum_{t=k+1}^{N+k} \square(\phi^{(t)}) \qquad \Rightarrow \overline{\square} = \langle \square \rangle + O(1/\sqrt{N})$$

Autocorrelations

Subsequent states in a Markov chain are correlated

$$\langle\langle \square^{(k)} \square^{(l)} \rangle\rangle \neq \langle\langle \square^{(k)} \rangle\rangle \langle\langle \square^{(l)} \rangle\rangle \qquad \square \equiv \square(\phi^{(k)}) \qquad \langle\langle \cdot \rangle\rangle \equiv \text{avg. indp. chains}$$

The error on time-averges

$$\sigma^2(\overline{\square}) = \langle\langle (\overline{\square} - \langle \square \rangle)^2 \rangle\rangle = \frac{1}{N^2} \sum_{k,l=1}^{N} \langle\langle \square^{(k)} \square^{(l)} \rangle\rangle - \langle \square \rangle^2 \qquad [\langle\langle \square^{(k)} \rangle\rangle = \langle \square \rangle]$$

can be written as

$$\sigma^2(\overline{\square}) = \frac{2\tau^{int,\square} \text{var}(\square)}{N} \qquad \text{with} \quad \text{var}(\square) = \langle \square^2 \rangle - \langle \square \rangle^2$$

Integrated autocorrelation time is given by

$$\tau^{int,\square} = \frac{1}{2} \left[1 + 2 \sum_{t=1}^{N-1} \frac{\Gamma^{(\square)}(t)}{\Gamma^{(\square)}(0)} \right]$$

and the **autocorrelation function**

$$\Gamma^{(\square(t))} = \langle\langle \square^{(t+i)} \square^{(i)} \rangle\rangle - \langle \square \rangle^2$$

- Error scales via $N/2\tau^{int}$
- for time-homogeneous chains the function only depends on the distance in Markov time

Autocorrelations

Spectral decomposition

$$\Gamma^{(\square)}(t) = \sum_{n>0} b_{n,\square} e^{-t/\tau_n} \qquad \tau_n = -1/\ln|\lambda_n| \qquad [\lambda \text{ eignv. of } T]$$

- τ_n only depends on the properties of the Markov chain

  $\Rightarrow \tau^{exp} = \tau_1$ is the "slowest" mode to decorrelate
- $b_{n,\square}$ determines the coupling of O to the n-th mode

  $\Rightarrow$ it can vary significantly among observables

Estimate of the autocorrelation function

$$\overline{\Gamma^{(\square)}}(t) = \frac{1}{N-t} \sum_{i=1}^{N-t} [(\square^{(i+t)} - \overline{\square})(\square^{(i)} - \overline{\square})]$$

Estimate of the integrated autocorrelation time

Relative error on the autocorrelation function grows exponentially -> we must choose a cutoff W

$$\tau^{int,\square,W} = \frac{1}{2}\left[1 + 2\sum_{t=1}^{W} \frac{\Gamma^{(\square)}(t)}{\Gamma^{(\square)}(0)}\right]$$

and find a compromise between statistical and systematic error

Autocorrelations

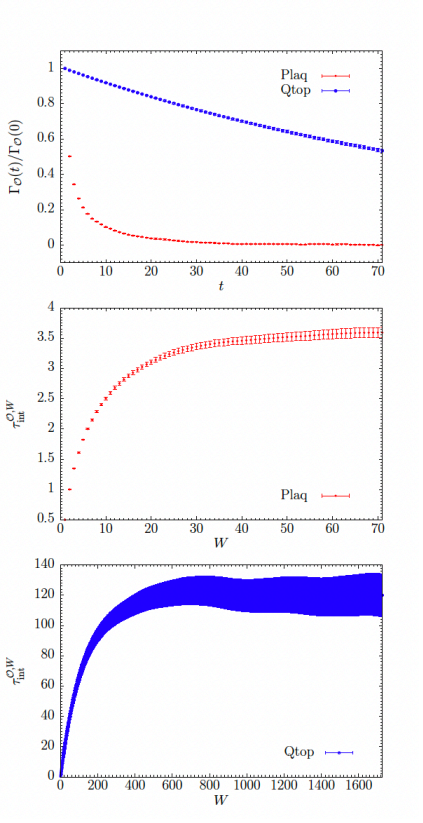
- Autocorrelations (AC) are unavoidable in Markov Chain Monte Carlo (MCMC)
- A proper estimate of AC is curical
  - no AC -> no error -> no result

Ideal:

- Length of simulation > O(100) * tau_exp
  - For thermalization O(10)*tau_exp

Otherwise risks:

- incomplete thermalization:
  - wrong sampling and a biased result
  - wrong estimation of AC, underestimation of errors



Estimation of tau^exp

Look for the observable O_slow with the largest AC, i.e. is very sensitive to slow modes

take $\tau^{\exp} \sim \tau^{int,\square^{\text{slow}}}$

Simulating Lattice QCD

Feynman Pathintegral

$$\langle \square \rangle = \frac{1}{Z} \int DU \; D\overline{\psi} D\psi \; e^{-Sg[U]} e^{-\overline{\psi} D[u] \psi} \cdot \square[U, \overline{\psi}, \psi]$$

$$= \frac{1}{Z} \int DU e^{-Sg[U]} \det(D[U]) \cdot \square[U, \overline{\psi}, \psi]$$

- pure gauge theory, quenched Simulation, det D = 1
- Action local : requires O(1) operations for a single link U update
  - Heat-bath
  - Overrelaxation
- Action non-local: requires O(V) operations for a single link uodate
  - Global update
- Global update must be **coherent** otherwise

$$\delta S \propto V \quad \Rightarrow P_A \propto \exp(-\delta S) \sim 0$$

Hybrid Monte Carlo

Add auxiliarry momentas

$$\pi(x,\mu) = T^a \pi^a(x,\mu) \in su(3) \qquad (\pi,\pi) = \sum_{x,\mu,a} |\pi^a(x,\mu)|^2$$

Hamiltonian system

$$\langle \square \rangle = \frac{1}{Z} \int DUD\pi \, e^{-S[U]} \, e^{-(\pi,\pi)/2} \qquad \text{with} \qquad \int D\pi e^{-(\pi,\pi)/2} = 1$$

$$= \frac{1}{Z} \int DUD\pi \, e^{-H[\pi,U]} \qquad \text{with} \qquad H = \frac{1}{2}(\pi,\pi) + S[U]$$

Now, we can use Molecular dynamics to update:

$$U(x,\mu) \rightarrow U(x,\mu)(t) \qquad \pi(x,\mu) \rightarrow \pi(x,\mu)(t)$$

using Hamiltons equations

$$\partial_t U(x,t) = \pi(x,\mu) U(x,\mu)$$

$$\partial_t \pi(x,\mu) = -F(x,\mu) \qquad F(x,\mu)^a = \partial_{x,\mu} S[U] \qquad [\partial^a{}_{x,\mu} \, U(y,\nu) = \delta_{xy} \, \delta_{\mu\nu} T^a U(x,\mu)]$$

Note that

$$P_H \propto exp{-H} \quad \text{and} \quad P_S \propto exp{-S} \quad \text{are equivalent for sampling } \square(U)$$

Introducing t is legitimate

$$\partial_t H = 0 \qquad \Rightarrow P_H(\pi(0), U(0)) = P_H(\pi(\tau), U(\tau))$$

Hybrid Monte Carlo

Ideal HMC algorithm

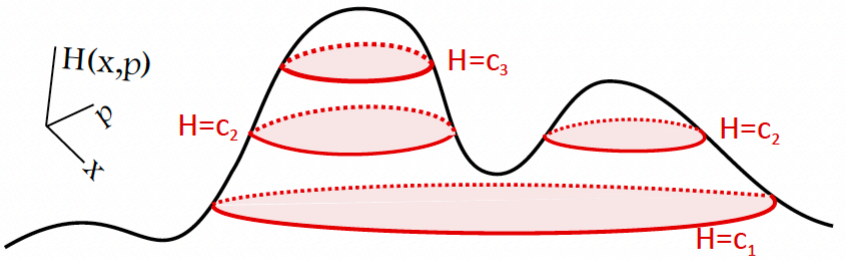
1. Start from a gauge-field U(0)
2. Sample a momentum field P(0) from the Gaussian distribution

$$P_\pi = e^{(\pi,\pi)/2}/Z$$

3. Solver Hamilton eqs. for a time t

$$(\pi(0), U(0)) \rightarrow (\pi(\tau), U(\tau))$$

4. Repeat 2. and 3. taking U(0)=U(t)



Hybrid Monte Carlo

Ergodicity:

First step is given by a heat-bath for the momenta's

$$P_\pi P_H = P_H$$

but the step is not ergodic in the total phase-space (only in the momentum part)

Second step is given by the Hamilton evolution

$$P_{MD}((\pi, U) \rightarrow (\pi', U')) = \delta(\pi' - \pi(\tau))\delta(U' - U(\tau))$$

it follows

$$P_{MD} P_H = P_H$$

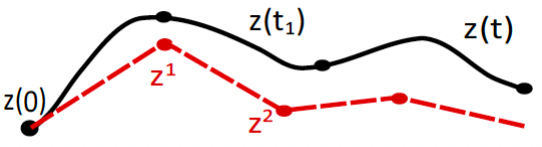
but is also not ergodic (H=const.)

However, the combination of first and second step is assumed to be ergodic

$$T = (P_{MD} P_\pi) \quad \text{has a fixed point and} \quad P_H \quad \text{is equilibrium distribution}$$

In practice

- Hamilton equations can not be solved exactly
  - use numerical integration
- H is not conserved
  - bias in equilibrium distribution



Hybrid Monte Carlo on the computer

HMC algorithm [Duane et al. 87]

1. Start from a gauge-field U(0)
2. Sample a momentum field P(0) from the Gaussian distribution

$$P_\pi = e^{(\pi,\pi)/2}/Z$$

3. Solve Hamilton eqs. numerically for a time t

$$(\pi^{(i)}, U^{(i)}) = (\pi(0), U(0)) \rightarrow (\pi(\tau), U(\tau)) = (\pi^{(f)}, U^{(f)})$$

4. Accept the configuration U'=U(t) with probability

$$P_A = \min[1, e^{\delta H}] \quad \text{with} \quad \delta H \equiv H(\pi^{(f)}, U^{(f)}) - H(\pi^{(i)}, U^{(i)})$$

   If reject start from the initial one U'=U(0)

5. Repeat 2. - 4. taking U(i)=U' and iterate

Hybrid Monte Carlo on the computer

- The numerical solution of Hamilton equations is used as a proposal in a Metropolis step
- the accept-reject step guarantees that PH is the equilibrium distribution, even if

$$\delta H \neq 0$$

- For the correctness of the HMC, the numerical integrator must preserve two **key properties** of Hamilton dynamics

  1. Time-reversibility

  $$P_{MD}((\pi, U) \rightarrow (\pi', U')) = P_{MD}((-\pi', U') \rightarrow (-\pi, U))$$

  Guarantess a symmetric proposal

  2. Phase-space measure preservation

  $$D\pi(0)\, DU(0) = D\pi(\tau) DU(\tau)$$

  in conjuction with 1. guarantees detailed balance

Molecular Dynamics integration

Hamiltonian

$$H(p,q) = \frac{1}{2}p^2 + S(q) = T(p) + S(q)$$

Time-evolution operator

$$\exp\left(\tau\frac{d}{dt}\right) f(p(t),q(t)) = f(p(t+\tau),q(t+\tau))$$

(taylor expansion) We can write

$$\exp\left(\tau\frac{d}{dt}\right) = \exp\left(\tau\left[\frac{dp}{dt}\frac{\partial}{\partial t} + \frac{dq}{dt}\frac{\partial}{\partial t}\right]\right) = \exp\left(\tau\left[-\frac{\partial H}{\partial q}\frac{\partial}{\partial t} + \frac{\partial H}{\partial p}\frac{\partial}{\partial t}\right]\right) \equiv \exp\left(\tau\hat{H}\right)$$

Hamiltonian vector field

$$\hat{H} = \left[\frac{\partial H}{\partial p}\frac{\partial}{\partial t} - \frac{\partial H}{\partial q}\frac{\partial}{\partial t}\right] = \hat{T} + \hat{S}$$

It follows

$$\exp(\tau\hat{H})H = H \quad \Rightarrow \quad \partial_t H = 0$$

and

$$\hat{T} = T'\frac{\partial}{\partial q} \quad \text{and} \quad \hat{S} = -S'\frac{\partial}{\partial p}$$

Molecular Dynamics integration

Integrable steps

$$\hat{e^{\tau T}} : f(p,q) \to f(p, q + \tau T'(p))$$

$$\hat{e^{\tau S}} : f(p,q) \to f(p - \tau S'(q), q)$$

Measure preserving/Volume preserving

$$J(\hat{e^{\tau T}}) = \frac{\partial \hat{e^{\tau T}}(p,q)}{\partial(p,q)} = \det \begin{bmatrix} 1 & \tau T''(p) \\ 0 & 1 \end{bmatrix} = 1$$

$$J(\hat{e^{\tau S}}) = \frac{\partial \hat{e^{\tau S}}(p,q)}{\partial(p,q)} = \det \begin{bmatrix} 1 & 0 \\ -\tau S''(q) & 1 \end{bmatrix} = 1$$

- $\hat{\exp(\tau T)}$ and $\hat{\exp(\tau S)}$ are exactly integrable for any τ
- can be combined to built symplectic integrators i.e. time-reversible and measure preserving

Leap Frog

$$[I_{LPFR}\ (h)]^n = \left(\hat{e^{\frac{h}{2}S}}\hat{e^{hT}}\hat{e^{\frac{h}{2}S}}\right)^n$$

which is reversible by construction and volume preserving

Integration error of symplectic integrators

Using Baker-Campbell-Hausdorff (BCH) formula

$$\ln(e^A e^B) = (A + B) + \frac{1}{2}[A, B] + \frac{1}{12}([A, [A, B]] - [B, [A, B]]) + \ldots$$

we find

$$[I_{LPFR}\ (h)]^n = \left(\exp[(\hat{T} + \hat{S})h - \frac{1}{24}([\hat{S}, [\hat{S}, \hat{T}]] + 2[\hat{T}, [\hat{S}, \hat{T}]])h^3 + O(h^5)]\right)^{\tau/h}$$

$$= \left(\exp[\tau((\hat{T} + \hat{S}) - \frac{1}{24}([\hat{S}, [\hat{S}, \hat{T}]] + 2[\hat{T}, [\hat{S}, \hat{T}]])h^2 + O(h^4))]\right)$$

$$\equiv \exp(\tau \tilde{H}) = \exp(\tau(\hat{T} + \hat{S}) + O(h^2))$$

Shadow Hamiltonian

The commutator of two Hamiltonian vector fields is a Hamiltonian vector field

$$\tilde{H} = \frac{\partial \tilde{H}}{\partial p}\frac{\partial}{\partial q} - \frac{\partial \tilde{H}}{\partial q}\frac{\partial}{\partial p}$$

Symplectic intergrators exactlu conserve a shadow Hamiltonian

Shadow Hamiltonian

It holds

$$[\hat{H_1}, \hat{H_2}] = \hat{H_3}$$

and its follows

$$H_3 = (H_1, H_2)_p = \frac{\partial H_1}{\partial p}\frac{\partial H_2}{\partial q} - \frac{\partial H_1}{\partial q}\frac{\partial H_2}{\partial p}$$

Now to find the shadow Hamiltonian, replace the commutators with Poisson brackets and it follows

Leap Frog

$$\Delta H_{LPFR} = \frac{1}{24}[(S,(S,T))_p + 2(T,(S,T))_p]h^2 + O(h^4)$$

$$= -\frac{1}{24}(S'^2(q) - 2p^2 S''(q))h^2 + O(h^4)$$

with

$$S'^2(q) = F^2 \quad \text{and} \quad S''(q) = F'$$

Remarks:

- BCH only gives an asymtotic expansion for tildeH
- existence of a conserved Hamiltonian tildeH along the trajectory means

$$\delta H = (H^{(f)} - \tilde{H}^{(f)}) - (H^{(i)} - \tilde{H}^{(i)}) = (\Delta H^{(f)} - \Delta H^{(i)}) = O(h^2)$$

Generalization of MD integrators

Second minimal norm scheme (OMF2)

$$I_{OMF2}(h) = e^{\lambda h \hat{S}} e^{h/2 \hat{T}} e^{(1-2\lambda) h \hat{S}} e^{h/2 \hat{T}} e^{\lambda h \hat{S}}$$

with

$$\Delta H_{OMF2} = (c_1(\lambda)(S,(S,T))_p + c_2(\lambda)(T,(S,T))_p) h^2 + O(h^4)$$

$$\text{Minimizing } c_1^2 + c_2^2 \quad \text{gives} \quad \lambda \approx 0.19$$

Fourth order integrator (OMF4) with 11 stages

$$I_{OMF4}(h) = e^{r_0 h \hat{S}} \cdots e^{r_0 h \hat{S}} \quad \Delta H_{OMF4} = O(h^4)$$

Remarks

- Measuring $var(\Delta H)$ in simulations and minimizing it allows for a systematic optimization

  [Clark et al. 11]

Multiple time-scale integration

Multiple actions

$$H(p,q) = \frac{1}{2}p^2 + S_1(q) + S_2(q) \qquad ||F_2|| \ll ||F_1||$$

If Cost(F2) >> Cost(F1) it may be convenient to use different step sizes h

Nested integrators [Sexton, Weingarten 92]

$$I(h) = e^{\frac{h}{2}\hat{S}_2}\left(e^{\frac{h}{2m}\hat{S}_1}e^{\frac{h}{m}\hat{T}}e^{\frac{h}{2m}\hat{S}_1}\right)^m e^{\frac{h}{2}\hat{S}_2}$$

Shadow Hamiltonian

$$\Delta H = [\alpha F_2^2 + \beta F_2' + \beta F_1 F_2 + \frac{1}{m^2}(\alpha F_1^2 + \beta F_1')]h^2 + O(h^4)$$

Remarks

- Correlation term between F1 and F2 is not suppressed by m

  -> efficiency depends on correlation between forces

- in lattice QCD,

  $$||F_G|| \gg ||F_{F,1}||$$

  and opposite for their cost

Some Remarks on MD integration

Gauge group integration

$$e^{h\hat{T}} : U(x,\mu) \rightarrow e^{h\pi(x,\mu)}U(x,\mu) \quad \pi(x,\mu) \rightarrow \pi(x,\mu)$$

$$e^{h\hat{S}} : U(x,\mu) \rightarrow U(x,\mu) \quad \pi(x,\mu) \rightarrow \pi(x,\mu) - hF(x,\mu)$$

Measure preservation

$$\langle e^{-\delta H} \rangle = 1 \quad \delta H = H^{(f)} - H^{(i)}$$

Reversibility:

$$\Delta = ||U' - U|| \quad (\pi', U') = F \circ [I(h)]^n \circ F \circ [I(h)]^n(\pi, U)$$

with

$$F(\pi, U) = (-\pi, U)$$

is violated by rounding errors

$$\Delta \propto h^{\nu} \quad \text{with} \quad \nu > 0 \quad \text{Liapunov exponent}$$

A too large h

$$\nu \propto h$$

and MD integration becomes unstable

Remarks on MD integration

Acceptance probability

$$P^{acc} = \langle \min[1, e^{-\delta H}] \rangle \overset{V\to\infty}{=} \operatorname{erfc}(\sqrt{\sigma^2(\delta H)/8})$$

With

$$\sigma^2(\delta H) = \langle (\delta H)^2 \rangle - \langle \delta H \rangle^2 \propto V h^{2n}$$

To tune the algorithm:

- Select stable integrator
- Minimize cost per trajectory at constant acceptance rate
  - Requires stable integrator
- $$P^{acc} = const. \Rightarrow \sigma^2 = const. \Rightarrow h \propto V^{-1/2n}$$

Critical slowing down

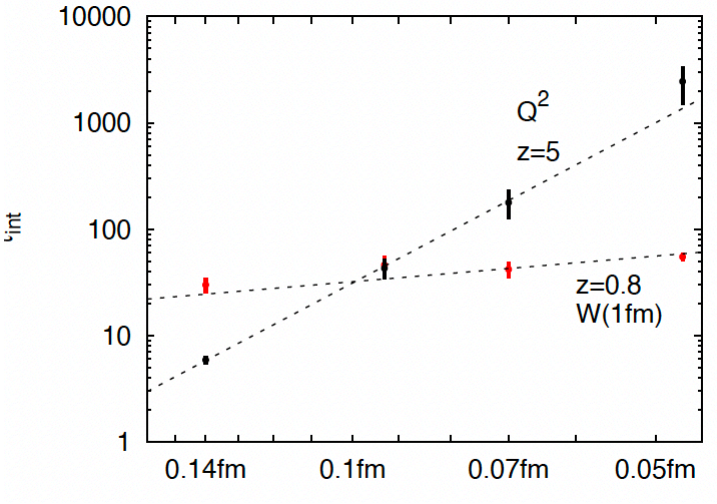
Approaching the continuum limit

$$\tau^{int,\square} \propto a^{-z}$$

where z depends on the algorithms

Status

- certain algorithms can be analyzed as QFTs :
- Simulation time is the (D+1)th dimension [Parisi, Wu 81, Zinn-Justin 86]
- HMC can not be analyzed this way: empirically z=2
- this might be true if topology issue is absent

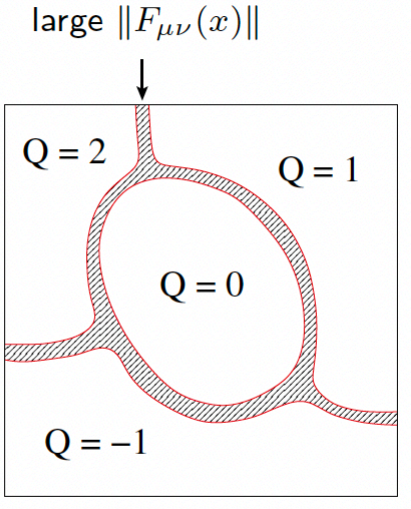


Topology freezing

- continuum path-integral with periodic bcs. for Fmunu is a sum over disconnected topological sectors
- on the lattice the field space "between" sectors rapidly vanishes as a->0
- Probability of changing sector in simulations rapidly deteriorating

  $\Rightarrow \tau^{int,Q}$ increases dramatically

- Ergodicity in simulations is compromised and so the results for any observablee
- One possible way, is to open the boundaries in time
- ...



field space

Fermions in simulations

Lattice QCD path-integral

$$\langle \square \rangle = \frac{1}{Z} \int DU \; D\overline{\psi} \; D\psi \; e^{-Sg[U]} e^{-\overline{\psi} D[U] \psi} \square[U, \overline{\psi}, \psi]$$

$$= \frac{1}{Z} \int DU \; e^{-Sg[U]} \det(D[U]) \square[U]$$

Fermionic observable

$$\square[U, \overline{\psi}, \psi] \rightarrow \square'[U] = \square[U, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \overline{\eta}}] e^{\overline{\eta} D^{-1}[U] \eta}$$

Determinant as observable:

$$\langle \square \rangle = \frac{\langle \det(D[U]) \square'[U] \rangle}{\langle \det D[U] \rangle}$$

- Calculation of det(D[U]) requires O(V^3) operations
- Overlap problem -> large statistical fluctuations

Fermions in simulations

Lattice QCD path-integral

$$\langle \square \rangle = \frac{1}{Z} \int DU \; D\overline{\psi} \; D\psi \; e^{-Sg[U]} e^{-\overline{\psi} D[U] \psi} \square[U, \overline{\psi}, \psi]$$

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Determinant in Metropolis

$$P_A \propto e^{-Sg[U'] - Sg[U]} \frac{\det D[U']}{\det D[U]}$$

- for a single link update

  $$\det(D[U + \delta U] D[U]^{-1})$$

  requires O(V) operation

  for a full sweep follows propotional to V^2
- det D[U] must be real and positiv

Fermions in simulations

Lattice QCD path-integral

$$\langle \square \rangle = \frac{1}{Z} \int DU \; D\overline{\psi} \; D\psi \; e^{-Sg[U]} \, e^{-\overline{\psi} D[U] \psi} \, \square[U, \overline{\psi}, \psi]$$

$$= \frac{1}{Z} \int DU \; e^{-Sg[U]} \det(D[U]) \square[U]$$

Fermionic observable

$$\square[U, \overline{\psi}, \psi] \rightarrow \square'[U] = \square[U, \frac{\partial}{\partial \eta}, \frac{\partial}{\partial \overline{\eta}}] e^{\overline{\eta} D^{-1}[U] \eta}$$

Determinant as effective action

$$S^{eff} = -\text{tr} \; \ln(D[U]) \qquad \Rightarrow \qquad F^{eff} = -\text{tr}(D[U]^{-1} \, \partial D[U])$$

- Difficult and impractical to mae the algorithm efficient (and exact)
- det D[U] must be real and positiv

Fermions in simulations

Pseudo-fermions [Weingarten, Petcher 81]

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

- det Q^2 is expressed in terms of a bosonic Gaussian integral with pseudo-fermions interacting non-locally
- $$\det(Q)^* = \det(Q^\dagger) = \det Q \in \mathbb{R}$$

  but for Wilson quarks not necessarily positiv
- positivity of the fermion kernel is needed for the convergence of the integral
- two degenerate quarks guarantee positivity and allow for an easy pseudo-fermion generation
- more difficult for single quarks

HMC with pseudo-fermions

Heat-bath

$$P_\eta[\eta] \propto \int D\eta^\dagger D\eta \; e^{-\eta^\dagger \eta} \qquad \Rightarrow \qquad \phi = Q\eta \qquad \Rightarrow P_\phi[\phi]$$

- At the beginning of a trajectory, we generate pseudo-fermions from Gaussian fields
- Averaging results over many trajectories effectively samples the contribution from the pseudo-fermion integral

Hamiltonian

$$H = \frac{1}{2}(\pi, \pi) + S \qquad S = S_G + S_{pf} \qquad S_{pf} = (Q^{-1}\phi, Q^{-1}\phi)$$

Dynamics

$$\partial_t U(x,\mu) = \pi(x,\mu)U(x,\mu) \qquad \partial_t \pi(x,\mu) = -F(x,\mu) \qquad F^a(x,\mu) = \partial^a{}_{x,\mu} S$$

Pseudo-fermions are held fixed during the Hamiltonian evolution

Fermionic forces

$$F_{pf}{}^a{}_{x,\mu} = \partial^a{}_{x,\mu}(\psi, \psi) = -2\mathrm{Re}(\chi, (\partial^a{}_{x,\mu} Q)\psi)$$

with

$$\psi = Q^{-1}\phi \qquad \text{and} \qquad \chi = Q^{-1}\psi$$

Challenges of simulating fermions

Solving the Dirac equation

- Computing Spf and Fpf requires solving linear systems:

$$D\chi = \eta \quad \Rightarrow \quad \chi = D^{-1}\eta$$

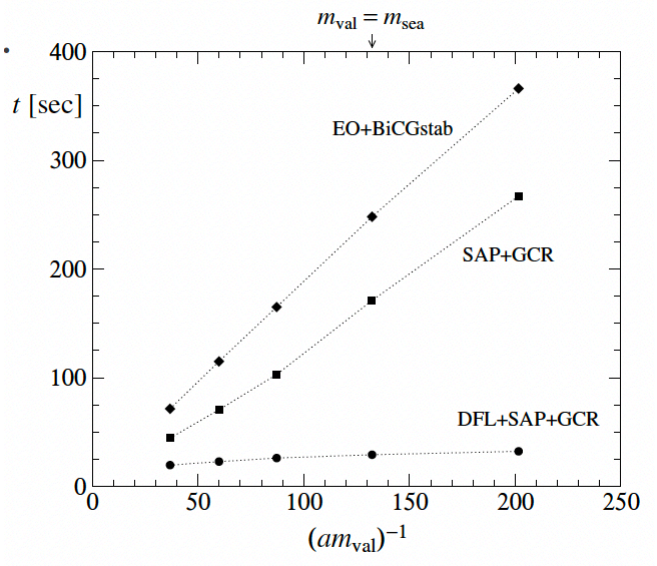
- D is a sparse matrix :

$$D\chi \quad \text{requires O(V) operations}$$

  iterative solvers are an effictive method to solve these stsmts

- Computational cost of conventional solvers rapidly grows with (a mq)^{-1}, system is quickly ill conditioned
- Multi-grid solvers are pratically solving this issues
  - lead to a speed up of O(10) - O(100)

Usually main computational challenge



Challenges of simulating fermions

Fermionic forces

- Single pseudofermion HMC is not competitive
- Consider

$$F_{pf} = (\phi, \partial Q^{-2}\phi) \qquad vs. \qquad F_F^{eff} = -2\partial \mathrm{trln}(Q)$$

  Fpf is a stochastic estimate of Feff at the start of the trajectory

$$\langle F_{pf} \rangle = F_F^{eff}$$

  - Fpf has very large fluctuations

1. $$||F_{pf}|| \gg ||F^{eff}{}_F||$$
2. $$var(||F_{pf}||) \gg var(F^{eff}{}_F)$$

  - Reall the shadow Hamiltonian

$$\Delta H_{OMF2} = (c_1 ||F||^2 + c_2 \pi^2 \partial^2 S) h^2 + O(h^4)$$

$$\text{large } var(||F_{pf}||) \quad \Rightarrow \text{ large } var(\Delta H) \quad \Rightarrow \text{ low } P_A \quad \Rightarrow \text{ small } h$$

  - large foces also trigger intabilities more easily -> limits the step size h

Even-odd reduction/preconditioning

If D only connects nearest-neighboring sites the fermionic problem can be effectively reduced to half the lattice

Checkerboard decomposition

Even or odd point

Schur decomposition

$$D = \begin{bmatrix} D_{ee} & D_{eo} \\ D_{oe} & D_{oo} \end{bmatrix} \qquad \det D = \det \hat{D} \det D_{oo} \qquad \hat{D} = D_{ee} - D_{eo} D^{-1}{}_{oo} D_{oe}$$

Even-odd action

$$S_{pf} \rightarrow S_{pfe} + S_{det} = (\hat{Q}^{-1} \phi_e, \hat{Q}^{-1} \phi_e) - 2\mathrm{tr} \ln(Q_{oo})$$

- Spfe involves pseudo-fermions residing only on the even sites of the lattice, helps in speed and reducing fluctuations
- Sdet and corresponding force can be evaluated exactly, i.e., without introducing pseudofermions

Hasenbusch mass-preconditioning

Frequency splitting [Hasenbusch 01, Hasenbusch, Jansen 03]

$$\det(Q^2) = \det(Q^2+\mu^2)\prod_{k=0}^{n-1}\det\left(\frac{Q^2+\mu_k^2}{Q^2+\mu^2{}_{k+1}}\right) \qquad 0=\mu_0<\ldots<\mu_n$$

Actions and forces

$$S_{pf,n} = (\phi_n, (Q^2+\mu_n^2)^{-1}\phi_n)$$

$$S_{pf,k} = (\phi_k, (Q^2+\mu^2{}_{k+1})(Q^2+\mu^2{}_k)^{-1}\phi_k) \qquad k=0,\ldots,n-1$$

$$(F_{pf,k})^a(x,\mu) = -2(\mu^2{}_{k+1}-\mu_k^2)\mathrm{Re}(\chi_k, (\partial^a{}_{x,\mu}Q)\psi_k)$$

- A proper tuning of mu can lead to a significant improvement
- $\text{smaller } var(||F_{pf}||) \Rightarrow \text{smaller } var(\Delta H) \Rightarrow \text{larger } P_A \Rightarrow \text{larger } h$
- for QCD, at the physical point,
- $$\mu_1 \sim m_q; \quad \mu_{k+1} \sim 10\mu_k$$

  Typically

  $$||F_{pf,k+1}|| \gg ||F_{pf,k}|| \quad \text{while opposite for their cost}$$

  Multiple time-step integration can be useful

Rational HMC

Single-quark determinante [Kennedy et al. 98, Clark, Kennedy 03]

$$\det(Q) \rightarrow \det(\sqrt{\overline{Q}^2}) = \det(W)\ \det R^{-1} \qquad W = |Q|R$$

where

$$R = r_b R^{n,\epsilon}(r_b^{-2} Q^2) \qquad \epsilon = (r_a/r_b)^2 \qquad \lambda(|Q|) \in [r_a, r_b]$$

Rational approximation

$$R^{n,\epsilon}(x) = A \frac{(x + a_1) \cdots (x + a_{2n-1})}{(x + a_2) \cdots (x + a_{2n})} \approx \frac{1}{\sqrt{x}} \qquad a_1 > \ldots > a_{2n} > 0$$

- Zolotarev rational function of degree (n,n)
- Guarantees smallest possible

$$\delta = \max_{\epsilon \le x \le 1} |1 - \sqrt{x} R^{n,\epsilon}(x)|$$

Frequency splitting (e.g. n=10)

$$\det(R^{-1}) \propto \det(P^{-1}{}_{1,4}) \det(P^{-1}{}_{5,7}) \det(P^{-1}{}_{8,10})$$

with

$$P_{k,l} = \prod_{j=k}^{l} \frac{Q^2 + \nu_j^2}{Q^2 + \mu_j^2} = 1 + \sum_{j=k}^{l} \frac{\rho_j}{Q^2 + \mu_j^2} \qquad \mu_1 > \ldots > \mu_n$$

Rational HMC

Actions and forces

$$S_{pf,k,l} = (\phi_{k,l}, P_{k,l}\,\phi_{k,l}) \qquad (F_{pf,k,l})^a(x,\mu) = \partial^a{}_{x,\mu} S_{pf,k,l}$$

Remarks

- ,We have to ensure \;$\det(Q) > 0$, this is ensured by measure the spectral range $[r_a, r_b]$ of Q^2

  If that fails, sign flip need to be included as reweighting factor (on some CLS ensembles thats the case [Mohler, Schaefer 19])

- Choose a large enough n to have a good approximation of R
- For Wilson quarks the RHMC is typically used for heavy quarks, (charm and strange)
- det(W) can be included in the accept-reject step or in the observable as a reweighting factor. It can be estimated stochastically

$$\langle \square \rangle_{|Q|} = \frac{\langle \square W \rangle_{R^{-1}}}{\langle W \rangle_{R^{-1}}} \qquad W = \langle e^{-\eta^\dagger [(1+Z)^{-1/2} - 1]\eta} \rangle_P$$

Costs

Approaching the continuum limit at constant physics, the cost to obtain a set of statistical independent configurations scales like

$$C \propto V a^{-4} \qquad V^{1/8} a^{-1/2} \qquad a^{-z} \propto V^{9/8} a^{4.5+z}$$

where the first term comes from the solver, the second from the integrator and the third from the autocorrelation

- OBC: z=2, PBC z=5

On a GPU machine with 4A100 this leads to

- O(1000) trajectories
- A physical volume of L=5.5 fm and a=0.05 fm
- Nf=2+1+1 twisted mass fermions at physical masses

$$C \approx 0.5 \text{ Mi node hours}$$

More techniques

- Pure-gauge algorithms
- Domain Decomposition
- Force gradient integrators
- Reweighting techniques
- Simulating chiral fermions
- Multi-level sampling
- …

References

This talk is based on Mattia Della Brida's Lattice Practice Contribution of 2021

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