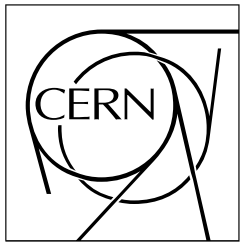
(Hybrid) Monte Carlo

Stefan Schaefer



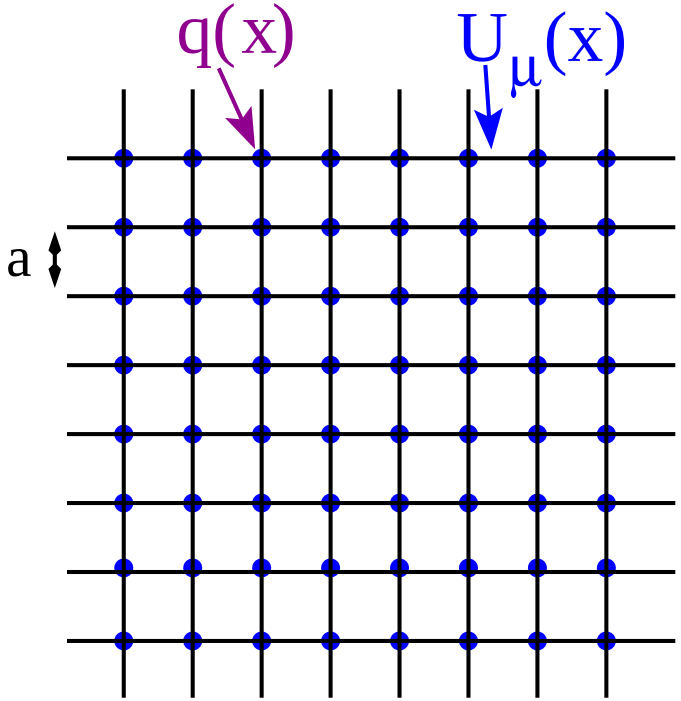
Lattice Practice 2012

Goal

$$\langle O \rangle = \frac{1}{Z} \int \prod_{i,\mu} dU_{i,\mu} e^{-S_g - S_{f,\text{eff}}} O[U]$$

with

$$Z = \int \prod_{i,\mu} dU_{i,\mu} e^{-S_g - S_{f,\text{eff}}}$$



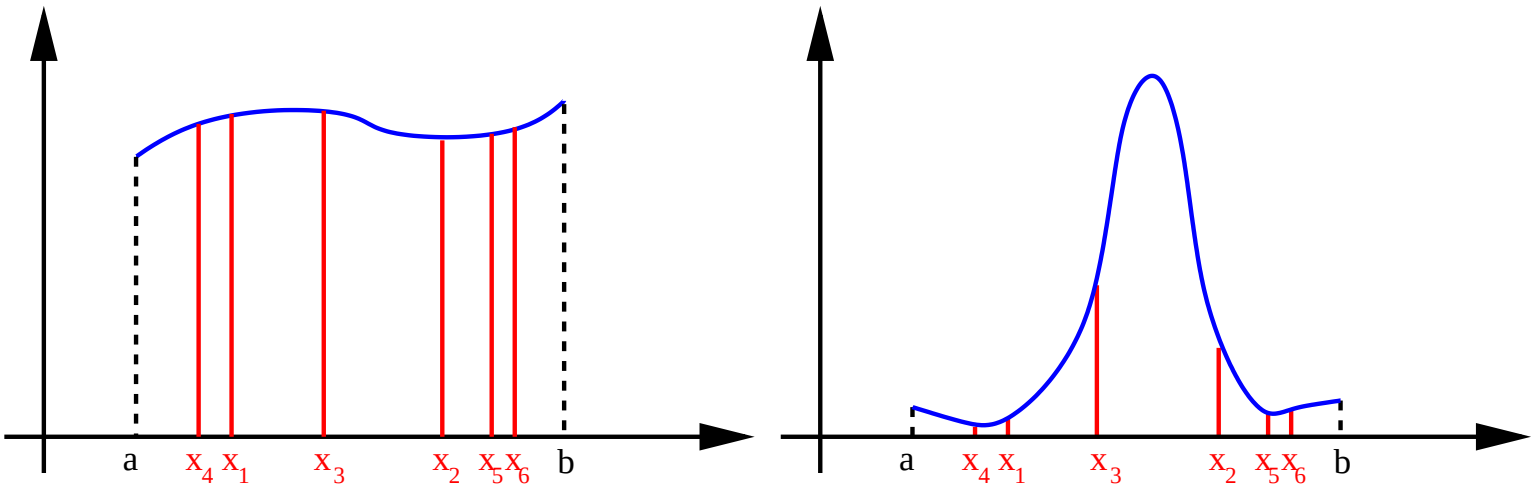
Importance sampling

General idea of Monte-Carlo integration

$$\int \mathrm{d}x\, f(x) = \left[\frac{1}{N}\sum_{i=1}^{N} f(x_i)\right] (1 + \mathcal{O}(N^{-1/2}))$$

with randomly chosen points x_i in the integration region

- good idea, if $f(x)$ approximately constant $\Rightarrow$ small fluctuations in $f(x_i)$.
- if $f(x)$ varies, large fluctuations, slow convergence for $N \to \infty$

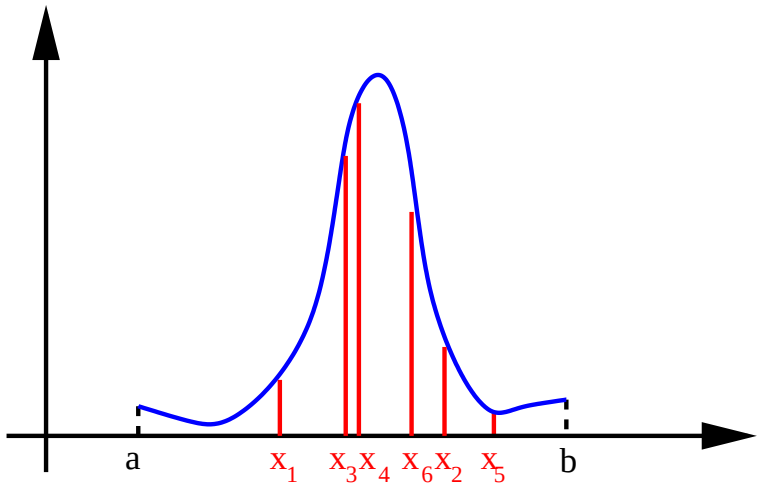


Importance sampling

$$\int \mathrm{d}x\, f(x) = \int \rho(x)\mathrm{d}x\, \frac{f(x)}{\rho(x)} = \left[\frac{1}{N}\sum_{i=1}^{N} \frac{f(x_i)}{\rho(x_i)}\right] (1 + \mathcal{O}(N^{-1/2}))$$

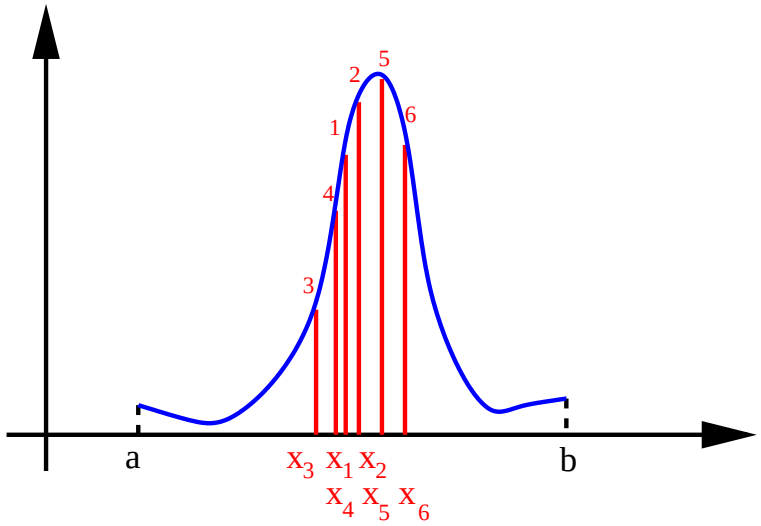
with points x_i chosen according to ρ.

- Choose points accoring to probablity distribution similar to function to be integrated
- variance is reduced — optimal, if distribution $\propto |f(x)|$
  ....need to know the integral for that.



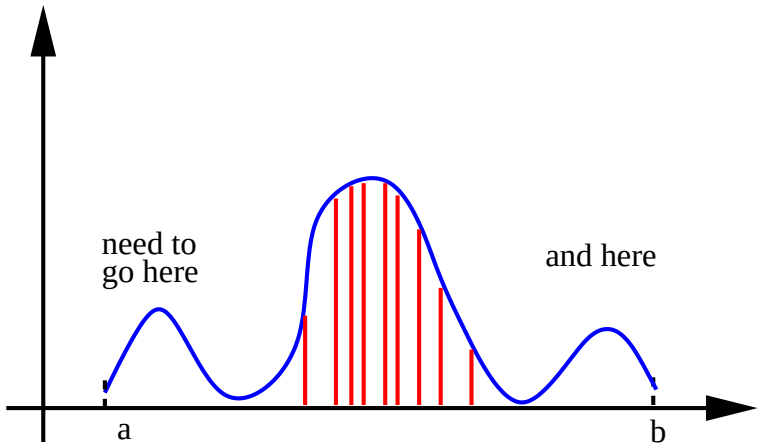
Importance sampling

- Need a method that uses only relative probabilities.
- Use Markov process: go from one point to the next with appropriate transition probability
- Take small steps $\rightarrow$ stay in the important region



Importance sampling

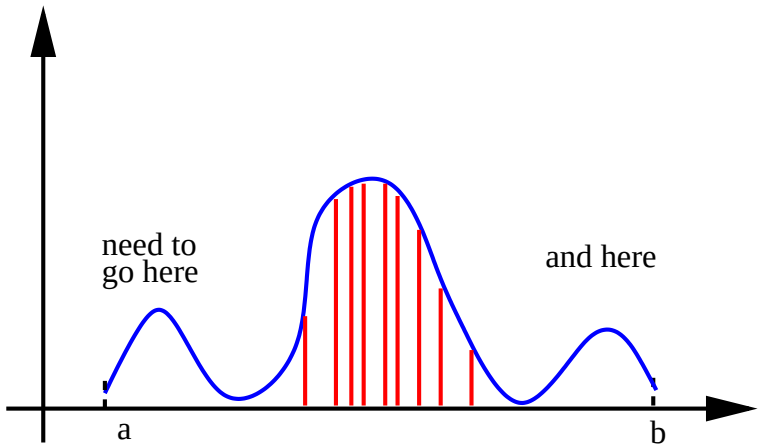
- Good as long as probability landscape simple
- Performs badly, when landscape structured
- Ergodicity $\leftarrow$ can be a problem in practical situations



Importance sampling

How do we tell?

- Eventually, we will visit all "valleys"
- Look at many observables, check for long range fluctuations
- Take into account in you error analysis
- Unfortunately, in a real world simulation, this need not be easy



Method

$$\langle O \rangle = \frac{1}{Z} \int \prod_{i,\mu} dU_{i,\mu} e^{-S_g - S_{f,\text{eff}}} O[U]$$

Lattice simulations split up in two steps

- Generate N *field configurations* U_i with probability density

$$P[U] = \frac{1}{Z} e^{-S_g - S_{f,\text{eff}}}$$

- Then get expectation values

$$\langle O \rangle = \frac{1}{N} \sum_{i=1}^{N} O[U_i](1 + \mathrm{O}(1/\sqrt{N}))$$

Comments

Probability

- Choice of probability $P[U]$ is not unique.
- Boltzmann factor natural, but can lead to problems.
- Surfaces with $S = \infty$
  $\rightarrow$ configuration space disconnected.
- Observables can show large fluctuations.

Update

- Direct determination of probability would need knowledge of integral Z.
- Methods that use **relative** probabilities necessary.

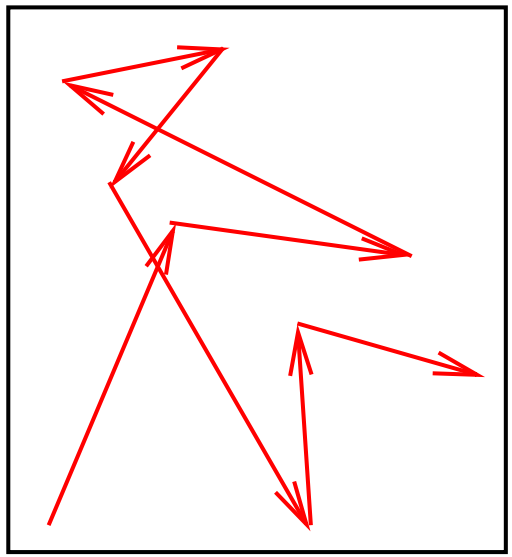
Markov Chain Monte Carlo

- Sequence of field configurations

$$U_1 \rightarrow U_2 \rightarrow U_3 \rightarrow \cdots \rightarrow U_N$$

- Generated by a **transition probability density**

$$T(U' \leftarrow U) \geq 0 \quad \text{for all } U, U'$$



- Stability

$$\int [dU]\, T(U' \leftarrow U)\, P[U] = P[U']$$

- Normalization

$$\int [dU']\, T(U' \leftarrow U) = 1$$

Generate sequence from T

$$U_1 \rightarrow U_2 \rightarrow U_3 \rightarrow \cdots \rightarrow U_N$$

- Stability
  If $\{U_i\}$ is an ensemble distributed according to P,
  so is $\{U_i'\}$, where $U \xrightarrow{T} U'$
- Show that starting from *any* configuration U_0

$$\{\, U_n \,|\, n \in [1, N]\}$$

  is distributed according to P for $N \rightarrow \infty$.
- Discuss this for observables $A[U]$

$$\overline{A}_N = \frac{1}{N} \sum_{i=1}^{N} A(U_i) \quad \rightarrow \quad \lim_{N \rightarrow \infty} \overline{A}_N = \langle A \rangle$$

Sketch of proof

- $T(U' \leftarrow U)$ a matrix on space of configurations

$$\int [dU]\, T(U' \leftarrow U)\, P[U] = P[U']$$

- $P[U]$ is an **eigenvector** of T with **eigenvalue** 1.

Perron–Frobenius theorem

For a normalized matrix like T, all eigenvalues $|\lambda_n| \leq 1$
There is exactly one eigenvalue λ_0 with $\lambda_0 = 1$.

Consequences

Let λ_i be eigenvalues of T

$$1 > |\lambda_1| \geq |\lambda_2| \geq \dots$$

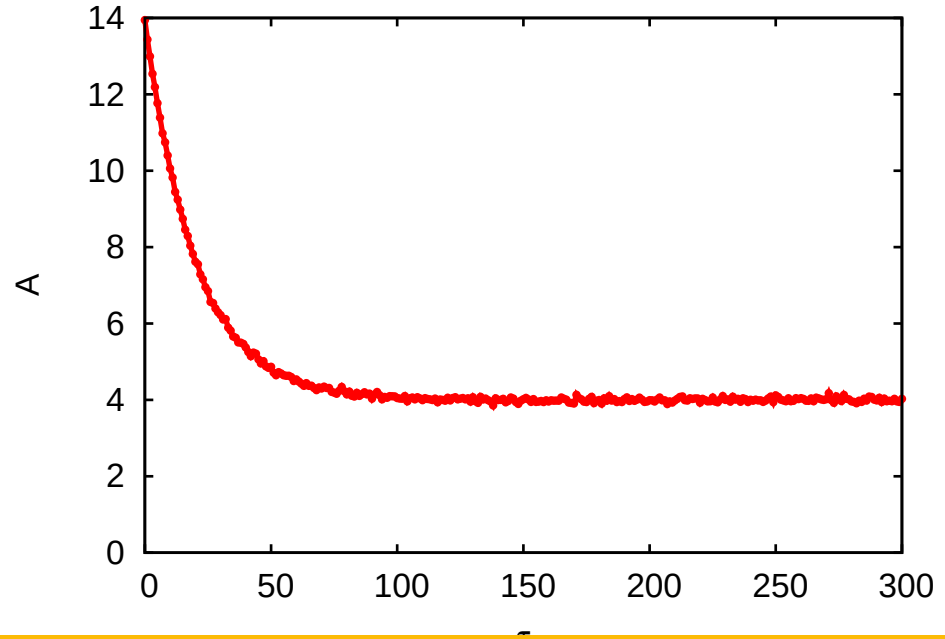
and η_i the corresponding eigenvectors.

- Start with any starting distribution P_0
- Apply matrix T a number of times t

$$P_t = T^t P_0 = \sum_n c_n \lambda_n^t \eta_n$$

- Because $|\lambda_{n>0}| < 1$, only the $\eta_0 = P$ survives.

Thermalization

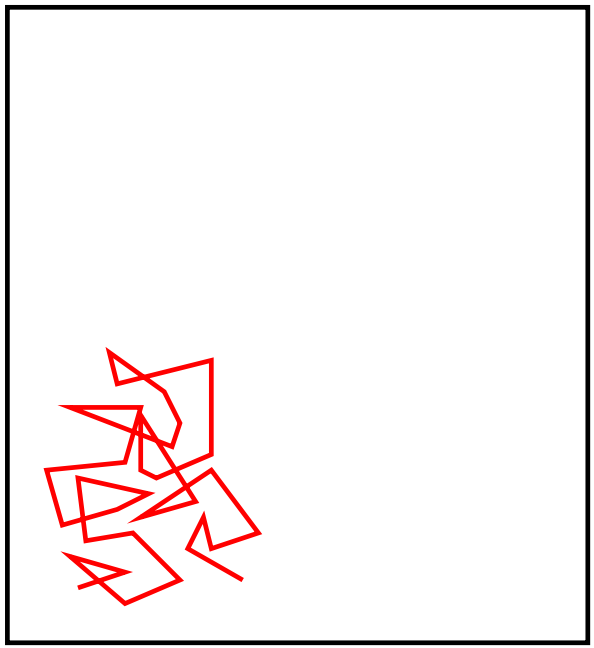


Procedure

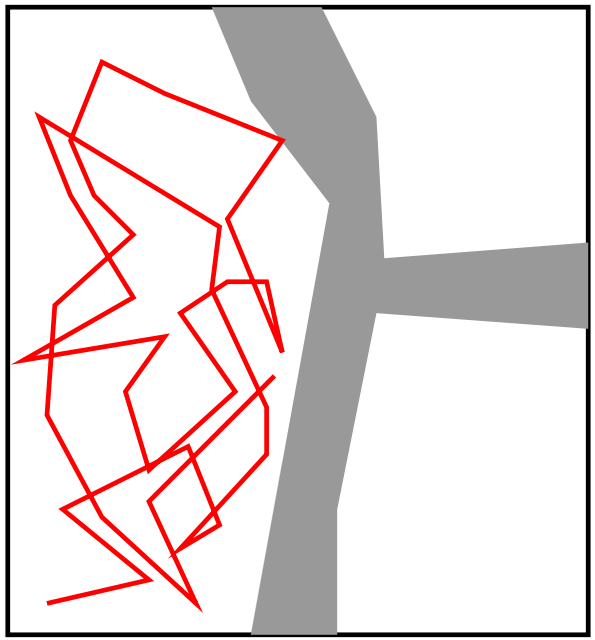
- Replace average over ensemble by time-series.
- Start with one configuration: $P_0(U) = \delta_{U,U_0}$
- Apply transition matrix N times
  $\rightarrow$ get sufficiently close to equilibrium
- Observe many observables $\rightarrow$ drifts.
- Ignore initial configurations.

Dangers

- Algorithm is slow.
- Detectable by measuring autocorrelations.



- There are barriers in field space.
- Hard to detect.



Autocorrelations

- Sequence of field configurations

$$U_1 \rightarrow U_2 \rightarrow U_3 \rightarrow \cdots \rightarrow U_N$$

- Measurements of observables are correlated

$$A_1 \rightarrow A_2 \rightarrow A_3 \rightarrow \cdots \rightarrow A_N$$

- Estimates

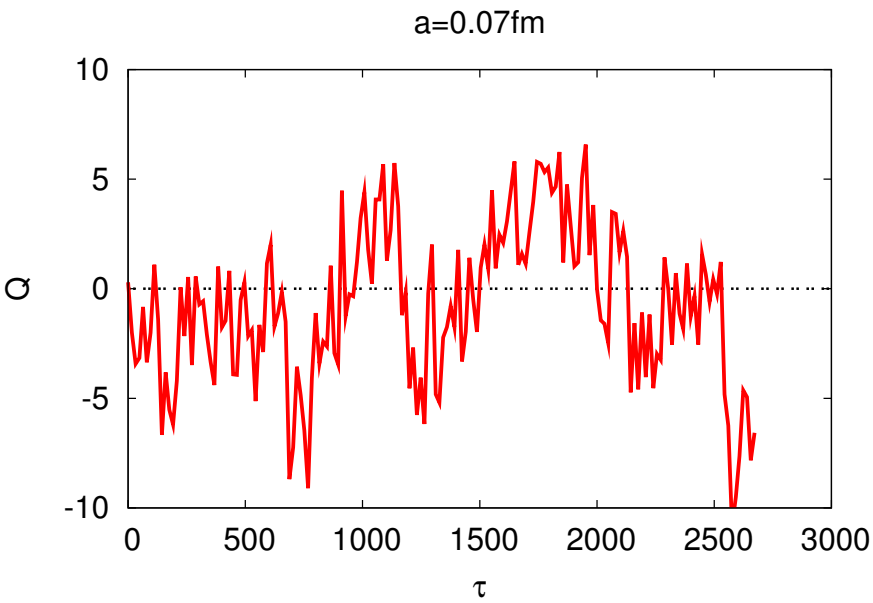
$$\langle A \rangle \approx \frac{1}{N} \sum_{i=1}^{N} A_i$$

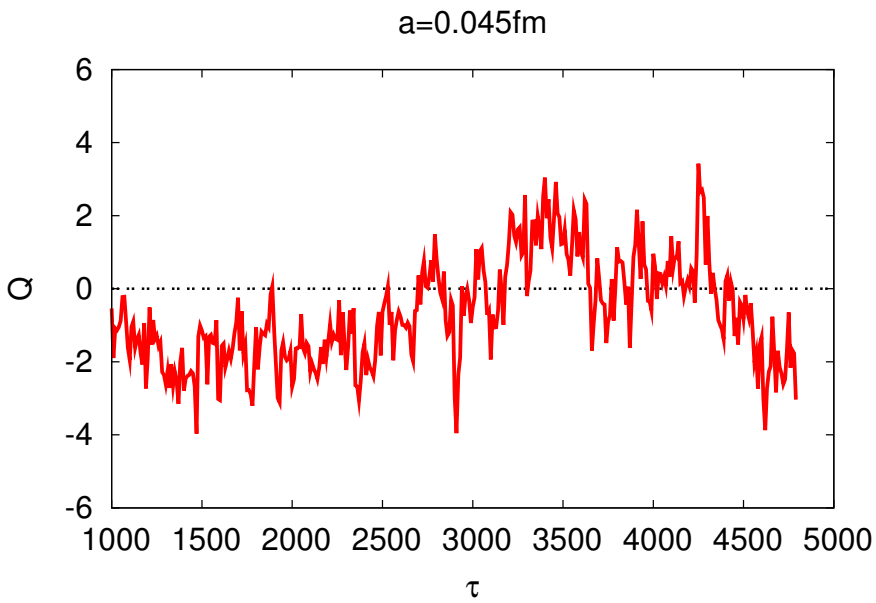
Autocorrelation function

$$\Gamma_A(t) = \langle (A_t - \bar{A})(A_0 - \bar{A}) \rangle$$

- Measures efficiency of algorithm.
- Can depend strongly on observable A.

Example


a=0.07fm
10
5
0
-5
-10
σ
0
500
1000
1500
2000
2500
3000
τ


a=0.045fm
6
4
2
0
-2
-4
-6
σ
1000
1500
2000
2500
3000
3500
4000
4500
5000
τ

Integrated autocorrelation time

$$\tau_{\text{int}}(A) = \int_0^\infty \frac{\Gamma(t)}{\Gamma(0)}\, dt$$

Time to make an "independent" configuration.

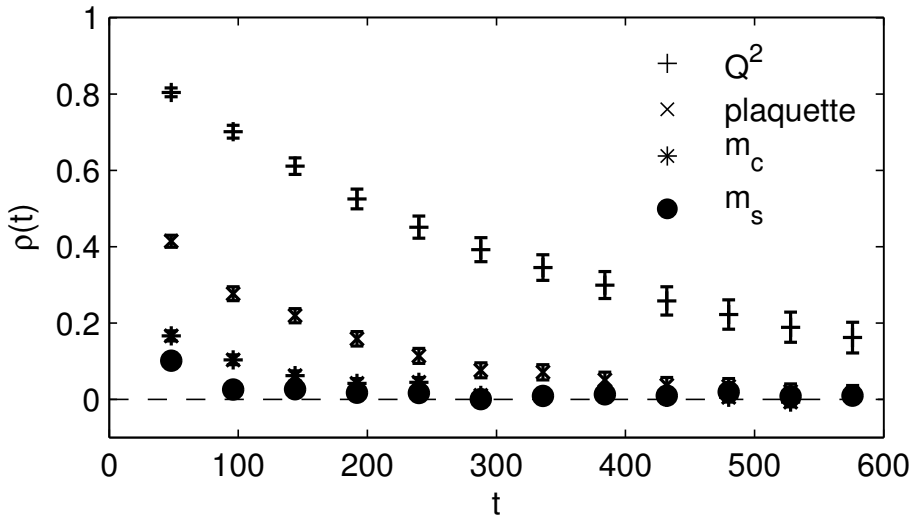
Statistical error

$$\sigma_A^2 = \frac{1}{N/2\tau_{\text{int}}} \langle (A - \bar{A})^2 \rangle = \frac{\mathbf{var}(A)}{N/2\tau_{\text{int}}}$$

Number of measurements effectively reduced by factor $2\tau_{\text{int}}$.

Example

Autocorrelation functions in pure YM theory



- Dependence on observable.
- Need long runs to measure precisely.

Next: theory of $\Gamma(t)$.

Detailed balance

Detailed balance

$$T(U' \leftarrow U)P[U] = P[U']T(U' \leftarrow U)$$

Implies stability

$$\int [dU] T(U' \leftarrow U)P[U] = \int [dU] P[U']T(U' \leftarrow U) = P[U']$$

Elementary steps frequently fulfill this condition.
As a consequence we have a symmetric matrix M

$$M(U' \leftarrow U) = P[U']^{-1/2} T(U' \leftarrow U) P[U]^{1/2}$$

If η eigenvector of T, ξ is eigenvector of M

$$\xi(U) = P^{-1/2}(U)\eta(U)$$

Autocorrelation Spectral decomposition

$$
\begin{aligned}
\Gamma_A(t) &= \left\langle \left(A_t - \bar{A}\right)\left(A_0 - \bar{A}\right) \right\rangle \\
&= \int [dU][dU'] \delta A(U')\, T^t(U' \leftarrow U)\, \delta A(U)\, P[U] \\
&= \int [dU][dU'] P^{1/2}[U'] \delta A(U') M^t(U' \leftarrow U) \delta A(U) P^{1/2}[U] \\
&= \sum_{n>0} (\lambda_n)^t \left[\xi_n(A)\right]^2
\end{aligned}
$$

With "matrix elements"

$$
c_n(A) = \int [dU] \xi_n(U) [P[U]]^{1/2} (A(U) - \bar{A})
$$

Spectral representation

$$\begin{aligned}\Gamma_A(t) &= \sum_n (\lambda_n)^t \left[c_n(A)\right]^2 \\ &= \sum_n (-)^{\mathrm{sign}\lambda_n} e^{-t/\tau_n} \left[c_n(A)\right]^2\end{aligned}$$

- $\tau_n = 1/\log|\lambda_n| > 0$
- For the analysis of algorithms it is useful to think of Monte Carlo time t as a fifth dimension.
- Autocorrelation function is a 2pt function.
- time constants $\tau_n \rightarrow$ inverse masses
- Slowest decay $\tau_1 \rightarrow$ exponential AC time

Comments

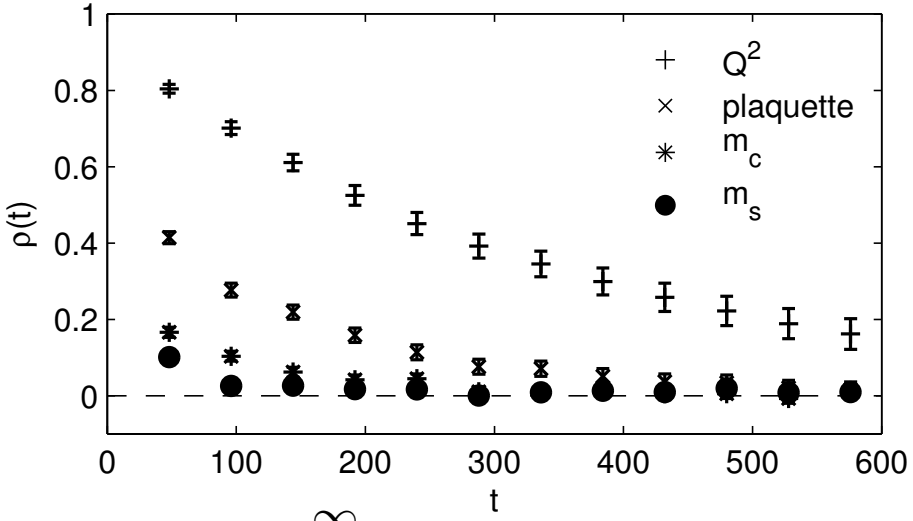
$$\Gamma_A(t) = \sum_n e^{-t/\tau_n} \eta_n^2$$

- τ_n depend only on algorithm
- Matrix elements c_n depend on observable.
- All observables affected by slow modes.

Length of a simulation

- Simulation must have length of at least $\mathrm{O}(100) \times \tau_0$.
- $\tau_{\mathrm{int}}(A)$ can be much smaller than τ_1
- Danger of
  - Incomplete thermalization.
  - Bias.
  - Wrong estimate of autocorrelations.

Measuring autocorrelations



$$\tau_{\mathrm{int}}(A) = \frac{1}{2} + \sum_{t=1}^{\infty} \langle (A(t) - \bar{A})\,(A(0) - \bar{A}) \rangle$$

We only have a limited precision estimate of the integrand.
Summing to $t = \infty$ leads to diverging variance.
$\rightarrow$ need to cut the summation
$\rightarrow$ biased estimate, neglecting (large?) contribution
Need to find a balance between stat. and syst. error.

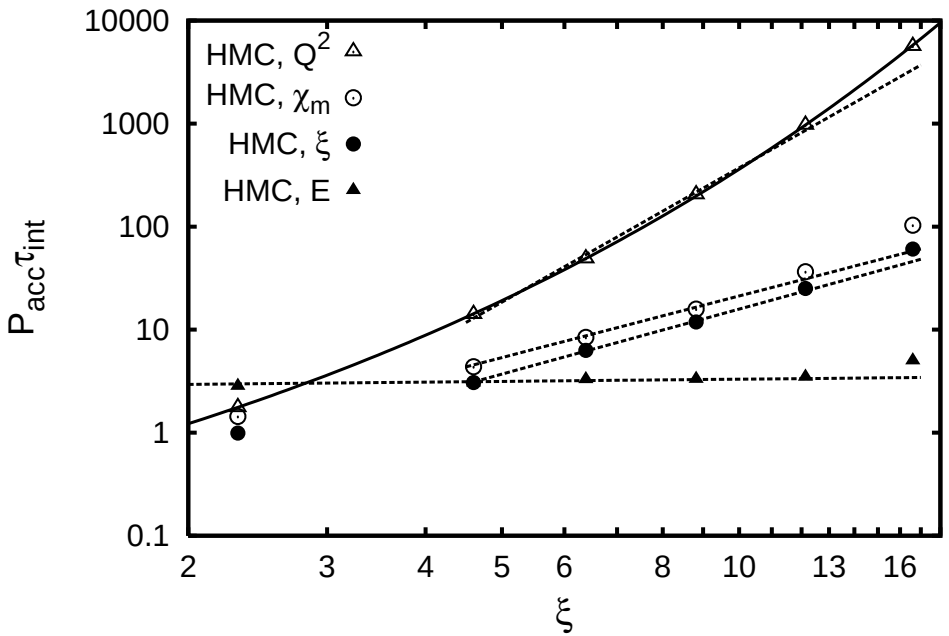
Comments

- All automatic methods are problematic.
- Cut where $\delta\Gamma > \Gamma$
  $\rightarrow$ large systematic error
- Sokal criterion
  $\rightarrow$ find compromise between stat and syst.
- ALPHA method (2010)
  Estimate τ_{exp} from various (slow) observables
  Add tail to all other observables before losing signal Γ_A

Topological charge

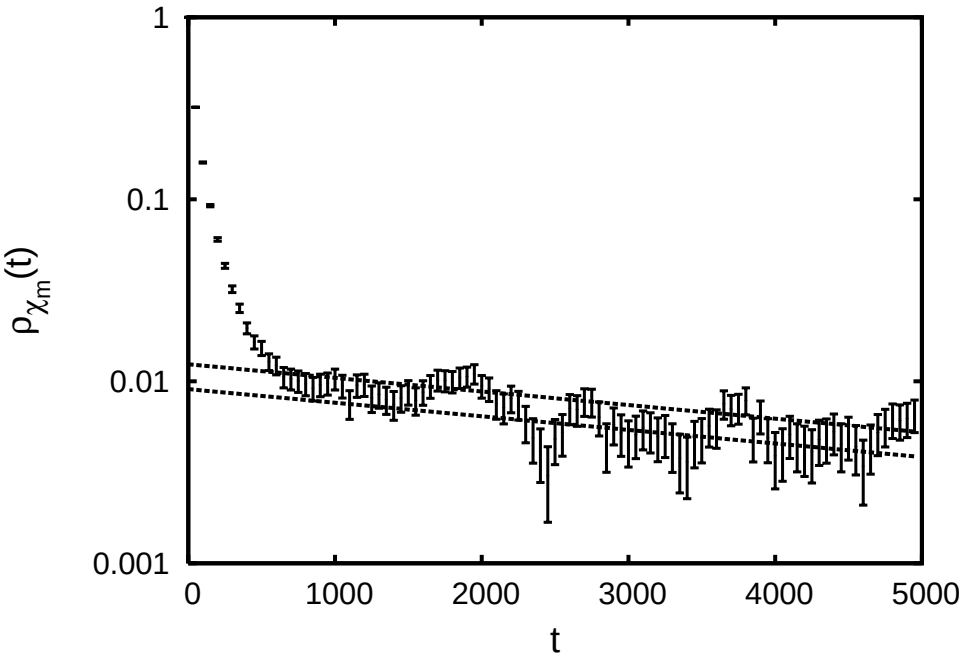
Best recipe: Avoid large autocorrelations τ_n.

- Special case: Topological charge
- In the continuum, topological sectors form.
- Happens very quickly as $a \to 0$.
- Has effect on all other observables.



Example from CP^{N-1} model

Topological charge AC dominates other observables.



Solution:
Use setup without topological sectors
$\rightarrow$ Open boundary conditions.

Summary Part I

General methods

- Importance sampling needed for high dim. integrals
- MCMC natural setup (only relative probabilities needed)
- Transition probability defined by algorithm

Suggested reading:
M. Lüscher, Computational Strategies in Lattice QCD, arXiv:1002.4232
U. Wolff, Monte Carlo errors with less errors, CPC 156 (2004) 143

Autocorrelations

- AC unavoidable consequence of approach
- Without knowledge of AC no control over results

Extended phase space

$$Z = \int [dU][d\pi]\, e^{-\frac{1}{2}(\pi,\pi) - S[U]}$$

- Expectation values of observables $A[U]$ remain the same.
- Momenta $\pi = \pi^a T^a \in \mathbf{su}(N)$, $\pi^a \in \mathbb{R}$
- $(\pi, \pi) = \sum_{x,\mu} \pi^a_{x,\mu} \pi^a_{x,\mu}$

- Make updates in this extended phase space.
  $\Rightarrow$ updates for U fields.

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.

Updates

$$Z = \int [dU][d\pi]\, e^{-\frac{1}{2}(\pi,\pi) - S[U]}$$

Momenta: Heatbath

- $(\pi,\pi) = \sum_{x,\mu} |\pi^a_{x,\mu}|^2$
  π^a are Gaussian random numbers.
- Normalization is known.
- Just for π this is the optimal update
  no correlation to previous config.
  Also true for combined system? (Kramers' rule,...)

Molecular dynamics

- Essential update step for the gauge fields: $(\pi, U) \to (\pi', U')$

Hamilton's equations of motion

- Hamiltonian

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

- E.o.m.

$$\dot{U}_{x,\mu} = \pi_{x,\mu} U_{x,\mu}$$

$$\dot{\pi}_{x,\mu} = -F_{x,\mu} \ , \qquad F^a_{x,\mu} = \frac{\partial S(e^\omega U)}{\partial \omega^a(x,\mu)}$$

Molecular dynamics

By Liouville's theorem, the classical dynamics

$$(\pi, U) \rightarrow (\pi', U')$$

maps areas of equal likelihood into eachother.

- Boltzmann factor e^{-H} is constant (energy conservation).
- Phase space is conserved.

An exact solution of the E.o.m is a valid update.

In practice: integration errors

Metropolis

Different viewpoint: Classic method by Metropolis et al'53

Metropolis

Construct update from

- Symmetric proposal

$$T_0[(\pi', U') \leftarrow (\pi, U)] = T_0[(\pi, U) \leftarrow (\pi', U')]$$

  area conserving $d\pi \wedge dU = d\pi' \wedge dU'$
- Acceptance step

Acceptance step

Molecular dynamics $(\pi, U) \to (\bar{\pi}, \bar{U})$

$$P_{\text{acc}} = \min(1, e^{-(H(\bar{\pi},\bar{U}) - H(\pi,U))})$$

New configuration $U' = \begin{cases} \bar{U} & \text{with prob. } P_{\text{acc}} \\ U & \text{with prob. } \quad 1 - P_{\text{acc}} \end{cases}$.

Comments

- Exact solution of MD equations has $\Delta H = 0$
  $\Rightarrow$ always accepted
- momentum heat-bath makes algorithm ergodic.
- Problems with ergodicity from $S = \infty$ surfaces.

Integration errors

- Numerical integration induces errors.
- Integration procedure must be symplectic
  symmetric and area ($dU \wedge dp$) conserving

Numerical integration

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

Splitting methods

$$H = \frac{1}{2}(\pi,\pi) + S[U] = H_1(p) + H_2(U)$$

- Eom for each part H_1, H_2 can be solved exactly $\rightarrow$ symplectic
- H_1, defines T_U

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

- H_2, defines T_p

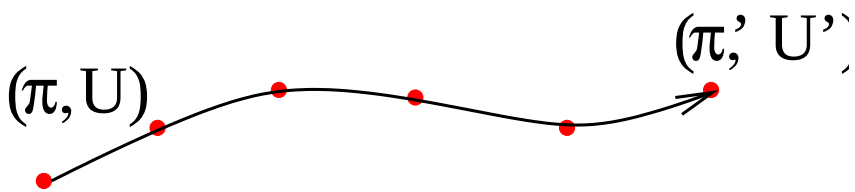
$$U_{x,\mu}(\tau) = U_{x,\mu}(0), \quad \pi(\tau) = \pi(0) - \tau F$$

Splitting methods

$$
\begin{aligned}
T_U: &\qquad U_{x,\mu}(\tau) = e^{\pi\tau} U_{x,\mu}(0), &&\qquad \pi(\tau) = \pi(0) \\
T_p: &\qquad U_{x,\mu}(\tau) = U_{x,\mu}(0), &&\qquad \pi(\tau) = \pi(0) - \tau F
\end{aligned}
$$

- Can be put together in any order.
- Legal integrator: time steps of T_U and T_p sum up to 1, symmetric
- Integration error automatically $\mathrm{O}(\epsilon^2)$
- 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
- Easy improvement without detailed knowledge of physics system.
  `Omelyan, Mrygold, Folk, 2003`
- Introduce parameters and optimize

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

- Performs roughly $2\times$ better than leapfrog
- 4th order integrators
- ...

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

Pseudofermions

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

$$\phi = Q\eta$$

$\rightarrow$ Pseudofermion heatbath, performed at beginning of each trajectory

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

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}

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

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 $\mu \rightarrow$ Noise reduction in force.
- success depends on choice of μ. URBACH ET AL'04

Numerical examples

Action

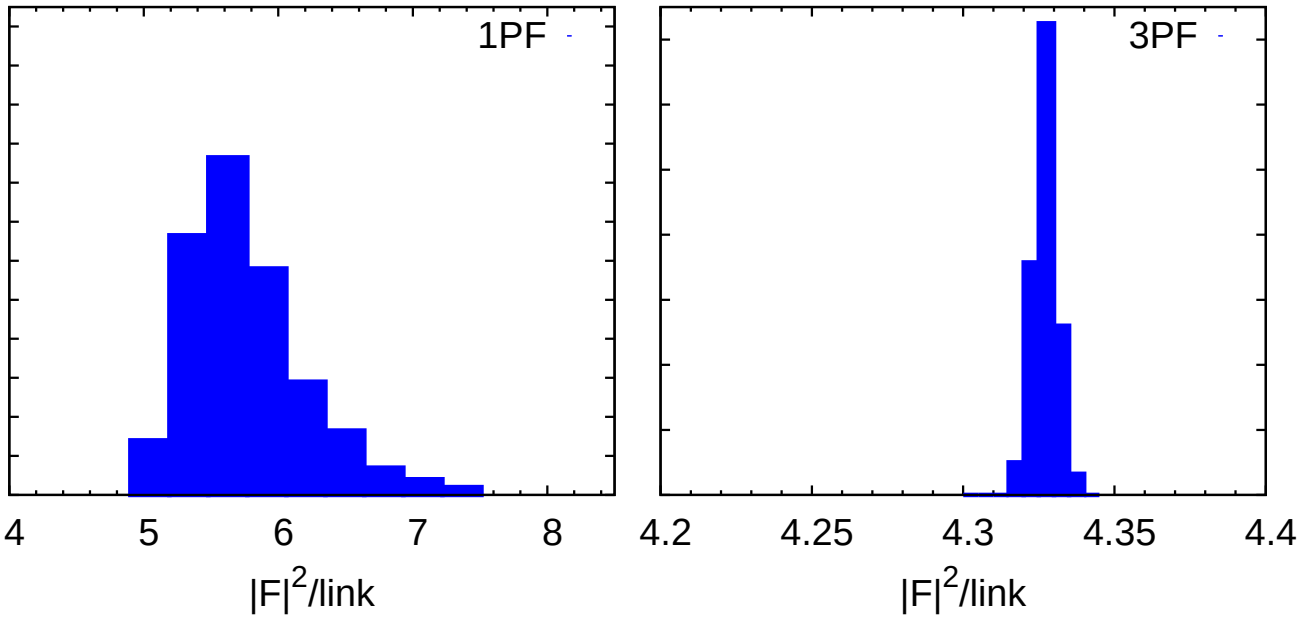
- $N_{\mathrm{f}} = 2 + 1$ NP improved Wilson fermions
- Iwasaki gauge action
- 64×32^3 lattice with $a = 0.09$fm
- studied extensively by PACS-CS — AOKI ET AL'09,'10
- $m_\pi = 200$MeV
- $m_\pi L = 3$

Algorithm — M. LÜSCHER, S.S.'12

- Reweighting to avoid stability problems.
- Generated with new 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

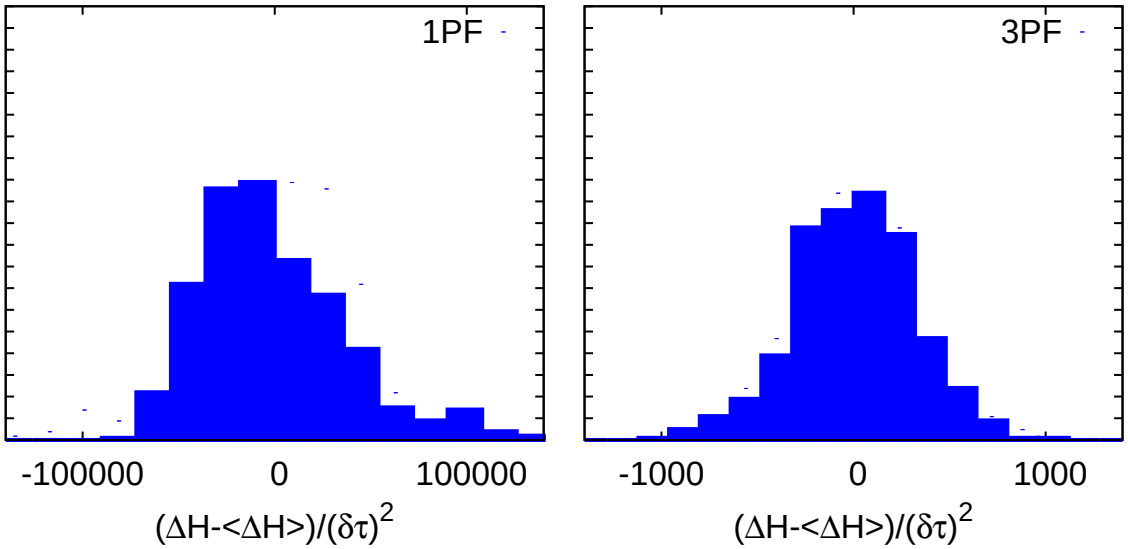
- Shadow Hamiltonian of symplectic integrators

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

- c_1 and c_2 depend on integrator.
- Large cancellation between the two terms
  $\rightarrow$ **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.

RHMC, PHMC

FREZZOTTI, JANSEN'97

HORVATH ET AL'00, CLARK, KENNEDY'07

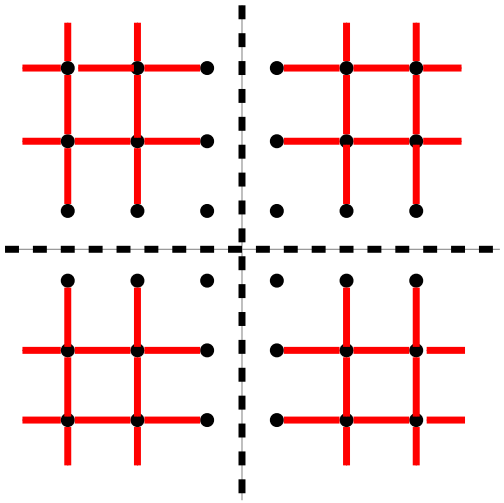
$$\det Q^2 = \prod_{i=1}^{n} \det \sqrt[n]{Q^2}$$

$$\approx \begin{cases} c_0 + \sum_n \frac{c_n}{Q^2 + b_n} & \text{RHMC} \\ \sum_n c_n Q^{2n} & \text{PHMC} \end{cases}$$

- Primary use: single flavors, $\det Q = \det \sqrt{Q^2}$
- PHMC: Polynomical approximation to square root.
- PHMC: Rational approximation.
- Used also to split fermion force in equal factors

Domain decomposition

LÜSCHER'04



- Domain decomposition
  $\rightarrow$ Divide the lattice in blocks

$$\det D = \det D_{\text{block}} \cdot \det D_{\text{R}}$$

- Do not update links connecting blocks
  $\rightarrow$ longer autocorrelations
- Good for slow communication.

Twisted mass reweighting

Wilson fermions: Dirac operator is not protected from zero eigenvalues.

$$S_f = -\mathrm{tr}\log Q^2$$

$\rightarrow$ action can become infinite
$\rightarrow$ field space separated in sectors

Consequences

- Thermalization difficult
- Problems with ergodicity
- Difficulties with numerical integration (spikes in forces)

Twisted mass reweighting

Solution:

- Run with protected Dirac operator
- Correct in the measurement

Reweighting (Ferrenberg & Swendsen '82)

$$\begin{aligned}\langle O \rangle &= \frac{1}{Z} \int \prod_{i,\mu} dU_{i,\mu} e^{-S_g - S_{f,\mathrm{eff}}} O[U] \\ &= \frac{Z'}{Z} \times \frac{1}{Z'} \int \prod_{i,\mu} dU_{i,\mu} e^{-S_g - S'_{f,\mathrm{eff}}} \left(O[U] e^{-(S_{f,\mathrm{eff}} - S'_{f,\mathrm{eff}})} \right) \\ &= \frac{\langle O e^{-(S_{f,\mathrm{eff}} - S'_{f,\mathrm{eff}})} \rangle'}{\langle e^{-(S_{f,\mathrm{eff}} - S'_{f,\mathrm{eff}})} \rangle'}\end{aligned}$$

Twisted mass reweighting

Want a reweighting factor with little fluctuation

Proposal by Lüscher & Palombi

$$\det Q^2 \to \begin{cases} \det Q^2 + \mu^2 \\ \det \frac{(Q^2+\mu^2)^2}{Q^2+2\mu^2} \end{cases}$$

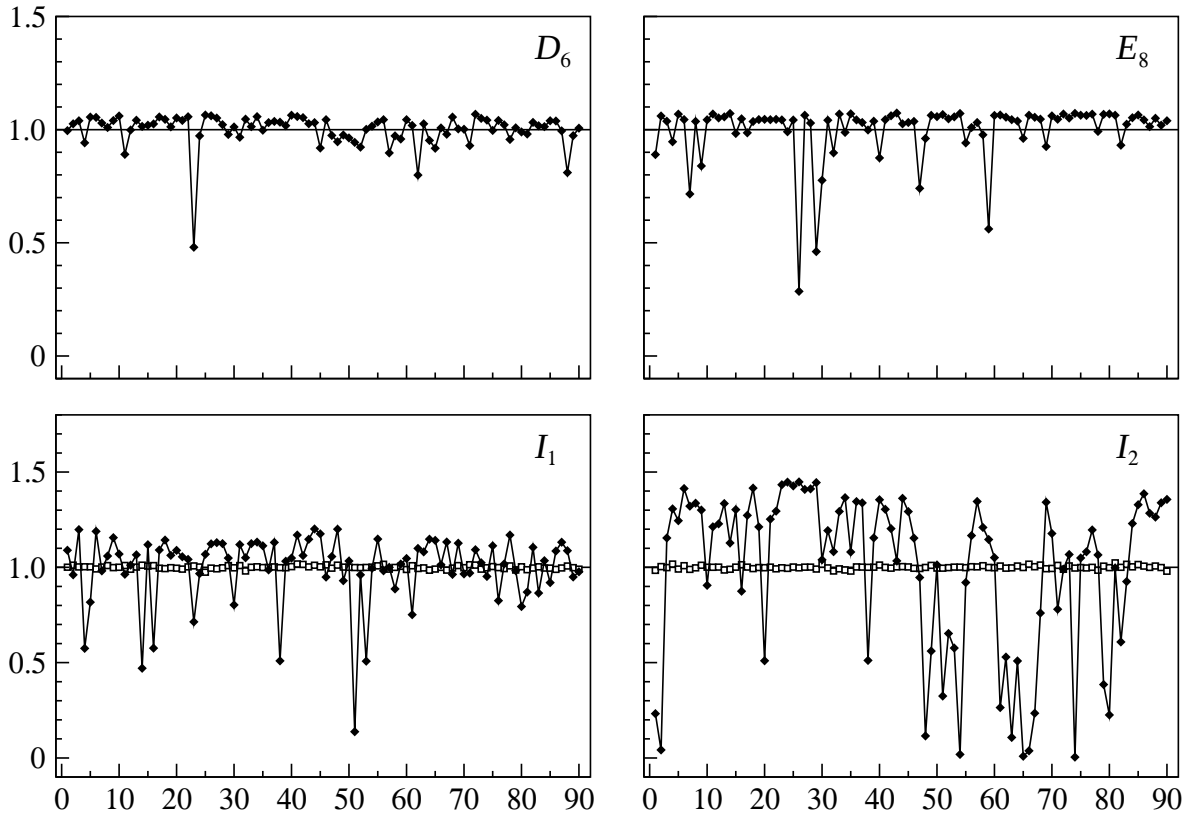
Reweighting factor

$$\det X^{-1} \to \begin{cases} \det 1 + \frac{\mu^2}{Q^2} & = \prod_\lambda 1 + \frac{\mu^2}{\lambda^2} \\ \det 1 + \frac{\mu^2}{Q^2}\frac{(Q^2+\mu^2)}{Q^2+2\mu^2} & = \prod_\lambda 1 + \frac{\mu^4}{\lambda^4} \end{cases}$$

Second term less sensitive to UV contribution.

Example

LÜSCHER, SCHAEFER'12



Summary and Outlook

Fermions

- Fermions are difficult $\rightarrow$ many approaches over the years.
  Mostly variants on pseudofermions
- Determinant splitting techniques reduce force fluctuations
- Intricate interplay between determinant estimate and integrator
- Large effort due to force computation.

Summary and Outlook

Scaling

- HMC is a specimen from a larger class of algorithms based on Stochastic Differential Equations.
- Towards the continuum limit, autocorrelation times scale as a^{-2}
- This is contrary to what has long been believed.
-
- Simulations get very expensive

$$\mathrm{Cost} \propto \underbrace{a^{-4}}_{\#\mathrm{points}} \underbrace{a^{-2}}_{\mathrm{HMC}} \underbrace{a^{-1}}_{\mathrm{integrator}} = a^{-7}$$

It would be good to find a viable alternative.