Introduction to the HMC

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Outline

1. Hamiltonian Monte Carlo: the basics
2. Speeding up the HMC for Lattice QCD
3. Tutorials with Pavel Buividovic

Lectures and Tutorials

1. Lectures: introduce the Theory
   - basic HMC algorithm and Schwinger model
   - algorithm improvements
   - recent developments
2. Tutorials with Pavel Buividovic: you can practice
   - example: Schwinger model
   - template code provided
   - online tutorial with step-by-step instructions
   - based on the lecture

Motivation

- Lattice QCD: solve high dimensional integral

$$\mathcal{Z}_{\mathrm{QCD}} = \int \mathcal{D}U\, \mathcal{D}\bar{\psi}\, \mathcal{D}\psi\, e^{-S_G[U] - \bar{\psi}\, D[U]\, \psi} \propto \int \mathcal{D}U\, \det(D[U]) e^{-S_G[U]}$$

- determinant can be represented by bosonic fields:

$$\det(D) \propto \int \mathcal{D}\phi^\dagger\, \mathcal{D}\phi\, e^{-\phi^\dagger\, D^{-1}\, \phi}$$

  ϕ fields also called pseudo-fermion fields

- can deal with $D^{-1}\, \phi$, but: non-local

Markov-Chain Monte Carlo

- stochastic method to solve the generic integral

$$\langle O \rangle = \int \mathcal{D}x \; O(x) \, e^{-S(x)}$$

- by generating a Markov-Chain $\{x_1, x_2, ...\}$ distributed as

$$e^{-S(x)}$$

- then

$$\langle O \rangle \approx \frac{1}{N} \sum_{i=1}^{N} O(x_i)$$

with statistical error:

$$\delta O \propto 1/\sqrt{N}$$

- how to generate such a chain $\{x_1, x_2, ...\}$?

Metropolis Algorithm

Metropolis Monte-Carlo algorithm

1. start with arbitrary x
2. chose a test x' with probability $P(x')$
   $P(x) > 0 \; \forall x$
3. accept x' with probability

$$P_A(x \to x') = \min\{1, \exp[-\Delta S = -(S(x') - S(x))]\}$$

4. continue with step 2

Fulfils detailed balance condition (easy exercise)

$$\exp(-S(x))P(x \to x') = \exp(-S(x'))P(x' \to x)$$

Metropolis Monte Carlo

- how to generate the proposal x'?
  1. chose x' randomly
     completely uncorrelated to previous x

  $\Rightarrow$ expect large $\Delta S \Rightarrow$ low acceptance $\Rightarrow$ large autocorrelation

  2. use $x' = x + \delta x$ with random but small δx
     δx can be tuned for ΔS to be small

  $\Rightarrow$ large autocorrelation

- if computation of ΔS is very expensive (like for QCD)
  both choices turn out to be not feasible

- desired: a global update combined with large acceptance

The Hamiltonian Monte Carlo (Hybrid Monte Carlo)

[Duane, Kennedy, Pendleton, Roweth, 1987]

- Introduce p_i conjugate to fundamental fields x_i and a Hamiltonian

$$\mathcal{H} = \frac{1}{2}\sum_i p_i^2 + S(x)$$

- $\mathcal{H}$ is conserved under Hamilton's EoM

$$\dot{x}_i = \frac{\partial \mathcal{H}}{\partial p_i} = p_i\,, \qquad \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial x_i} = -\frac{\partial \mathcal{S}}{\partial x_i}$$

$\Rightarrow$ use Hamilton's EoM for global update (molecular dynamics):

$$(p, x) \quad \rightarrow \quad (p', x')$$

- Accept with probability

$$P_A(\mathcal{H} \rightarrow \mathcal{H}') = \min\{1, \exp(\mathcal{H}(p,x) - \mathcal{H}(p',x')\}$$

- Energy conservation guarantees large acceptance!

Detailed Balance for HMC

- Need to proof detailed balance

$$e^{-S(x)} P(x \to x') = e^{-S(x')} P(x' \to x)$$

- $P(x \to x')$ is a convolution of

$$P(x \to x') = \int \mathcal{D}p \; \mathcal{D}p' \; P_{\mathrm{G}}(p) \; P_{\mathrm{MD}}[(x,p) \to (x',p')] P_A(\mathcal{H} \to \mathcal{H}')$$

with (x', p') fixed given (x, p) and

$$P_{\mathrm{G}}(p) = \exp\left\{ -\sum_i p_i^2 \right\}, \qquad P_{\mathrm{G}}(p)\, e^{-S(x)} = e^{-\mathcal{H}(x,p)}$$

- we require molecular dynamics (MD) integration to be reversible

$$P_{\mathrm{MD}}[(x,p) \to (x',p')] = P_{\mathrm{MD}}[(x',-p') \to (x,-p)]$$

Detailed Balance for HMC

- $\mathcal{H}$ is quadratic in p

$$\mathcal{H}(x,p) = \mathcal{H}(x,-p)$$

- and we have the identity

$$\begin{aligned}
\exp(-\mathcal{H})P_A[(x,p) \to (x',p')] &= \exp(-\mathcal{H})\min\{1, \exp(\mathcal{H}-\mathcal{H}')\} \\
&= \min\{\exp(-\mathcal{H}), \exp(-\mathcal{H}')\} \\
&= \exp(-\mathcal{H}')\min\{\exp(\mathcal{H}'-\mathcal{H}), 1\} \\
&= \exp(-\mathcal{H}')P_A[(x',p') \to (x,p)]
\end{aligned}$$

which is basically detailed balance for the Metropolis algorithm

Detailed Balance for HMC

- using all these we obtain

$$
\begin{aligned}
e^{-S(x)}\, P(x \to x') = & \\
&= \int \mathcal{D}p\, \mathcal{D}p'\, e^{-\mathcal{H}(x,p)}\, P_{\mathrm{MD}}[(x,p) \to (x',p')] P_A(\mathcal{H} \to \mathcal{H}') \\
&= \int \mathcal{D}p\, \mathcal{D}p'\, e^{-\mathcal{H}(x',-p')}\, P_{\mathrm{MD}}[(x',-p') \to (x,-p)] \times \\
&\quad \times P_A(\mathcal{H}(x',-p') \to \mathcal{H}(x,-p))
\end{aligned}
$$

- change of variables $-p' \to p'$ and $-p \to p$

$$
\begin{aligned}
e^{-S(x)}\, P(x \to x') = & \int \mathcal{D}p\, \mathcal{D}p'\, e^{-\mathcal{H}(x',p')}\, P_{\mathrm{MD}}[(x',p') \to (x,p)] \times \\
& \times P_A(\mathcal{H}' \to \mathcal{H}) \\
= & e^{-S(x')}\, P(x' \to x) \qquad \text{q.e.d.}
\end{aligned}
$$

Detailed Balance for HMC

from the proof one learns

- MD must be reversible
- measure must invariant

$$\mathcal{D}p \times \mathcal{D}p' = \mathcal{D}(-p) \times \mathcal{D}(-p')$$

  (area preserving)
- if $\mathcal{H}$ is conserved, the $P_A = 1$

in practice we use

- a numerical integration scheme
- accept/reject step corrects for discretisation errors

$\Rightarrow$ need to find a reversible and area preserving integration scheme

Symplectic Integrators

- by linking together x and p in $z = (x, p)$ we can write

$$\dot{z} = \mathbf{J} \cdot \frac{\partial \mathcal{H}(z)}{\partial z}$$

- with symplectic matrix

$$\mathbf{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

- symplectic mans intertwined (see **J**)

- time evolution $z(t_0) \rightarrow z(t)$ represents a canonical transformation $\mathbf{A}(t_0, t)$

$$z(t) = \mathbf{A} \cdot z(t_0)$$

Symplectic Integrators

- such a transformation conserves the energy
- but the symplectic form

$$s(z_1, z_2) \equiv z_1^T \, \mathbf{J} \, z_2$$

  is conserved under this mapping

- geometrically:
  the area of the parallelogram spanned by $z_{1,2}$ is preserved
- for the harmonic oscillator you can easily show

$$z_1(t_0)^T \mathbf{J} \, z_2(t_0) = z_1(t)^T \mathbf{J} \, z_2(t)$$

  by writing down the mapping $\mathbf{A}$.

$\Rightarrow$ s is conserved if $\mathbf{A}^T \mathbf{J} \mathbf{A} = \mathbf{J}$

Symplectic Integrators

- is this useful for a numerical integration scheme?
- yes! (surprise) one can show:
  symplectic integrators do conserve a Hamiltonian $\mathcal{H}_s$ different from, but close to the given Hamiltonian $\mathcal{H}$

$\Rightarrow$ consequence: $\Delta\mathcal{H} = \mathcal{H}_s - \mathcal{H}$ depends only on step size $\Delta\tau$, not on the length of the integration

- simplest example and exercise for you:

$$x_{n+1} = x_n + \Delta\tau\, p_n \qquad p_{n+1} = p_n - \Delta\tau \frac{\partial\mathcal{H}}{\partial x_{n+1}}$$

is symplectic and conserves for the harmonic oscillator

$$\mathcal{H}_s = p^2/2 + x^2/2 + \Delta\tau\, p\, x/2$$

exactly!

Symplectic Integrators

- however, the simple example is not reversible
- but the leap-frog integration scheme
- Discrete updates for time step $\Delta\tau$

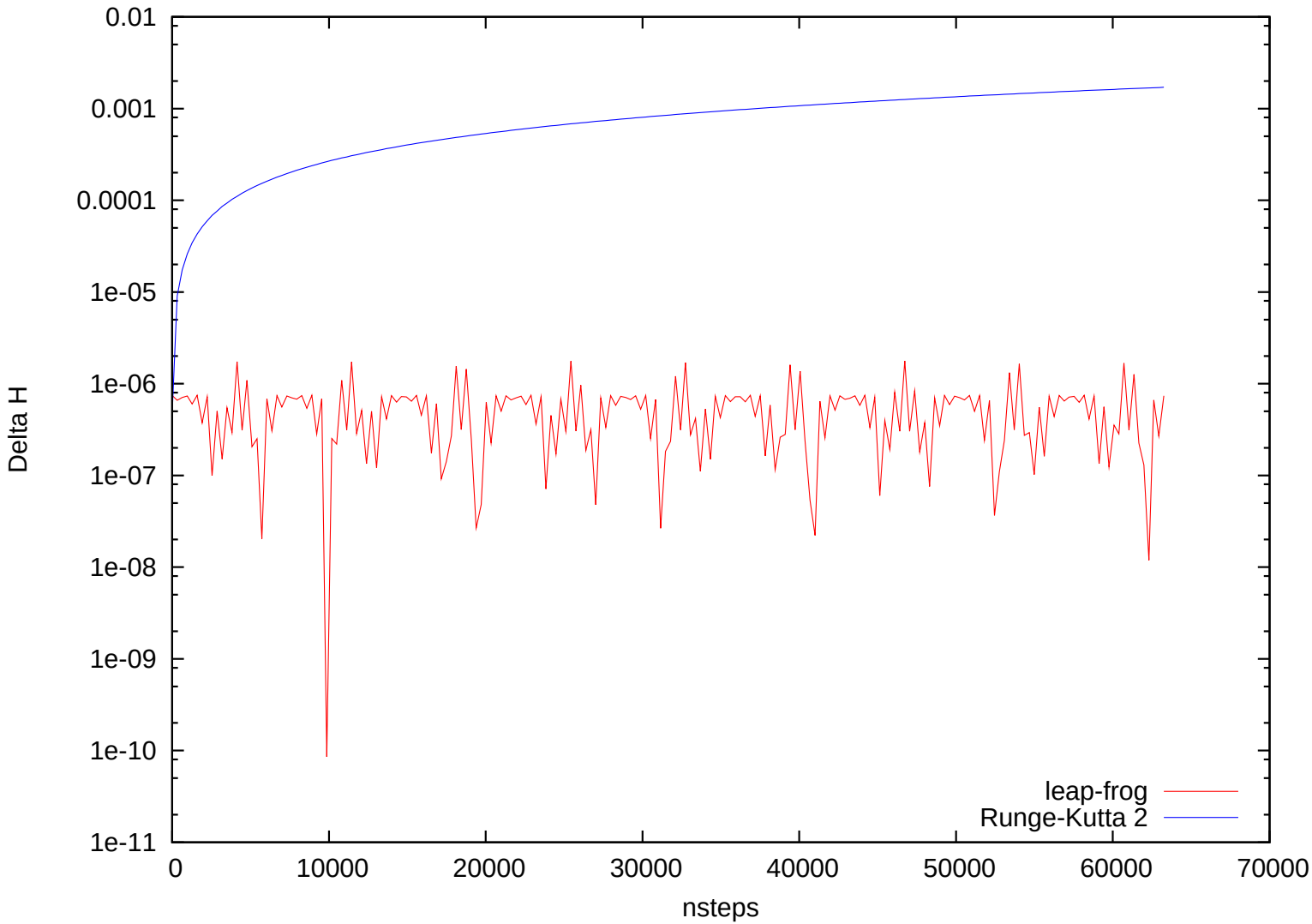
$$T_{\mathrm{x}}(\Delta\tau): \quad x \quad \rightarrow \quad x' = x + \Delta\tau p$$
$$T_{\mathrm{p}}(\Delta\tau): \quad p \quad \rightarrow \quad p' = p - \Delta\tau \frac{\partial \mathcal{H}}{\partial x}$$

- basic Leap Frog time evolution step

$$T = T_{\mathrm{p}}(\Delta\tau/2)\; T_{\mathrm{x}}(\Delta\tau)\; T_{\mathrm{p}}(\Delta\tau/2)$$

- trajectory of length τ: $N_{\mathrm{MD}} = \tau/\Delta\tau$ successive applications of T
- $\Delta\mathcal{H}$ independent of τ!

Symplectic Integrators



Integration Errors

- how does $\Delta\mathcal{H}$ scale with $\Delta\tau$?
- introduce time evolution operator $\exp\{\Delta\tau\hat{\mathcal{H}}\}$ with

$$\hat{\mathcal{H}}\, f(p,x) \equiv -\{\mathcal{H}, f\} = \frac{\partial\mathcal{H}}{\partial p}\frac{\partial f}{\partial x} - \frac{\partial\mathcal{H}}{\partial x}\frac{\partial f}{\partial p}$$

- write $\mathcal{H} = T(p) + S(x)$
- the leap-frog scheme has time evolution

$$e^{\Delta\tau/2\,\hat{S}}\, e^{\Delta\tau\,\hat{T}}\, e^{\Delta\tau/2\,\hat{S}} =$$

$$= \exp\{\Delta\tau(\hat{\mathcal{H}} + \Delta\tau^2([[\hat{S},\hat{T}],\hat{S}] + [[\hat{S},\hat{T}],\hat{T}]) + \mathcal{O}(\Delta\tau^3)\}$$

using the Baker-Campbell-Hausdorff formula

$\Rightarrow\ \Delta\mathcal{H} = \mathcal{O}(\Delta\tau^2)$

Summary basic HMC algorithm

1. generate momenta p_i randomly from Gaussian distribution

$$P \sim e^{-p^2/2}$$

   and compute initial Hamiltonian $\mathcal{H}$.

2. Integrate the equations of motion

$$\dot{x}_i = \frac{\partial \mathcal{H}}{\partial p_i} = p_i \qquad \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial x_i} = -\frac{\partial S}{\partial x_i} \quad \forall i$$

   by means of the leap-frog integration scheme
3. the Hamiltonian is conserved up to $\mathcal{O}(\Delta\tau^2)$
4. compute final Hamiltonian $\mathcal{H}'$ and accept/reject

$$P_A = \min\{1, \exp(-\Delta\mathcal{H})\}$$

   to correct for discretisation errors

Some Diagnostics

Things one can use to test an implementation

- if you get acceptance something must be correct
  unless $\Delta\tau$ too small
- check that $\Delta\mathcal{H}$ scales with $\Delta\tau^2$
- perform a reversibility test
  by integrating forward and backward (reverse time)
- one can show

$$\langle \exp(-\Delta\mathcal{H}) \rangle = 1$$

  useful to check

Some Diagnostics

- when to start measuring?
  - $N \longrightarrow \infty$ is not possible

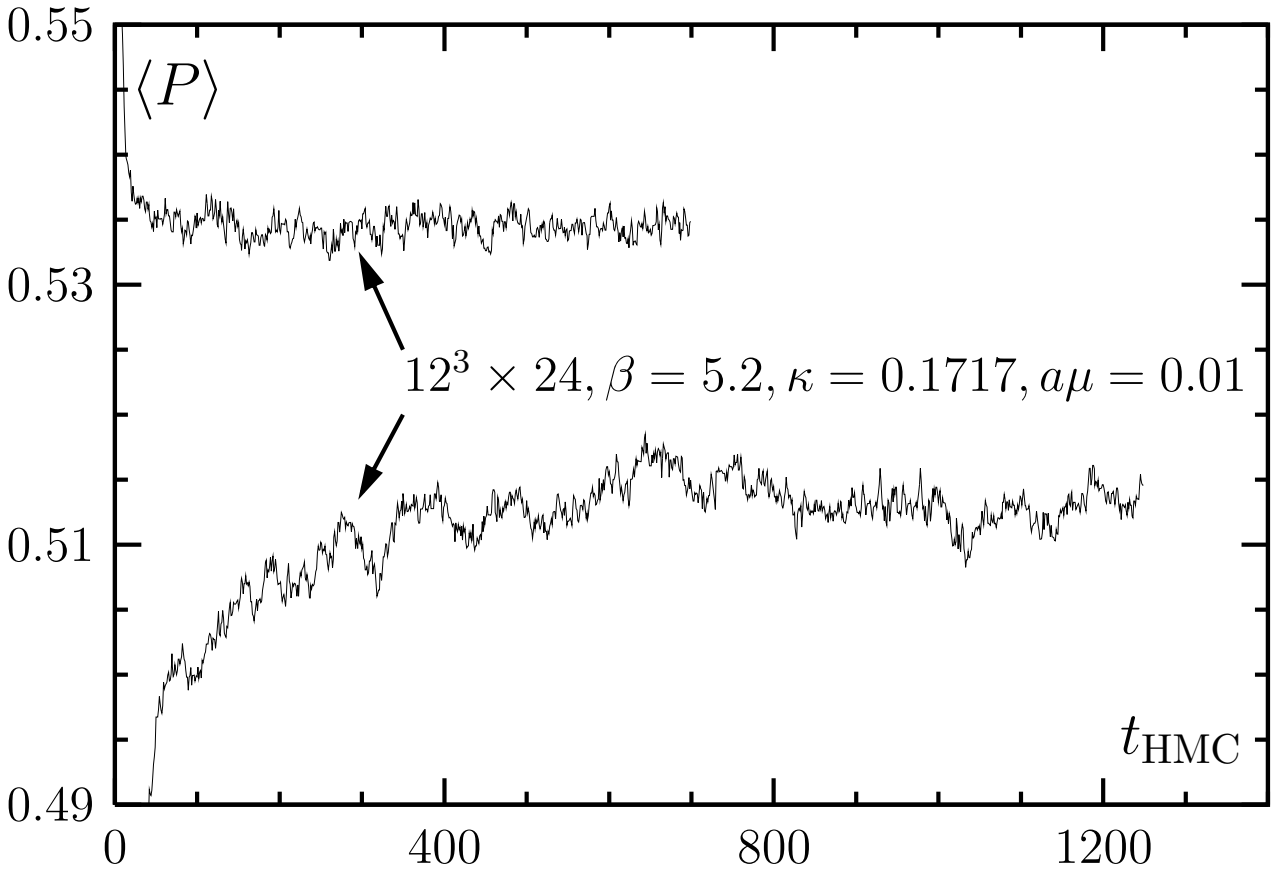
  $\Rightarrow$ we have to equilibrate N_{therm} updates
  - there is no sound theoretical tool for N_{therm}
  - N_{therm} is different for different observables!
- start from several initial configurations until they merge

$\Rightarrow$ expensive

- monitor the moving average until it does not change
- monitor history

Bad Example

This is not just in theory...! Take care!



[Farchioni et. al, Eur.Phys.J. C39 (2005)]

Schwinger Model

- our model for the tutorials:
  QED in 2 dimensions with $N_f = 2$ dynamical fermions
- we use a two-dimensional lattice with extend $L_x \times L_t$
- label the sites with $n = tL_x + x$
- we use periodic boundary conditions for fermion and gauge fields in both directions (for simplicity only)

$\Rightarrow$ the fermionic fields should have anti-periodic b.c.

- the link variables $U_{n,\mu}$ connect sites n and $n + \hat{\mu}$
- they are $U(1)$ phase factors

$$U_{n,\mu} = \exp\{iA_{n,\mu}\}\,, \qquad A_{n,\mu} \in [-\pi, \pi[$$

- lattice action looks identical to QCD

$$S = \beta \sum_P \left[1 - \frac{1}{2}(U_P - U_P^\dagger) \right] + \phi^\dagger \frac{1}{MM^\dagger} \phi = S_G + S_F$$

- with plaquette variable

$$U_P \equiv U_{n,\mu} U_{n+\hat{\mu},\nu} U^\dagger_{n+\hat{\nu},\nu} U^\dagger_{n,\nu}$$

- n is site index and $\mu, \nu \in \{x, t\}$ the directions
- M is the Wilson Dirac operator

Wilson Fermions

- the Wilson Dirac operator

$$M_{n\alpha,m\beta} = (m_0 + 2r)\delta_{nm}\delta_{\alpha\beta} - \frac{1}{2}\sum_{\mu}\left[(r-\gamma_\mu)_{\alpha\beta}U_{n,\mu}\delta n, m-\hat{\mu} + (r+\gamma_\mu)_{\alpha\beta}U^{\dagger}_{m,\mu}\delta_{n,m+\hat{\mu}}\right]$$

- in $d = 2$ dimensions the γ-matrices are

$$\gamma_1 = \sigma_1\,, \quad \gamma_2 = \sigma_2\,, \quad \gamma_5 = \sigma_3$$

  with Pauli matrices σ_i

- they fulfil

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$$

- M is γ_5 hermitian

$$M^{\dagger} = \gamma_5 M \gamma_5$$

- with $N_f = 2$ flavours of Wilson fermions

$$\det \begin{pmatrix} M & 0 \\ 0 & M \end{pmatrix} = \det(MM) = \det(M\gamma_5 M\gamma_5) = \det(MM^\dagger)$$

$\Rightarrow$ $MM^\dagger \equiv Q^2$ is positive definite (with $Q = M\gamma_5$ and $Q = Q^\dagger$)

$\Rightarrow$ fermionic action is real

- and fermion weight is Gaussian

$$\exp\{-\phi^\dagger \frac{1}{Q^2}\phi\} = \exp\{-R^\dagger R\}\,, \qquad \phi = QR$$

$\Rightarrow$ Can generate R from Gaussian distribution and compute ϕ by applying Q

- what about the derivative with respect to $A_{n,\mu}$?
- $\partial S_G / \partial A_{n,\mu}$ is simple
- the pseudo-fermion action is slightly more involved
- the variation for an inverse matrix

$$\delta(A^{-1}) = -A^{-1}\delta(A)A^{-1}$$

$\Rightarrow$ so, for S_F

$$\delta S_F \;=\; -\phi^\dagger \frac{1}{Q^2}\delta(Q^2)\frac{1}{Q^2}\phi \;\equiv\; -\eta^\dagger \delta(Q^2)\eta$$

- with

$$\eta \;\equiv\; \frac{1}{Q^2}\phi$$

HMC for the Schwinger Model

introduce conjugate momenta $p_{n,\mu}$ for every angle $A_{n,\mu}$

1. generate $p_{n,\mu}$ Gaussian distributed
2. generate R Gaussian distributed
3. compute $\phi = Q\,R$
4. MD update with EoM

$$\eta = (Q^2)^{-1}\phi$$
$$\dot{A}_{n,\mu} = p_{n,\mu}$$
$$\dot{p}_{n,\mu} = -\frac{\partial S_G}{\partial A_{n,\mu}} + \eta^\dagger \frac{\partial (Q^2)}{\partial A_{n,\mu}} \eta$$

using the leap-frog algorithm (ϕ unchanged)

5. accept/reject step with

$$\mathcal{H}(A,p) = \sum p^2/2 + S_G(A) + R^\dagger R$$
$$\mathcal{H}(A',p') = \sum p^2/2 + S_G(A') + R'^\dagger R' \,, \qquad R' = (Q(A'))^{-1}\phi$$

HMC for the Schwinger Model

- Q^2 or Q must be inverted on a source
  - in each time step for $\eta = (Q^2)^{-1}\phi$
  - in the acceptance step for $R' = (Q(A'))^{-1}\phi$

- so in total N_{MD} inversions per trajectory

- typically the conjugate gradient (CG) method is used

$\Rightarrow$ requires $\mathcal{O}(1000)$ applications of Q^2 per inversion (depending on lattice spacing, mass, etc...)

Exercises

- for the symplectic integrator (see before!) use

$$\mathcal{H}(x,p) = p^2/2 + x^2/2$$

  and show that the integrator is symplectic and $\mathcal{H}_s$ is conserved
- show that

$$\eta^\dagger \frac{\partial(Q^2)}{\partial A_{n,\mu}} \eta = 2\mathrm{Re}\left[\eta^\dagger \frac{\partial Q}{\partial A_{n,\mu}} Q\eta\right]$$

- compute

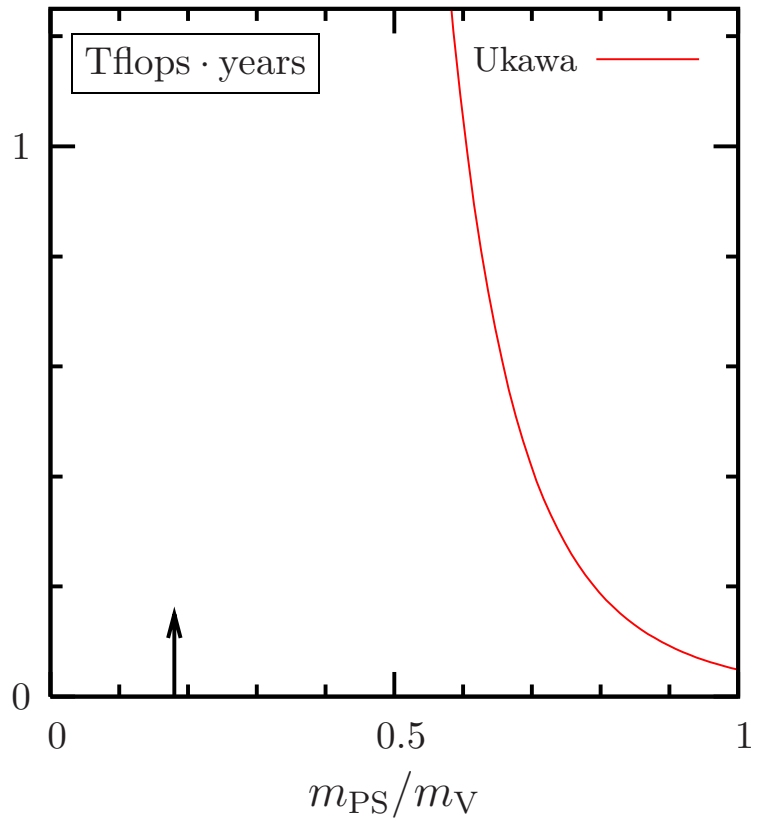
$$\frac{\partial Q}{\partial A_{n,\mu}}$$

  explicitly
- the slides are available at

  `http://www.itkp.uni-bonn.de/~urbach/urbach1.pdf`

Scaling of the HMC

Computer time for 1000 independent configurations
$a \approx 0.08$ fm, $L \approx 2$ fm, Wilson fermions



- Cost $\propto K\,(m_{\mathrm{PS}}/m_{\mathrm{V}})^{-6} L^5 a^{-7}$

  [Ukawa, 2001]

- arrow indicates physical point

- even today not feasible

$\Rightarrow$ Improvements needed!

Scaling of the HMC

What is the source of the bad scaling?

- with decreasing quark mass
  condition number $\kappa \equiv \lambda_{\max}/\lambda_{\min}$ of Q increases

$\Rightarrow$ number of iterations in the CG increases with κ

$\Rightarrow$ fermionic force increases with κ
potentially magnified by noise from the one ϕ-field

- need to reduce
  - condition number κ
  - number of Q^{-2} applications
  - noise from pseudo-fermion fields

Preconditioning

- Most expensive part: fermion determinant
- Precondition by factorisation (with suitable C and E):

$$\det Q^2 = \det(C) \cdot \det(E)$$

  with C and E have both smaller κ than Q^2.

- optimally C and E should be easy to implement and to handle
- by using two independent ϕ-fields for C and E fluctuations are smoothed out

n^{th}-root Trick

- use the following (exact) factorisation

$$\det Q^2 = \sqrt{\det Q^2} \cdot \sqrt{\det Q^2}$$

[Hasenbusch, Hasenbusch and Jansen, Sommer]

- in terms of condition numbers

$$\kappa \qquad \rightarrow \qquad 2\sqrt{\kappa}$$

- of more general with n^{th}-root

$$\det Q^2 = [(\det Q^2)^{1/n}]^n$$

[Clark, de Forcrand, Kennedy (2006)]

- allows to significantly reduce κ

Hasenbusch Trick

- one particularly easy implementation of this idea:

$\Rightarrow$ Mass or Hasenbusch preconditioning

- factorise as follows:

$$\det Q^2 = \det\left[Q^2 + \mu^2\right] \cdot \det\left[\frac{Q^2}{Q^2 + \mu^2}\right].$$

[Hasenbusch, 2001]

- corresponding effective action:

$$S_{\text{eff}} = S_{\text{G}} + \phi_1^\dagger \frac{1}{Q^2 + \mu^2}\phi_1 + \phi_2^\dagger \frac{Q^2 + \mu^2}{Q^2}\phi_2 = S_{\text{G}} + S_{\text{PF}_1} + S_{\text{PF}_2}\,.$$

- can be extended to $N_{\text{PF}} > 2$ pseudo-fermion fields

- tune μ such that the two condition numbers become equal
  exercise: show that this corresponds to the squareroot trick!

Scaling of the HMC

What is the source of the bad scaling?

- with decreasing quark mass
  condition number $\kappa \equiv \lambda_{\max}/\lambda_{\min}$ of Q increases

$\Rightarrow$ number of iterations in the CG increases $\propto \kappa^2$

$\Rightarrow$ fermionic force increases roughly $\propto \kappa$
potentially magnified by noise from the one ϕ-field

- need to reduce
  - condition number κ (✓)
  - number of Q^{-2} applications (✓)
  - noise from pseudo-fermion fields ✓

Separating Scales

- recall Hasenbusch trick:

$$S_{\text{eff}} = S_{\text{G}} + \phi_1^\dagger \frac{1}{Q^2+\mu^2}\phi_1 + \phi_2^\dagger \frac{Q^2+\mu^2}{Q^2}\phi_2 = S_{\text{G}} + S_{\text{PF}_1} + S_{\text{PF}_2}\,.$$

- S_{PF_1} is cheap compared to S_{PF_2}
  it involves only inversions of $Q^2+\mu^2$

- μ could be tuned such that S_{PF_2} has smaller κ than S_{PF_1}

$\Rightarrow$ could try to integrate

  - S_{PF_1} (cheap) with small $\Delta\tau_1$
  - S_{PF_2} (expensive) with large $\Delta\tau_2 \gg \Delta\tau_1$

$\Rightarrow$ separation of Scales

Multiple Time Scale Integration

[Sexton, Weingarten, 1992]

- assume: $\mathcal{H} = \frac{1}{2}\sum p^2 + S_0(x) + S_1(x)$
- define ($j = 0, 1$):

$$T_x(\Delta\tau): \quad x \quad \rightarrow \quad x' = x + \Delta\tau p$$

$$T_{S_j}(\Delta\tau): \quad p \quad \rightarrow \quad p' = p - \Delta\tau \frac{\partial S_j}{\partial x}$$

- and recursively:

$$T_0 = T_{S_0}(\Delta\tau_0/2)\; T_x(\Delta\tau_0)\; T_{S_0}(\Delta\tau_0/2)\,,$$

$$T_1 = T_{S_1}(\Delta\tau_1/2)\; [T_0]^{N_0}\; T_{S_1}(\Delta\tau_1/2)$$

- trajectory of length τ: $\left[T_1\right]^{N_1}$

Multiple Time Scale Integration

- time steps must fulfil: $N_1 = \tau / \Delta\tau_1 \,, \qquad N_0 = \Delta\tau_1 / \Delta\tau_0$
- S_0 must be computed $N_0 \cdot N_1$ times
  S_1 only N_1 times
- note the recursive structure!

$$\left[T_1\right]^{N_1} = \left[T_{S_1}(\Delta\tau_1/2)\ [T_0]^{N_0}\ T_{S_1}(\Delta\tau_1/2)\right]^{N_1}$$

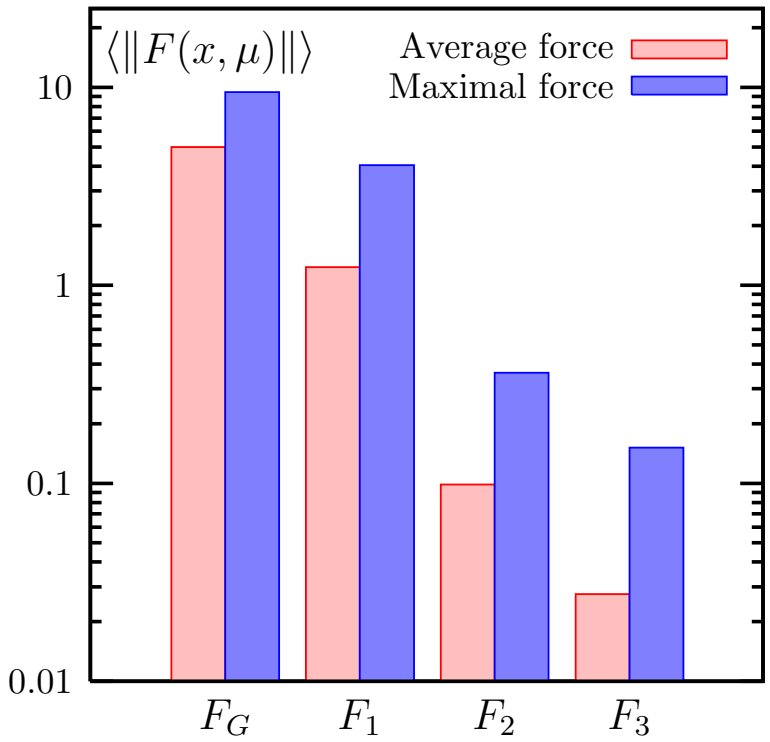
- take

$$\Delta\tau_j \|F_j\| = \Delta\tau_i \|F_i\| \qquad \forall\, i,j$$

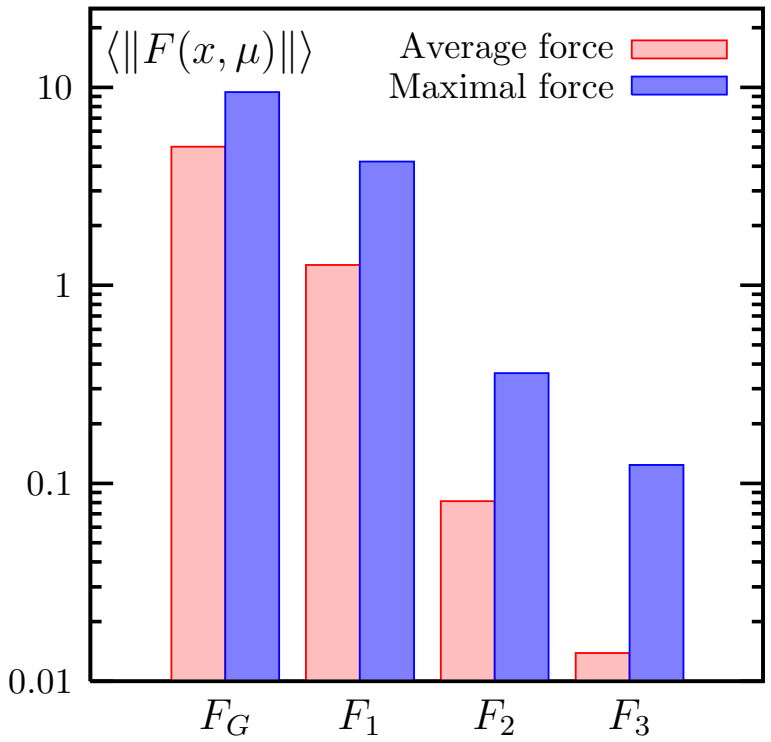
  as a tuning guidline
- for a generalisation with N_i relatively prime to N_j
  see [Kamleh, Peardon (2011)]

Molecular Dynamics Forces

run with $m_{\mathrm{PS}} \approx 485$ MeV:



run with $m_{\mathrm{PS}} \approx 294$ MeV:



Scaling of the HMC

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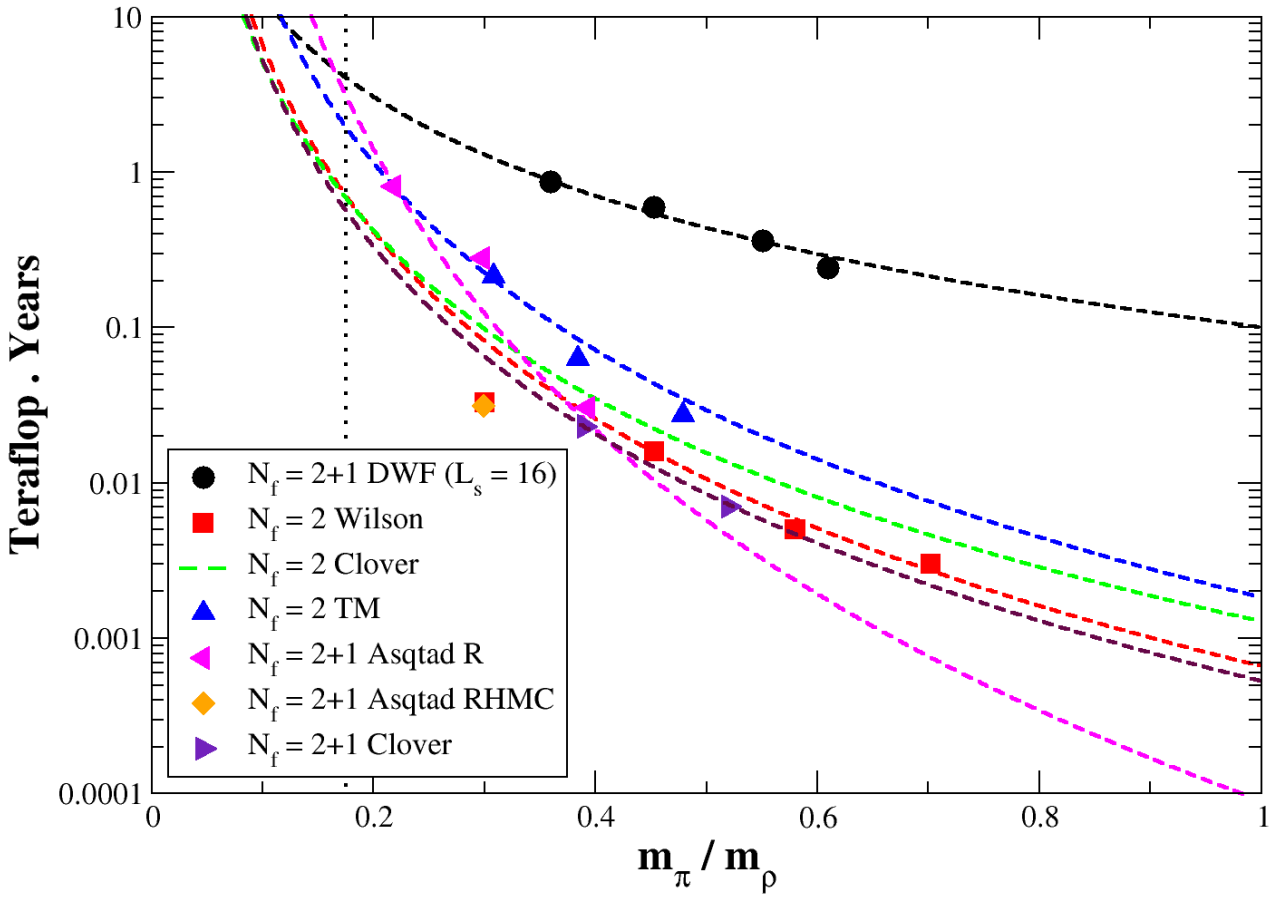
- need to reduce
  - condition number κ ✓
  - number of Q^{-2} applications ✓
  - noise from pseudo-fermion fields ✓

Scaling of the HMC

Updated Berlin Wall plot [Clark (2006)]



Preconditioning

There are alternatives to mass preconditioning

- domain decomposition

  [Lüscher (2005)]

- filtering with rational approximations

  [Clark, Kennedy]

- polynomial filtering

  [Kamleh, Peardon, (2006,2011)]

2MN integration scheme

- $\Delta\tau$ errors can be reduced by higher order integrators
- second order minimal norm (2MN) integration scheme

$$T_{\mathrm{2MN}} = T_{\mathrm{S}}(\lambda\Delta\tau)\; T_{\mathrm{x}}(\Delta\tau/2)\; T_{\mathrm{S}}((1-2\lambda)\Delta\tau)\; T_{\mathrm{x}}(\Delta\tau/2)\; T_{\mathrm{S}}(\lambda\Delta\tau)$$

- trajectory of length τ: $N_{\mathrm{MD}} = \tau/\Delta\tau$ successive applications of T_{2MN}
- λ additional real tunable parameter
- choice $\lambda = 1/6$ is called Sexton-Weingarten integration scheme
- $\lambda \approx 0.21$ is known to be close to optimal

[Takaishi, De Forcrand, hep-lat/0505020]

Other Knobs to twiddle

- vary the trajectory length

$\Rightarrow$ longer trajectory length seems to be favourable

[Meyer et al. (2007)]

- reduced precision in the MD integration
  looking at the detailed balance proof you'll notice the
  - only reversibility and aread preserving properties are used

  $\Rightarrow$ a *guiding* Hamiltonian $\mathcal{H}_g$ can be used instead of $\mathcal{H}$ itself
  - but reversibility *must* be monitored

- use of a chronological solver for better initial guesses for the CG solver

[Brower et al, (1995,1997)]

$\Rightarrow$ the history of solution is used
to create an optimal initial guess for the next inversion
- again reversibility *must* be monitored

Variants of the HMC

- Polynomial HMC (PHMC)

  [Frezzotti, Jansen (1999)]

  $$\det Q = \det(P(Q^2)^{-1})$$

  with a polynomial approximation

  $$Q \cdot P(Q^2) = 1$$

$\Rightarrow$ allows for simulations with odd flavours

$\Rightarrow$ allows for more improvements

- Rational HMC (RHMC)

  [Clark, de Forcrand, Kennedy (2006)]

  like PHMC but with rational approximation

- Domain-decomposed HMC (DD-HMC)

  [Lüscher (2005)]

Critical Slowing Down

- well known: algorithms show critical slowing down as a phase transition is approached

$\Rightarrow$ for QCD

$$\tau_{\text{int}} \quad \propto \quad a^{-z_a}$$

z_a depending on algorithm and observable

- in QCD topological charge is serverly affected

[S. Schäfer et al (2011)]

- possible solution: open boundary conditions

[Lüscher, Schäfer (2011)]

$\Rightarrow$ still: something to think about for young and keen students!

A Study-Case for the Tutorials

- Schwinger model in $d = 2$ dimensions has dimenisonful coupling

$$\beta = \frac{1}{a^2 e^2}$$

- The mass spectrum contains a pion Iso-triplett
- m_π can be determined from pseudo-scalar correlation function
- in the continuum one knows ($m_f \equiv$ quark mass)
  - for small masses

$$\frac{m_\pi}{e} = 2.008 \left(\frac{m_f}{e}\right)^{2/3}$$

[Smilga (1997)]

  - for large masses

$$\frac{m_\pi}{e} = 2.163 \left(\frac{m_f}{e}\right)^{2/3}$$

[Gattringer (1995)]

- note, m_f does not need renormalisation

so, if you are keen and have time, you might want to look at

- continuum limit of m_π at fixed m_f

$\Rightarrow$ $m_\pi\sqrt{\beta}$ as a function of $1/\sqrt{\beta}$ at fixed $(m_f\sqrt{\beta})^{2/3}$ and $L/\sqrt{\beta}$

- you can implement Wilson and Wilson-twisted mass fermions and practice what you learned this week
- check the asymptotic formulae for m_π in the continuum
- for details see:
  [N. Christian et al, Nucl.Phys. B739 (2006) 60-84, hep-lat/0510047]

Have fun with the tutorial!

Tutorial at

`http://www.lattice.itep.ru/~pbaivid/dubna/`

These slides can be found at

`http://www.itkp.uni-bonn.de/~urbach/urbach1.pdf`

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