Status and challenges of simulations with dynamical fermions

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Lattice 2012

Progress

Typical simulation 2002

- $L = 1.8\,\text{fm}$
- $a = 0.09\,\text{fm}$
- $m_\pi \approx 600\,\text{MeV}$

Typical simulation 2012

- $L = 3\,\text{fm}$
- $a = 0.06\,\text{fm}$
- $m_\pi \approx 250\,\text{MeV}$

Progress

Typical simulation 2002

- $L = 1.8\,\text{fm}$
- $a = 0.09\,\text{fm}$
- $m_\pi \approx 600\,\text{MeV}$

Typical simulation 2012

- $L = 3\,\text{fm}$ . . . and up
- $a = 0.06\,\text{fm}$ . . . down to $0.045\,\text{fm}$
- $m_\pi \approx 250\,\text{MeV}$ . . . down to $m_\pi = m_\pi^{\text{phys}}$

Techniques

Update algorithms

- determinant splitting
- better-than-leapfrog integrators

Solvers

- local deflation
- multigrid

Computers

- Computers have become faster.

UPDATE ALGORITHMS

Theme: Choose the right action

Generalities

- All large scale simulations use the **Hybrid Monte Carlo**.

  DUANE ET AL'87
- Variants from specific **action during trajectory**.
  $\rightarrow$Representation of quark determinant.

Guide for improvement

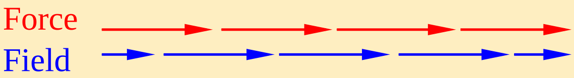
- Frequency splitting.
- Determinant estimate.

Molecular dynamics

- Hamiltonian equations of motion

$$\dot{\pi} = -\frac{\delta S}{\delta U} \quad \text{and} \quad \dot{U} = \pi$$

- Numerical solution



- Conventional wisdom:

  Large Forces $\Rightarrow$ Small step size

- Fluctuations of force more important.
- Influences choice of S.

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}

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

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

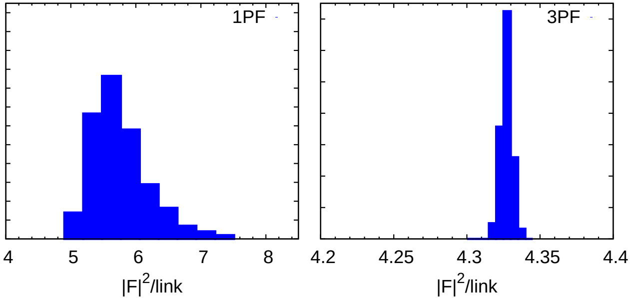
- $N_\mathrm{f} = 2 + 1$ NP improved Wilson fermions
- Iwasaki gauge action
- 64×32^3 lattice with $a = 0.09$fm
- studied extensively by PACS-CS AOKI ET AL'09,'10
- $m_\pi = 200$MeV
- $m_\pi L = 3$

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 in **norm** squared of force.
  Spread reduced by more than factor 100.
  (Different scale!)

Understanding the improvement

Framework — CLARK, JOO, KENNEDY, SILVA'11

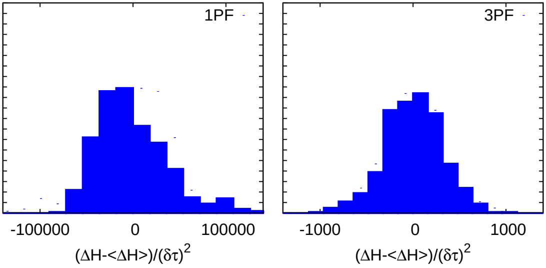
- Shadow Hamiltonian of symplectic integrators

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

- 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.

Other decompositions

RHMC

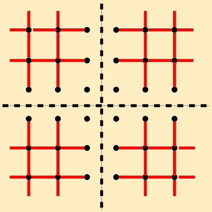
Horvath et al'00, Clark, Kennedy'07

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

- Primary use: single flavors
- Splitting in equal factors
- Need n-th root function
  $\rightarrow$ rational approximation

DD-HMC

Lüscher'04



- Domain decomposition
- Divide the lattice in blocks
- Inactive links
  $\rightarrow$ longer autocorrelations

Reweighting

Problem

- Wilson fermions do not have solid spectral gap.
- Affects stability of the algorithm.
  $\rightarrow$ large fluctuations in forces ("spikes").

Basic idea

FERRENBERG, SWENDSEN'88

- Action S_0 inconvenient in simulations.
- Simulate different action S_1.
- Include correction factor in measurement.

$$\langle A \rangle_0 = \frac{\langle A \; e^{-(S_0 - S_1)} \rangle_1}{\langle e^{-(S_0 - S_1)} \rangle_1}$$

Stability of Wilson fermion simulations

Twisted mass reweighting — LÜSCHER, PALOMBI'09

- Simulate with finite action

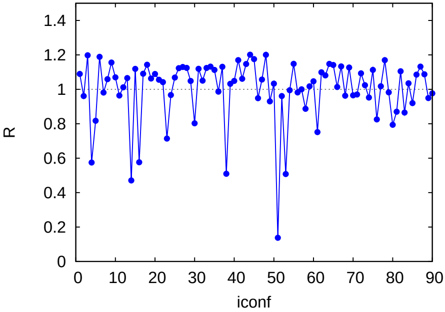
$$\det Q^2 \to \begin{cases} \det(Q^2+\mu^2) & \text{Type I} \\ \det(Q^2+\mu^2)^2/\det(Q^2+2\mu^2) & \text{Type II} \end{cases}$$

- Include reweighting factor in measurement.
- Ensures that all sectors of field space can be reached.

Example

- 2+1 improved Wilson fermions, Iwasaki gauge
- $L = 2.9\,\mathrm{fm}$, $m_\pi = 200\,\mathrm{MeV}$
- $\mu \approx Z_A m_q$

PLOT: LÜSCHER, S.S.'12



SEE ALSO MIAO ET AL'11

- Reweighting factor well behaved.

Reweighting

Further Applications

- Corrections in quark mass tuning — PACS-CS, RBC
- QED effects — TALK BY IZUBUSHI
- Low mode sampling efficiency — HASENFRATZ ET AL'08

SOLVERS

Theme: Block decomposition

Solution of the Dirac equation

$$(D + m)\psi = \phi$$

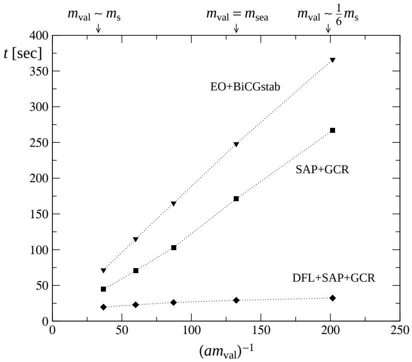
- Most expensive part of simulation.
- Traditional solvers(CG,...) inefficient as $m \to 0$.
- Essential to treat low-energy part of spectrum separately.

Block methods

- Successful methods: block decomposition
  - Schwarz Alternating Procedure — LÜSCHER'04, TALK BY ISHIKAWA
  - Local deflation — LÜSCHER'07
  - Adaptive multigrid (groups in Boston and Wuppertal) — BABICH ET AL'10, FROMMER ET AL'12

Example: Local deflation

PLOT: M. LÜSCHER, JHEP 0707 (2007) 081



- Critical slowing down almost absent for defl. solver.
- Deteminant split-up needs multiple solves per gauge field → **solver's setup cost negligible**.

Summary: Light quark simulations

QCD in the chiral regime

- Simulations at physically light quark masses possible
  $\rightarrow$ PACS-CS, BMW, ...
- **Combination** of several improvements
  - Better treatment of quark determinant
    $\rightarrow$ split in several contributions
  - Advanced solvers (local deflation, multigrid)
    Setup cost easily amortized over multiple solutions.
  - Improved integrators profit from reduced fluctuations.
    $\rightarrow$4th order/force gradient integrators
- Wilson fermions have particularly profited.
- Tool to argue about performance.

Continuum Limit

Continuum limit

Cost of a simulation

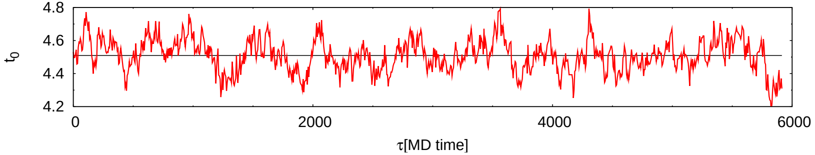
- For 2nd order integrator

$$\text{cost} \propto (V/a^4)^{5/4} \cdot a^{-z}$$

V/a^4	number of lattice points
$V^{0.25}/a$	step size for constant acceptance
z	dynamical critical exponent z of algorithm (approaching continuous phase transition)

- Number of points inevitable
- Noise reduction as $a \to 0$.
- **How does Monte Carlo time behave as $a \to 0$?**
- HMC in Langevin universality class LÜSCHER, S.S.'11
  $\Rightarrow \quad z = 2$

Autocorrelation time

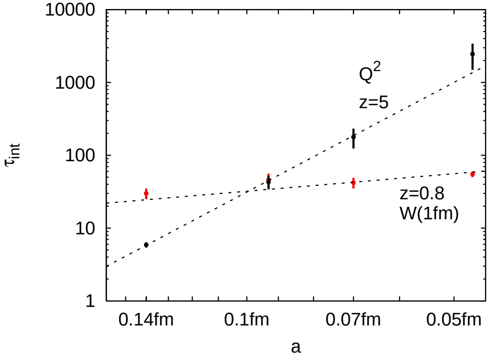


Autocorrelation function

$$\Gamma(\tau) = \langle (A(\tau) - \bar{A})(A(0) - \bar{A}) \rangle$$

Integrated Autocorrelation Time

$$\tau_{\mathrm{int}}(A) = \int_{-\infty}^{\infty} \mathrm{d}\tau \, \rho(\tau) \quad \text{with} \quad \rho(\tau) = \frac{\Gamma(\tau)}{\Gamma(0)}$$

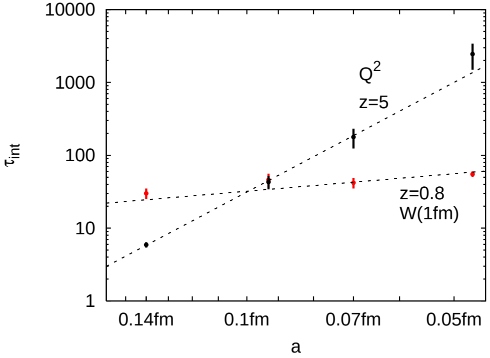


SOMMER, VIROTTA, S.S.'10

SEE ALSO DEL DEBBIO ET AL'02, LÜSCHER'10

- Pure gauge theory, Wilson action, $L = 2.4\,\text{fm}$
- $1\text{fm} \times 1\text{fm}$ Wilson loop $\to \tau_{\text{int}} \propto a^{-0.8}$
- Topological charge $Q^2 \to \tau_{\text{int}} \propto a^{-5}$

Observed scaling: Pure gauge theory



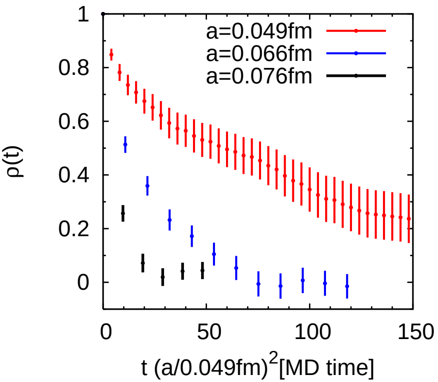
Sommer, Virotta, S.S.'10

see also Del Debbio et al'02, Lüscher'10

- Even in pure gauge theory, measurements below 0.05 fm difficult
- Does not match $z = 2$ expectation.

Autocorrelations: Fermions

DATA: F. VIROTTA, CLS

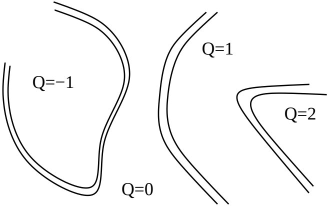


- $N_\mathrm{f} = 2$ improved Wilson fermions, Wilson gauge action
- For $a < 0.05\,$fm, Q^2 slower than other observables.

Topological charge

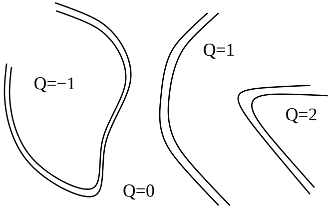
$$Q = -\frac{a^4}{32\pi^2} \int \mathrm{d}\,x\, \epsilon_{\mu\nu\rho\sigma}\, \mathrm{tr}\, F_{\mu\nu} F_{\rho\sigma}$$

- In continuum limit, disconnected **topological sectors**.
- Consequence of periodic boundary conditions.
- Simulations stuck in one sector.



Topological charge

- **Tunneling is a cut-off effect.**
- The probability of configurations "in between" sectors drops rapidly as $a \to 0$:
  Roughly with a^{-6} in fixed volume. M. LÜSCHER, '10
- All quasi continuous algorithms affected.
  Independent of the lattice action.
- Insufficient sampling of field space,
  prevents simulations on fine lattices.



Solutions I

Fixed topological charge

- Modify action so that algorithm does not change Q.
- Deal with finite volume effects BROWER ET AL'03

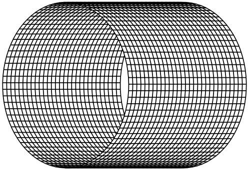
$$\langle A \rangle_{Q=Q_0} = \langle A \rangle \cdot \{1 + \frac{c_{Q_0}}{V} + \dots)\}$$

- Theory no longer unitary.
- Used by JLQCD in the dynamical overlap project.

Solutions II

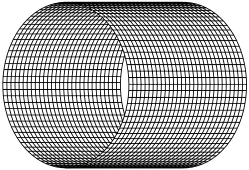
Open boundary conditions — M. LÜSCHER, S.S. 2011

- open boundary condition in time direction
  → same transfer matrix, same particle spectrum
- periodic boundary condition in spatial directions
  → momentum projection possible
- Charge can flow over temporal boundaries.
- **Field space connected also in the continuum.**



Open boundary conditions

- Lattices of size $T \times L^3$.
- Neumann boundary conditions in time.
- Fermions like Schrödinger functional



- Gauge fields

$$F_{0k}|_{x_0=0} = F_{0k}|_{x_0=T} = 0, \quad k = 1,2,3$$

- Fermion fields

$$P_+\psi(x)|_{x_0=0} = P_-\psi(x)|_{x_0=T} = 0 \qquad P_\pm = \frac{1}{2}(1 \pm \gamma_0)$$

$$\bar{\psi}(x)P_-|_{x_0=0} = \bar{\psi}(x)P_+|_{x_0=T} = 0$$

STUDYING AUTOCORRELATIONS

Smooth observables with continuum limit

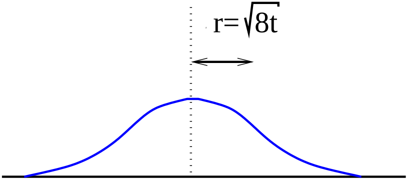
Gradient flow

LÜSCHER'10, LÜSCHER&WEISZ'11

- Smoothing with **gradient flow** with flow time t

$$\partial_t V_t(x,\mu) = -g_0^2 \left[\partial_{x,\mu} S(V_t)\right] V_t(x,\mu); \quad V_t(x,\mu)|_{t=0} = U(x,\mu)$$

- Gaussian smoothing over $r \sim \sqrt{8t}$.
- "continuous stout smearing" with physical range
- Renormalized quantities with continuum limit.
- Good tool to reveal slow modes of simulation.



Observables

$$\partial_t V_t(x,\mu) = -g_0^2 \left[\partial_{x,\mu} S(V_t)\right] V_t(x,\mu); \quad V_t(x,\mu)|_{t=0} = U(x,\mu)$$

$$\overline{E}(x_0) = -\frac{a^3}{2V} \sum_{\vec{x}} \mathrm{tr}\, G_{\mu\nu} G_{\mu\nu}$$

$$\overline{Q}(x_0) = -\frac{a^3}{32\pi^2} \sum_{\vec{x}} \epsilon_{\mu\nu\rho\sigma} \mathrm{tr}\, G_{\mu\nu} G_{\rho\sigma}$$

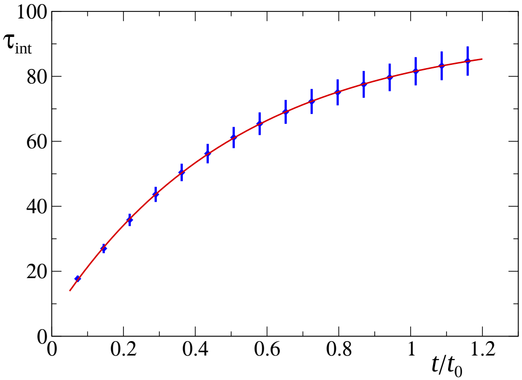
$$Q = -\frac{a^4}{32\pi^2} \sum_{x} \epsilon_{\mu\nu\rho\sigma} \mathrm{tr}\, G_{\mu\nu} G_{\rho\sigma}$$

- $G_{\mu\nu}$: field strength tensor constructed from V_t
- Define t_0 for smoothing radius $r \approx r_0 = 0.5\,\mathrm{fm}$

$$t^2 \langle \overline{E} \rangle_{t=t_0} = 0.3$$

Effect of the smoothing

Autocorrelation time of $\bar{E}$ vs. smoothing range (a=0.05fm).

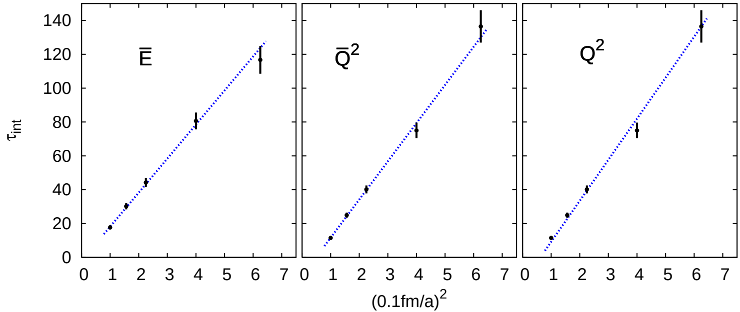


- $\sqrt{8t}$ smoothing radius $\rightarrow t = t_0$ smoothing over $r \approx r_0$
- $\tau_{\rm int}$ saturates with $\tau_{\rm int} = 93 + ae^{-c/t}$.

Test of open boundary conditions

Theme: They work as expected.

Scaling towards continuum limit: $\tau_{\rm int}$ vs a^{-2}



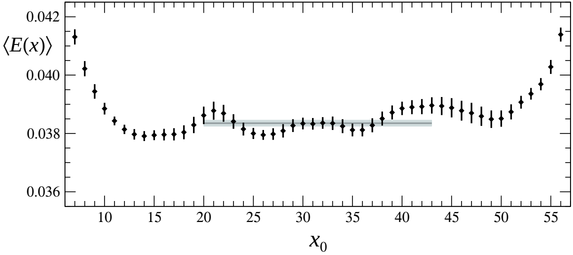
SMD algorithm scale $\tau_{\rm int}$ with 1.37 for HMC.

- Pure gauge theory, Wilson gauge action, $L = 1.6$ fm.
- $\tau_{\rm int}$ **for all observables linear in** a^{-2}.
- Moderate autocorrelation times.

Action

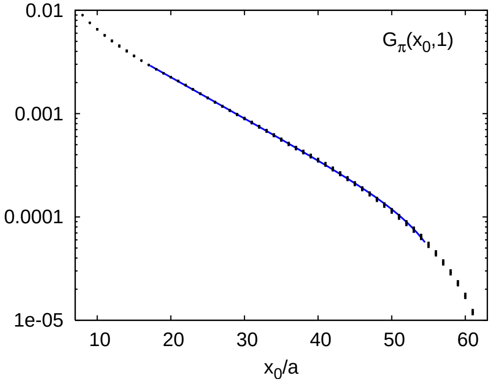
- $N_\mathrm{f} = 2 + 1$ NP improved Wilson fermions
- Iwasaki gauge action
- 64×32^3 lattice with $a = 0.09\,$fm
- $L \approx 2.9\,$fm
- $m_\pi = 200$MeV; $m_\pi L = 3$

Effect of the boundary: gauge observables



- Wilson flow time $t = t_0$
- Smoothing radius $r = \sqrt{8t} \approx 0.5$ fm.
- Correlation length $1/(am_\pi) \approx 11$
- Plateau starting ~ 1 fm from boundary.

Fermions and open boundary conditions



source at $y_0/a = 1$

- Chiral perturbation theory with Dirichlet b.c.

$$G(x_0, y_0) \propto \sinh(m(T - x_0)) \sinh(m y_0) \qquad \text{for} \quad y_0 < x_0$$

- Valid if sufficiently away from boundary (≈ 0.5 fm).

Summary: Algorithms

Current state

Combination of several innovations

- Quark determinant factorization reduces noise in forces.
- Advanced solvers.
  Setup cost amortized over several solutions.
- Advanced MD integrators profit from stable forces.

Methods are widely used and work for most actions.

Summary: Continuum limit

Scaling

- Molecular dynamics based algorithms:
  MD time scales with $1/a^2$.

Topological charge

- Topological charge freezes as $a \to 0$.
- Property of continuum theory.
- All discretizations affected.
- Open boundary conditions solve this problem:
  Field space connected in continuum.

MORE EXAMPLES FOR OPEN B.C.$\to$TALK BY A. RAMOS

What can we expect?

Experience

- Improved Wilson fermions, Iwasaki gauge action.
- 64×32^3 lattice, $a = 0.09$ fm
- **physical light and strange quark mass**, $m_\pi L = 2$
- $\tau_{\text{int}}(E) \sim \text{O}(20)$

Estimate

- Twice larger lattice for $m_\pi L = 4$, $L \approx 6$ fm.
- Run length $100 \cdot \tau_{\text{int}}(E) = 2000 \cdot (a/0.09\text{fm})^{-2}$.

$$\text{cost} = 3\,\text{Tflops} \cdot \text{years} \cdot (a/0.09\text{fm})^{-7}$$

- $a = 0.045$ fm still cost 400 Tflops·years.