Status and challenges of simulations with dynamical fermions

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Lattice 2012
## Typical simulation 2002

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

## Typical simulation 2012

- $L = 3 \text{ fm}$
- $\alpha = 0.06 \text{ fm}$
- $m_\pi \approx 250 \text{ MeV}$
Typical simulation 2002

- $L = 1.8$ fm
- $\alpha = 0.09$ fm
- $m_\pi \approx 600$ MeV

Typical simulation 2012

- $L = 3$ fm . . . and up
- $\alpha = 0.06$ fm . . . down to 0.045 fm
- $m_\pi \approx 250$ 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**.
  - 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
  - Force
  - Field

- Conventional wisdom:
  - Large Forces \(\Rightarrow\) Small step size
  - Fluctuations of force more important.
  - Influences choice of \(S\).
Pseudofermions

\[ \det Q^2 \propto \int d\phi e^{-\left(\phi, Q^{-2}\phi\right)} \]

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

\[ F_{\text{pf}} = \delta(\phi, Q^{-2}\phi) \quad \text{and} \quad F_{\text{ex}} = -\delta \text{tr log } Q^2 \]

- **\( F_{\text{pf}} \) is “stochastic estimate” of \( F_{\text{ex}} \)**
  
  At beginning of the trajectory \( \langle F_{\text{pf}} \rangle_\phi = F_{\text{ex}} \)

- **Very large fluctuations in \( F_{\text{pf}} \)**

\[ |F_{\text{pf}}| \gg |F_{\text{ex}}| \]
Insight

- Need better estimate of determinant.
- Frequency splitting.

Mass preconditioning  

\[
det Q^2 = det \left( \frac{Q^2}{Q^2 + \mu^2} \right) \det(Q^2 + \mu^2)
\]

- Each determinant represented by pseudo-fermion
- "Pauli-Villars" for fermion force
- More intermediate \( \mu \rightarrow \) Noise reduction in force.
- Success depends on choice of \( \mu \).
### Numerical examples

#### Action

- $N_f = 2 + 1$ NP improved Wilson fermions
- Iwasaki gauge action
- $64 \times 32^3$ lattice with $a = 0.09\text{fm}$
- Studied extensively by PACS-CS [Aoki et al.’09,’10](#)
- $m_\pi = 200\text{MeV}$
- $m_\pi L = 3$

#### Algorithm

- Reweighting to avoid stability problems.
- Generated with new public openQCD code. [http://cern.ch/luscher/openQCD](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

- **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 → **potential for optimization**.

- **2nd order minimum norm integrators:**
  minimum of \(c_1^2 + c_2^2\)  

- **Symplectic integrators profit from reduced fluctuations in norm of force.**

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*CLARK, JOO, KENNEDY, SILVA’11*

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*OMELYAN, MRYGOLD, FOLK’03*
Numerical examples

\[ \Delta H = \tilde{H} - H, \text{ fermions only.} \]

- Second order min. norm Omelyan integrator.
- Much larger step-size possible.

\[ \frac{(\Delta H - \Delta H)}{(\delta \tau)^2} \]

1PF

\[ \frac{(\Delta H - \Delta H)}{(\delta \tau)^2} \]

3PF
Other decompositions

**RHMC**

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

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

**DD-HMC**

- 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.
  → large fluctuations in forces ("spikes").

Basic idea

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

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

Lüscher, Palombi’09

- Simulate with finite action

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

- Include reweighting factor in measurement.
- Ensures that all sectors of field space can be reached.
2+1 improved Wilson fermions, Iwasaki gauge

\( L = 2.9 \text{ fm}, m_\pi = 200 \text{ MeV} \)

\( \mu \approx Z_A m_q \)

Reweighting factor well behaved.
### Further Applications

- Corrections in quark mass tuning
- QED effects
- Low mode sampling efficiency

**PACS-CS, RBC**  
**TALK BY IZUBUSHI**  
**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
    - Babich et al’10
    - Frommer et al’12
  - (groups in Boston and Wuppertal)
Critical slowing down almost absent for defl. solver.

Determinant 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
  → PACS-CS, BMW, ...
- **Combination** of several improvements
  - Better treatment of quark determinant
    → split in several contributions
  - Advanced solvers (local deflation, multigrid)
    Setup cost easily amortized over multiple solutions.
  - Improved integrators profit from reduced fluctuations.
    → 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
  \[ \text{cost} \propto \left( \frac{V}{a^4} \right)^{5/4} \cdot a^{-z} \]

- \( V/a^4 \): 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
  \[ \Rightarrow z = 2 \]

Lüscher, S.S.’11
Autocorrelation function

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

Integrated Autocorrelation Time

\[ \tau_{\text{int}}(A) = \int_{-\infty}^{\infty} d\tau \, \rho(\tau) \quad \text{with} \quad \rho(\tau) = \frac{\Gamma(\tau)}{\Gamma(0)} \]
Observed scaling: Pure gauge theory

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

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

- $N_f = 2$ improved Wilson fermions, Wilson gauge action
- For $a < 0.05$ fm, $Q^2$ slower than other observables.
Topological charge

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

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

![Diagram showing topological charge sectors](image_url)
- **Tunneling is a cutoff effect.**
- The probability of configurations "in between" sectors drops rapidly as \( a \to 0 \):
  Roughly with \( a^{-6} \) in fixed volume.  
  
  \[ Q = -1 \quad Q = 0 \quad Q = 1 \quad Q = 2 \]

- All quasi continuous algorithms affected.
  Independent of the lattice action.

- Insufficient sampling of field space, prevents simulations on fine lattices.

\[ \text{M. L"uscher, '10} \]
Fixed topological charge

- Modify action so that algorithm does not change $Q$.
- Deal with finite volume effects

\[
\langle A \rangle_{Q=Q_0} = \langle A \rangle \cdot \left\{ 1 + \frac{cQ_0}{V} + \ldots \right\}
\]

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

- 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

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

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

Smooth observables with continuum limit
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.

$r = \sqrt{8t}$
\[ \partial_t V_t(x, \mu) = -g_0^2 \left[ \partial_{x, \mu} S(V_t) \right] V_t(x, \mu); \quad V_t(x, \mu)|_{t=0} = U(x, \mu) \]

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

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

\[ Q = -\frac{a^4}{32\pi^2} \sum_x \epsilon_{\mu\nu\rho\sigma} \text{tr} \, G_{\mu\nu} G_{\rho\sigma} \]

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

\[ t^2 \langle \overline{E} \rangle_{t=t_0} = 0.3 \]
Effect of the smoothing

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

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

Theme: They work as expected.
Scaling towards continuum limit: $\tau_{\text{int}}$ vs $a^{-2}$

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

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

- $N_f = 2 + 1$ NP improved Wilson fermions
- Iwasaki gauge action
- $64 \times 32^3$ 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 $r = \sqrt{8t} \approx 0.5 \text{ fm}$.
- Correlation length $1/(am_\pi) \approx 11$
- Plateau starting $\sim 1 \text{ fm from boundary}$.
Fermions and open boundary conditions

Chiral perturbation theory with Dirichlet b.c.

\[ G(x_0, y_0) \propto \sinh(m(T - x_0)) \sinh(my_0) \quad \text{for} \quad y_0 < x_0 \]

Valid if sufficiently away from boundary (\( \approx 0.5 \text{ fm} \)).

Source at \( y_0/a = 1 \)
## 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.
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. → TALK BY A. RAMOS
What can we expect?

Experience

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

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.