Stabilised Wilson fermions for QCD on very large lattices

A. Francis, P. Fritzsch, M. Lüscher, A. Rago
Master-field & large-scale simulations

Are we well prepared for very large lattices?

\[ \sim (V/a^4)^p \]

Known obstacles

- algorithmic stability
  - Hybrid Monte-Carlo algorithm
  - integration schemes
  - global Metropolis accept-reject step
  - ...

- fermion discretisation
  - spectral gap of Dirac operator
  - near zero-modes: MD evolution of smallest eigenvalue
  - solver stopping criteria
  - ...

strongly influence costs & may decrease reliability
Algorithmic improvements for stability

General caveats: volume dependence, sampling, reversibility, … → Suggestion:

**Stochastic Molecular Dynamics (SMD) algorithm**\(^{[1–4]}\)

Refresh \(\pi(x, \mu), \phi(x)\) by random field rotation

\[
\pi \rightarrow c_1 \pi + c_2 v , \quad c_1 = \exp(-\epsilon \gamma) , \quad c_2 = (1 - c_1^2)^{1/2}
\]

\[
\phi \rightarrow c_1 \phi + c_2 D^\dagger \eta , \quad (\gamma > 0: \text{friction parameter}; \epsilon: \text{MD integration time})
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+ MD evolution + accept-reject step + repeat
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- ergodic\(^{[5]}\) for sufficiently small \(\epsilon\)
- exact algorithm
- significant reduction of unbounded energy violations \(|\Delta H| \gg 1\)
- a bit “slower“ than HMC but compensated by shorter autocorrelation times
- smooth changes in \(\phi_t, U_t\) improve update of deflation subspace
Algorithmic improvements for stability

- Solver stopping criteria

\[ \| D\psi - \eta \|_2 \leq \rho \| \eta \|_2 , \quad \| \eta \|_2 = \left( \sum_x (\eta(x), \eta(x)) \right)^{1/2} \propto \sqrt{V} \]

- Global accept-reject step

\[ \Delta H \propto \epsilon^p \sqrt{V} \] (numerical precision must increase with \( V \))
Algorithmic improvements for stability

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✓ uniform norm \( \| \eta \|_\infty = \sup_x \| \eta(x) \|_2 \) V-independent

- global accept-reject step

\( \Delta H \propto \epsilon^p \sqrt{V} \)

✓ quadruple precision in global sums

- well-established techniques

✓ SAP, local deflation, multi-grid, mass-preconditioning, multiple time-scales, …
Bulk O(a)-improved Wilson–Dirac operator

\[ D = \frac{1}{2} \left\{ \gamma_\mu (\nabla^*_\mu + \nabla_\mu) - a \nabla^*_\mu \nabla_\mu \right\} + ac_{sw} \frac{i}{4} \sigma_{\mu \nu} \hat{F}_{\mu \nu} + m_0 \]

Even-odd preconditioning:

\[ \hat{D} = D_{ee} - D_{eo} (D_{oo})^{-1} D_{oe} \]

with diagonal part

\[ D_{ee} + D_{oo} = M_0 + c_{sw} \frac{i}{4} \sigma_{\mu \nu} \hat{F}_{\mu \nu} \]

\( M_0 = 4 + m_0 \)

\( \checkmark \) not protected from arbitrarily small eigenvalues

small mass, rough gauge field, large lattice promote instabilities in \((D_{oo})^{-1}\)
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\[ D_{ee} + D_{oo} = M_0 + c_{sw} \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu} \sim M_0 \exp \left\{ \frac{c_{sw}}{M_0} \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu} \right\} \]

\( \checkmark \) not protected from arbitrarily small eigenvalues
small mass, rough gauge field, large lattice promote instabilities in \((D_{oo})^{-1}\)

\( \times \) Employ bounded counterterm operator
  - valid Symanzik improvement
  - guarantees invertibility
Improvement coefficient $c_{SW}$

Revised Wilson–Dirac operator

- $N_f = 3$ simulations with

$$M_0 \exp \left\{ \frac{c_{SW}}{M_0} \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu} \right\}$$

- tree-level impr. Symanzik gauge
- standard determination$^{[6, 7]}$ in massless Schrödinger Functional
- still employing HMC, …

✓ stable inversions of $D_{oo}$ at any time (1 M traj., $\tau = 2$)
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Comparison with previous result\(^{[8]}\)

- arrows indicate $a \sim 0.095$ fm

$$(c_{sw}^{new} < c_{sw}^{old})$$

- similar picture in $N_f = 0$ theory, with reduction of except. cnfgs.

✓ stable inversions of $D_{oo}$ at any time (1 M traj., $\tau = 2$)
Towards large scale simulations

First investigations with (2+1)-flavour simulations

\[ \phi_4 \equiv 8t_0\left(\frac{1}{2}m^2_\pi + m^2_K\right) = \text{const} \sim \text{Tr}[M_q] \]

| \( a/\text{fm} \) | \( \beta \) | \( T \cdot L^3 \) | \( m_\pi \) MeV | \( m_K \) MeV | \( Lm_\pi \) | b.c. | status | \( \langle P_{\text{acc}} \rangle \) | \( P_{|\Delta H| \geq 1} \) |
|-----------------|---------|-----------------|-----------|-----------|-----------|------|--------|----------------|----------------|
| 0.095           | 3.8     | 96 \cdot 32^3   | 410       | 410       | 6.3       | P    | ✓      | 97.5%          | 0.2%            |
| 96 \cdot 32^3   |         | 294             | 458       | 4.5       | P         | ✓    | 98.6%          | 0.1%            |
| 96 \cdot 32^3   |         | 220             | 478       | 3.4       | P         | ✓    | 98.1%          | 0.1%            |
| 144 \cdot 64^3  |         | 135             | 494       | 4.2       | P         | tuned| 98.1%          | 0.1%            |
| 0.064           | 4.0     | 96 \cdot 48^3   | 410       | 410       | 6.4       | P    | tuned|                |                 |
| 0.055           | 4.1     | 96 \cdot 48^3   | 410       | 410       | 5.5       | O    | therm.|                |                 |

to be compared to Coordinated Lattice Simulations (CLS) effort\textsuperscript{[9–11]}

\( \beta = 3.8 \) SMD simulations: \( (\gamma = 0.3, \epsilon = 0.31, 2\text{-lvOMF-4, } N_{pf} \leq 8, R_{\text{deg}} \leq 10) \)
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Physical \(m_{\pi}\) possible at such coarse lattice spacing (CL scaling missing)
Towards large scale simulations

How does the lowest eigenvalue distribution scale with quark mass?

\[ \alpha = 0.095 \text{ fm}, \ V = 96 \times 32^3 \]

(historical data missing for detailed comparison)

\[ m_\pi = 410 \text{ MeV}, \ m_\pi L = 6.3 \]

Overall behaviour of smallest eigenvalue

- \[ \alpha \lambda = \min \{ \text{spec}(D_u^\dagger D_u)^{1/2} \} \]
  \[ (\alpha \lambda = 0.001 \sim 2 \text{ MeV}) \]
- median \[ \mu \propto Zm \]
- width \[ \sigma \] decreases with \[ m \]
- somewhat similar to \( N_f = 2 \) case \([12]\)
  (unimproved Wilson)
- (non-)Gaussian ?
- empirical: \([12]\) \[ \sigma \sim a/\sqrt{V} \]

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$m_\pi = 294 \text{ MeV}, m_\pi L = 4.5$

$m_\pi = 220 \text{ MeV}, m_\pi L = 3.4$
Stabilising very large volume simulations

- Stochastic Molecular Dynamics
- uniform norm in stopping criteria
- quadruple precision in global sums
- modified $O(a)$-improved Dirac op.

Stay tuned

- larger lattices are on the way

Thank you for your attention!


