Stabilised Wilson fermions for QCD

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In collaboration with A. Francis, P. Fritzsch and M. Lüscher
Motivations

A large part of the success of Lattice Gauge Theory is inherently tied with advances in Monte Carlo simulations.

Monte Carlo methods used in Lattice Gauge Theory are importance sampling methods.

- Generating an ensemble of configurations through a Markov process and estimating the expectation values on the ensemble averages.

- On very large lattices translation averages in presence of a single gauge field (the master field) provide an alternative way of calculating the expectation values.

However, when the gap of the lattice Dirac operator shrinks, algorithmic instabilities and precision issues hamper the stability of the configurations generation and affect the estimate of observables.

Ways to overcome these problems are described in this talk for the case of the O(a)-improved Wilson formulation of lattice QCD.
Identifying the critical aspects

- **Algorithmic stability:**
  - Update algorithm: Hybrid Monte-Carlo.
  - 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.

All the above have a strong influence on the simulation cost and affects the reliability of the simulation.
Summary: Stabilized Wilson fermions

The proposed stabilizing measures include:

1. A modification of the standard O(a)-improved lattice Dirac operator.

2. The use of the Stochastic Molecular Dynamics (SMD) simulation algorithm.

3. Tuning of the numerical precision required to guarantee a sufficient level of accuracy on large lattices.

I will present results of some representative simulations of the theory with $2 + 1$ flavours of quarks, to demonstrate the viability of the framework.
$O(a)$-improvement revisited

The traditional Wilson Dirac $O(a)$-improved operator is

$$D = \frac{1}{2}\{\gamma_\mu(\nabla_\mu^* + \nabla_\mu - a\nabla_\mu^*\nabla_\mu)\} + c_{sw}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu} + m_0.$$ 

If the lattice points are classified as even-odd

$$D = \begin{pmatrix} D_{ee} & D_{eo} \\ D_{oe} & D_{oo} \end{pmatrix}$$

with the diagonal part

$$D_{ee} + D_{oo} = 4 + m_0 + c_{sw}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}.$$ 

The even-odd preconditioned form

$$\hat{D} = D_{ee} - D_{eo}(D_{oo})^{-1}D_{oe}.$$
$O(\alpha)$-improvement revisited

- The coefficient $c_{sw}$ is equal to 1 at tree-level PT and grows monotonically with the gauge coupling ($\sim 2$ on coarse lattices).

- The Pauli term in these equations can be fairly large, particularly so on coarse lattices (saturating the bound).

$$\left| i \sigma_{\mu\nu} \hat{F}_{\mu\nu} \right|_2 \leq 3$$

- Positive and negative eigenvalues of the Pauli term are equally distributed. $D_{oo}$ is not protected by small eigenvalues especially for small masses and rough gauge fields.

- EO preconditioning occasionally fails with probability growing with the lattice size.

- Impossible to use in master-field simulations.
$O(a)$-improvement revisited

The improved Wilson-Dirac is not positive: is this why it tends to promote the instabilities?

- An alternative definition of the Wilson Dirac $O(a)$-improved operator is

$$D_{ee} + D_{oo} = (4 + m_0) \exp \left( \frac{c_{sw}}{4 + m_0} \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu} \right).$$
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- Moreover, $\det D = \det \hat{D}$ up to a field-independent proportionality constant.
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- The exponential and the associated force can be evaluated with negligible computational effort.
Improved $c_{SW}$ tuning

Is this a viable choice of Dirac-Wilson improvement?

We need extensive simulations of the modified theory.

- $N_f = 2 + 1$ QCD simulations with a tree level improved Symanzik action.
- Tuning of the $c_{SW}$ through the standard massless Schröedinger Functional scheme
- Scan up to very large $\beta$ to make contact with PT.

![Graph showing $c_{SW}$ vs $\beta$]

\[ c_{SW} \]
Comparison with the traditional $c_{SW}$ term

How does it compare with the traditional $c_{SW}$ tuned values?

- The scale setting is different. Arrows indicate $a \sim 0.095\text{fm}$
- For equal lattice spacing $c_{sw}^{\text{new}} < c_{sw}^{\text{old}}$
- A similar outcome is obtained also for the quenched theory
Comparison of the critical mass

- It is analogously possible to compare the critical mass: 
  $$am_{cr} = \frac{1}{2\kappa_{cr}} - 4$$

- Also in this case the scale setting is different.
- A similar outcome is obtained also for the quenched theory.
The SMD algorithm

The SMD algorithm is rather similar to the HMC algorithm.

Start with:

\[ U(x, \mu), \text{ the momentum } \pi(x, \mu) \text{ and the pseudo-fermion } \phi(x) \text{ with action } S_{pf} = \phi(D^\dagger D)^{-1})\phi \]

One cycle consists of:

- A random rotation of the momentum and the pseudo-fermion

\[ \pi \to c_1 \pi + c_2 v \quad \quad \phi \to c_1 \phi + c_2 D^\dagger \eta \]

\[ \text{with } v \text{ and } \eta \text{ random normally distributed, } c_1^2 + c_2^2 = 1 \text{ and } c_1 = e^{-\epsilon \gamma}. \]

Where \( \epsilon \) is the MD integration time and \( \gamma \) is the friction parameter.

- A short molecular-dynamics evolution

- an accept-reject step that makes the algorithm exact
Generally: More spikes in $H$ means longer autocorrelation times.

**The SMD algorithm**

**HMC**
- Momenta redrawn
- Integration errors accumulate
- Possible long jumps in $\Gamma$
- Possible path switch after jump

**SMD**
- Momenta rotated
- Shorter traj. length
- Acc./Rej. after each
- High acc. required
- Less integration errors accumulated
- Stochastic path

\[ \vec{p}_{new} = \vec{p}_{rand} \]

\[ \vec{p}_{new} = R(\vec{p}_{rand}, \vec{p}_{old}) \]
Considerations on the SMD algorithm

- At fixed $\epsilon$ and large $\gamma$, the SMD algorithm coincides with the HMC algorithm.
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Significant reduction of the unbounded energy violations $|\Delta H| \gg 1$
Other algorithmic improvements

- **Convergence criterion for the solver**
  The solver uses an iterative procedure that is being stopped when the approximate solution \( \tilde{\psi} \) satisfies

\[
||\eta - D\tilde{\psi}||_2 \leq w||\eta||_2 \quad \text{with} \quad ||\eta||_2 \propto V
\]

- **Global reductions**
  Sum over all lattice points can cause accumulations errors.

\[
\Delta H \propto \sqrt{V} \quad \text{the numerical precision has to increase with } V.
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  with

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  ✓ Replaced with the uniform norm: $||\eta||_\infty = \sup_x ||\eta(x)||_2$ (V-independent)

- Global reductions
  Sum over all lattice points can cause accumulations errors.

  $$\Delta H \propto \sqrt{V}$$

  the numerical precision has to increase with $V$.

  ✓ Use quadruple precision in global sums
Ongoing investigations

Once $c_{sw}$ is tuned and with all the algorithmic measures in place
We performed a set of (2+1)-flavour simulations

<table>
<thead>
<tr>
<th>$a$/fm</th>
<th>$\beta$</th>
<th>$T \times L^3$</th>
<th>$m_\pi$/MeV</th>
<th>$m_K$/MeV</th>
<th>$Lm_\pi$</th>
<th>BC</th>
<th>status</th>
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<td>0.095</td>
<td>3.8</td>
<td>$96 \times 32^3$</td>
<td>410</td>
<td>410</td>
<td>6.3</td>
<td>P</td>
<td>✓</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$96 \times 32^3$</td>
<td>294</td>
<td>458</td>
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<td>✓</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$96 \times 32^3$</td>
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<td>478</td>
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</tr>
<tr>
<td></td>
<td></td>
<td>$144 \times 64^3$</td>
<td>135</td>
<td>494</td>
<td>4.2</td>
<td>P</td>
<td>planned</td>
</tr>
<tr>
<td>0.064</td>
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<td>$96 \times 48^3$</td>
<td>410</td>
<td>410</td>
<td>6.4</td>
<td>P</td>
<td>✓</td>
</tr>
<tr>
<td>0.055</td>
<td>4.1</td>
<td>$96 \times 48^3$</td>
<td>410</td>
<td>410</td>
<td>5.5</td>
<td>O</td>
<td>thermalized</td>
</tr>
</tbody>
</table>

The runs are in direct comparison with ensembles from Coordinated Lattice Simulations (CLS) collaboration.

- The scale setting is on the symmetric point for the continuum limit:

$$\phi_4 \equiv 8t_0 \left( \frac{1}{2} m_\pi^2 + m_K^2 \right) = \text{const} \propto \text{tr}(M_q)$$

- We have also planned a single $\beta$ set of runs up to the physical point on the coarsest lattice.
Details of the SMD runs

- The runs have shown no issues of instability

- Parameters setup: $\gamma = 0.3, \epsilon = 0.31$, 2-lvls of OMF-4, $N_{pf} \leq 8$, $\text{deg}(R) \leq 10$

| $m_\pi$/MeV | $P_{acc}$ | $P(|\Delta H| \geq 2)$ |
|-------------|-----------|-------------------------|
| 410         | 97.5%     | 0.15%                   |
| 294         | 98.6%     | 0.15%                   |
| 220         | 98.2%     | 0.05%                   |

- Physical $m_\pi$ seems possible also at such coarse lattice spacing.

- The lowest eigenvalue of $\sqrt{D^\dagger D}$ was measured with a precision greater than 0.5%.
Spectral gap of the Dirac operator

- Width ($\sigma$) of the distribution is generally smaller than the traditional case.
- $\sigma$ decreases for lighter pions (as observed with $N_f = 2$)
- Empirically $\sigma \propto 1/\sqrt{V}$
- No data for a direct comparison.
- For $R_1$ $m_\pi = 410$
Spectral gap of the Dirac operator

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  - For $R_2 \ m_\pi = 294$
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No data for a direct comparison.

For $R_1$ $m_\pi = 410$

For $R_2$ $m_\pi = 294$

For $R_3$ $m_\pi = 220$

These simulations are all about equally expensive, as we lower $m_u$ and raise $m_s$ the cost balance stays constant.
A direct comparison is easier in a quenched setup

- Quenched improved Wilson action, $\beta = 6.0$
Quantifying $O(a^2)$ effects

With the generation of the continuum limit trajectories still ongoing we can give estimates of the size of the cutoff effects.

CLS continuum extrapolation of symmetric point $f_{\pi K}$ data  

\[ \sqrt{8t_0 F_\pi} \]

\[ 0.215 \quad 0.220 \quad 0.225 \]

Fig. 4. Lattice-spacing dependence of $\sqrt{8t_0 F_\pi}$ at $m_0$, $u = m_0$, $d = m_0$, $s$. Open squares represent results previously obtained in ref. [32] at $\phi_4 = 1$ using the traditional setup of the $O(a^2)$-improved theory. A linear extrapolation of these data yields a value in the continuum limit (cross), which coincides with the results obtained in the runs $A_1, B_1$ (black circles) and $X_1$ (open circle). The latter moves down if the axial-current renormalization constant is replaced by the one used in ref. [32] (grey open circle).

6.7 Higher-order lattice effects

All simulated lattices are in a range of parameters, where $O(a^2)$ lattice effects cannot be expected to be very small, independently of which Dirac operator is chosen. The values of $t_0/a^2$, for example, would change by 15% on the $A_1$ lattice and by 6% on the $B_1$ lattice, if defined with the Wilson plaquette instead of the symmetric ("clover") expression for the Yang–Mills action density.

The dimensionless combination $\sqrt{8t_0 F_\pi}$ is potentially more sensitive to the choice of the lattice Dirac operator than gluonic quantities like $t_0$. In Fig. 4 there results for $\sqrt{8t_0 F_\pi}$ obtained at the SU(3)-symmetric point (i.e. in the runs $A_1, B_1$ and $X_1$) are compared with data published in ref. [32]. For a sensible comparison, $\phi_4$ should

NOTE: The CLS current has been renormalized with the $Z_A$ from the chirally rotated SF  [M. Dalla Brida et al. Eur. Phys. J. C79 (2019)]. We Use $Z_A$ determined with the fermion flow [M. Lüscher,JHEP 1304 (2013) 123].
Lattice effects

A fixed bare quark masses trajectory will show deviations in the observables of order $\mathcal{O}(a m)$

[M. Bruno et al. Phys. Rev. D 95, 074504 ]

More about lattice effects
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Stabilized Wilson CLS runs

... Significant lattice effects were also seen in the ratios $t_0/t_0^{\text{sym}}$ and $f_{\pi K}/f_{\pi K}^{\text{sym}}$.

In the runs 96x32x32x32-20{1,2,3}, the lattice spacing is about 0.094 fm and thus even larger, but the lattice effects in the ratios considered in [1] appear to be smaller:

Fig.7: Results for $\phi_4$, $t_0$, $F_{\pi K}=(F_{\pi}+2F_K)/3$ and $\text{tr}\{MR\}=m_{00_R}/2+m_{01_R}$ obtained in the runs 96x32x32x32-20{1,2,3}, all given in units of their values at the symmetric point (run 96x32x32x32-201), plotted as a function of $\phi_2=8 t_0 m_{\pi}^2$. The decay constants are the renormalized ones and the renormalization of the quark masses does not include $Z_P$ and the associated $\mathcal{O}(a m)$ factors.

By and large, the behaviour of the $t_0$, $F_{\pi K}$ and $\text{tr}\{MR\}$ ratios is similar to the ones plotted on the left of Fig.4 of [1] at $\beta=3.55$ (where $a=0.064$ fm). One should however take into account that the decay constants include an $\mathcal{O}(a m)$ factor.

More about lattice effects
--------------------------

The runs 96x32x32x32-20{1,2,3} are at fixed sum of the bare quark masses. As already emphasized by Bruno et al. [1], this is a trajectory where the sum of the renormalized quark masses may not be strictly constant, the deviations being an $\mathcal{O}(a m)$ lattice effect. The effects shown in the bottom-left plot in Fig.4 of [1] are actually quite big on the coarsest lattice considered there, where the lattice spacing is 0.086 fm. Significant lattice effects were also seen in the ratios $t_0/t_0^{\text{sym}}$ and $f_{\pi K}/f_{\pi K}^{\text{sym}}$.

Where

$$\phi_4 \equiv 8 t_0 \left( \frac{1}{2} m_{\pi}^2 + m_K^2 \right)$$

$$\phi_2 = 8 t_0 m_{\pi}^2$$

H101,H102,H105,C101, blue squares.

N202,N203,N200,D200, red diamonds.
Summary and Perspectives

Our measures to stabilize the Wilson Dirac improved action comprise

- A modified $O(a)$ improvement of the action.
- Stochastic Molecular Dynamics
- Uniform norm and quadruple precision

So far:

✓ Good behaviour of the proposal even on very coarse lattices
✓ Comparable runtime with respect to the traditional formulation
✓ No indication of unusually large lattice effects

Ongoing:

- Continuum limit scaling behaviour
Modified $c_{SW}$ implementation

- The Cayley-Hamilton theorem can be used to express a $n \times n$ matrix as:

$$\exp_N(A) = \sum_{m=0}^{N} \frac{1}{m!} \sum_{i=0}^{n-1} c_i(m, A) A^i = \sum_{i=0}^{n-1} b_i(N, A) A^i.$$ 

- The Horner method states that for a sequence of polynomial $q_i(X)$ the iteration

$$q_N = c_N$$
$$q_i = Xq_{i+1} + c_i \quad i = N - 1, \ldots, 0$$
$$c_i = 1/i!$$

will converge and the last polynomial $q_0$ will coincide with the evaluation of the recursive sum up to grade $N$. 

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Modified $c_{SW}$ implementation

- Specialising to the case of $6 \times 6$ matrices and the Cayley-Hamilton representation

$$q_{N,0} = c_N = 1/N! \quad q_{N,1...5} = 0$$

$$q_{n,0} = -p_0 q_{n+1,5} + 1/n!$$

$$q_{n,i} = -p_i q_{n+1,5} + q_{n+1,i-1} \quad i = 1, \ldots, 5,$$

where the $p_i$ are the coefficients of the characteristic polynomial.

- Rapid convergence:

![Graph showing rapid convergence](image-url)