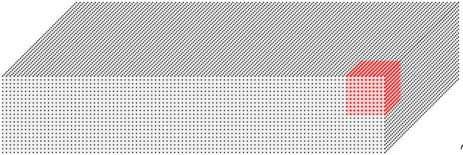
Stabilised Wilson fermions for QCD on very large lattices

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, … $\to$ Suggestion:

Stochastic Molecular Dynamics (SMD) algorithm[1–4]

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

$$\pi \to c_1\pi + c_2 v\,, \qquad c_1 = \exp(-\epsilon\gamma)\,, \quad c_2 = (1-c_1^2)^{1/2}$$

$$\phi \to c_1\phi + c_2 D^\dagger\eta\,, \qquad (\gamma > 0\text{: friction parameter; }\epsilon\text{: MD integration time})$$

+ MD evolution + accept-reject step + repeat

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- ergodic[5] for sufficiently small ϵ
- 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 ϕ_t, U_t improve update of deflation subspace

Algorithmic improvements for stability

- Solver stopping criteria

$$\|D\psi - \eta\|_2 \leq \rho\|\eta\|_2\ , \qquad \|\eta\|_2 = \Big(\sum\nolimits_x \big(\eta(x), \eta(x)\big)\Big)^{1/2} \propto \sqrt{V}$$

- global accept-reject step (numerical precision must increase with V)

$$\Delta H \propto \epsilon^p \sqrt{V}$$

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$$\|D\psi - \eta\|_2 \le \rho\|\eta\|_2 \;, \qquad \|\eta\|_2 = \Big(\sum\nolimits_x (\eta(x), \eta(x))\Big)^{1/2} \propto \sqrt{V}$$

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

- global accept-reject step (numerical precision must increase with V)

$$\Delta H \propto \epsilon^p \sqrt{V}$$

✓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

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

Even-odd preconditioning:

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

with diagonal part $(M_0 = 4 + m_0)$

$$D_{\mathrm{ee}} + D_{\mathrm{oo}} = M_0 + c_{\mathrm{sw}}\tfrac{\mathrm{i}}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}$$

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

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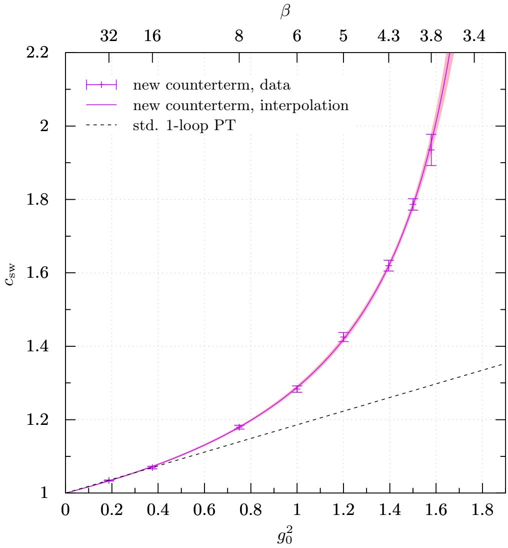
✗ not protected from arbitrarily small eigenvalues

small mass, rough gauge field, large lattice promote instabilities in $(D_{\rm oo})^{-1}$

✓ Employ bounded counterterm operator

- valid Symanzik improvement
- guarantees invertibility

Improvement coefficient c_{sw}



Revised Wilson–Dirac operator

- $N_{\mathrm{f}} = 3$ simulations with

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

- 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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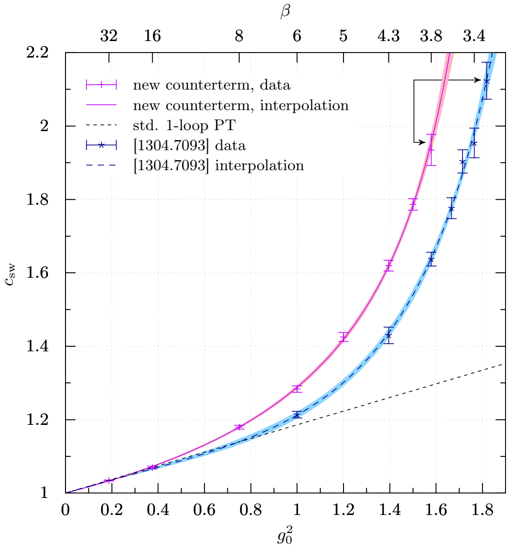

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Comparison with previous result[8]

- arrows indicate $a \sim 0.095\,\mathrm{fm}$ ($c_{\mathrm{sw}}^{\mathrm{new}} < c_{\mathrm{sw}}^{\mathrm{old}}$)
- similar picture in $N_{\mathrm{f}} = 0$ 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

$$\phi_4 \equiv 8t_0(\tfrac{1}{2}m_\pi^2 + m_\mathrm{K}^2) = \text{const} \quad \sim \quad \mathrm{Tr}[M_\mathrm{q}]$$

a/fm	β	$T \cdot L^3$	$\frac{m_\pi}{\mathrm{MeV}}$	$\frac{m_\mathrm{K}}{\mathrm{MeV}}$	Lm_π	b.c.	status	$\langle P_\mathrm{acc}\rangle$	$P_{\lvert\Delta H\rvert\geq 1}$
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		
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[9–11]

$\beta = 3.8$ SMD simulations: ($\gamma = 0.3$, $\epsilon = 0.31$, 2-lv OMF-4, $N_\mathrm{pf} \leq 8$, $R_\mathrm{deg} \leq 10$)

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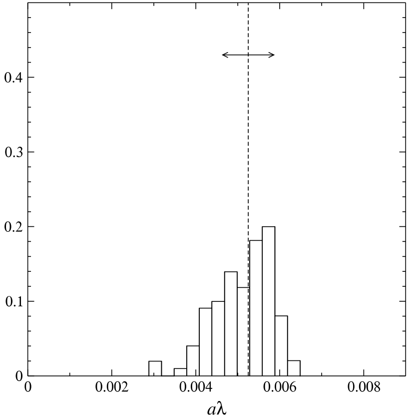
physical m_π possible at such coarse lattice spacing (CL scaling missing)

Towards large scale simulations

How does the lowest eigenvalue distribution scale with quark mass?

$a = 0.095\,\mathrm{fm},\ V = 96 \times 32^3$



$m_\pi = 410\,\mathrm{MeV},\ m_\pi L = 6.3$

(historical data missing for detailed comparison)

Overall behaviour of smallest eigenvalue

- $a\lambda = \min\left\{\mathrm{spec}(D_u^\dagger D_u)^{1/2}\right\}$

  $(a\lambda = 0.001 \sim 2\,\mathrm{MeV})$
- median $\mu \propto Zm$
- width σ decreases with m
- somewhat similar to $N_\mathrm{f} = 2$ case[12] (unimproved Wilson)
- (non-)Gaussian ?
- empirical:[12] $\sigma \simeq a/\sqrt{V}$

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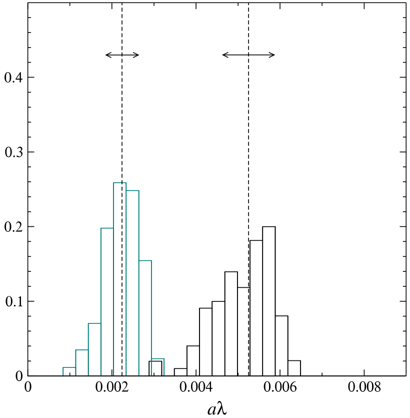

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$m_\pi = 294\,\mathrm{MeV},\ m_\pi L = 4.5$

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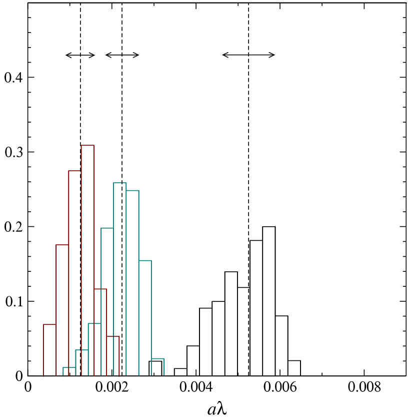

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Thank you for your attention!

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

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