# Simulating Stabilised Wilson fermions: Status and prospects

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Comput.Phys.Commun. 255 (2020) 107355
e-Print: 1911.04533 [hep-lat]

in collaboration with
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# What are *Stabilised Wilson fermions* good for?

## More than just another lattice action.

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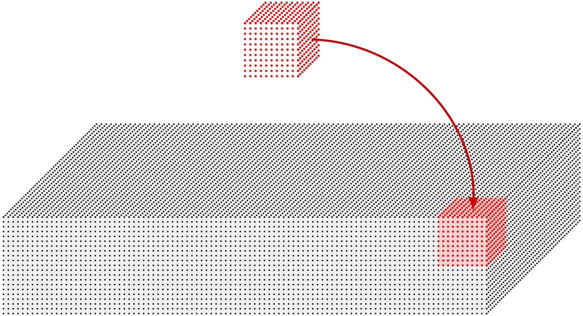


- *negligible finite-volume effects*
- *evade topological-freezing problem*
- *access to new kinematic regimes*
- *ideal for position-space methods*
- *better exploitation of exascale machines*
  (large memory footprint $\Rightarrow$ weak-scaling case)
- *new tool to perform different/new calculations*

# The standard lattice QCD approach

**Markov Chain Monte Carlo simulations of QCD**

Goal: produce sequence of gauge fields $\{U_i | i = 1, \dots, N_U\}$


$\Rightarrow$ expectation values of physical observables $\mathcal{O}$ from ensemble-average

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[U]\, \mathcal{O}\, e^{-\mathcal{S}_{\mathrm{G}}[U] - \mathcal{S}_{\mathrm{eff}}[U]}$$

$$\approx \frac{1}{N_U} \sum_{i=1}^{N_U} \mathcal{O}[U_i] \,,$$

with Wilson–Dirac operator $Q$ and

$$e^{-\mathcal{S}_{\mathrm{eff}}} \simeq \prod_f \det(Q_f) \,, \qquad f \in \{u, d, s, \dots\}$$

employs **Hybrid Monte-Carlo (HMC) algorithm**

- with importance sampling
- draw conjugate momenta $\pi$ & integrate molecular dynamics (MD) equations
- made exact by (global) Metropolis accept-reject step ($\Delta H = \Delta \mathcal{S}$)
- ergodicity maintained by redrawing the momenta

and **advanced techniques to solve large linear systems**:

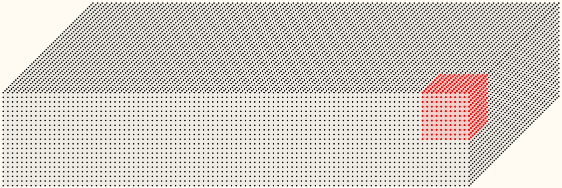
- various (Krylov) solvers
- precondition techniques (eo, det-splitting, ...)
- mixed-precision arithmetic
- symplectic integrators w/ multiple time-scales
- architecture dependent optimisations
- ...

# The master-field approach[1]

**Master-field lattice**

single master-field replaces classical (Markov chain) ensemble

$$N_V = \frac{V_4^{\mathrm{mf}}}{V_4} = \prod_{i=0}^{3} N_i \simeq 100 - 1000 \approx N_U$$



$\Rightarrow$ expectation values from translation average $\langle\langle \mathcal{O} \rangle\rangle$

$$\langle \mathcal{O}(x) \rangle = \langle\langle \mathcal{O}(x) \rangle\rangle + \mathrm{O}(N_V^{-1/2}) \,,$$
$$\langle\langle \mathcal{O}(x) \rangle\rangle = \frac{1}{N_V} \sum\nolimits_z \mathcal{O}(x+z)$$

based on **stochastic locality** due to short-range interaction

- QCD field variables in distant regions fluctuate largely independent
- their distribution is everywhere the same (with periodic bc.)
- translation averages replace ensemble averages provided localisation range of $\mathcal{O} \ll L$ (lattice extent)
- uncertainties estimated using standard methods through correlations in space

Concept successfully applied to SU(3) YM theory.[2]

It isn't straightforward to simulate QCD on very large lattices!

# Critical aspects of lattice QCD simulations

Various choices (strongly) impact cost and reliability of a simulation.

**Discretisation aspects**

- gauge action (impacts UV fluctuations)
- fermion action (lattice Dirac operator $D$)
- spectral gap of $D \sim \lambda_{\rm min}$ (near zero-modes in MD evolution)

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- update algorithm: Hybrid Monte-Carlo (exploration of phase space)
- integration schemes and length (symplectic integrators)
- numerical precision, e.g. in global sums (Metropolis step) (double precision)
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**Physical aspects**

- coarse $a$ $\rightsquigarrow$ promote large fluctuations of gauge field (roughness of $U$ fields)
- small $m_{\mathrm{ud}}$ $\rightsquigarrow$ result in small eigenvalues $\lambda_{\min}(m_{\mathrm{ud}})$ of lattice Dirac operator
- large $(L/a)^4$ $\rightsquigarrow$ increase risk of exceptional behaviour (e.g. from MD force)

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Large potential for algorithmic instabilities and precision issues. $\Rightarrow$ Additional stability measures required.[3]

# Stabilising measures for QCD[1, 3]

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include …

- new fermion action / Wilson–Dirac operator $\rightsquigarrow$ +1 page
- new algorithm: stochastic molecular dynamics (SMD) algorithm[4–7] $\rightsquigarrow$ +3 pages
- solver stopping criteria

$$\|D\psi - \eta\|_2 \leq \rho\|\eta\|_2 \ ,$$

$$\|\eta\|_2 = \left(\sum\nolimits_x \big(\eta(x), \eta(x)\big)\right)^{1/2} \propto \sqrt{V}$$

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

$\|\eta\|_\infty$ for all forces (res$_F = 10^{-12} \ldots 10^{-10}$) and some actions (res$_\phi = 10^{-12}$)

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

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

✓ quadruple precision in global sums

- well-established techniques

✓ Schwarz Alternating Procedure, local deflation, multi-grid, …
even-odd & mass-preconditioning, multiple time-scales, …

$$D = \frac{1}{2}\gamma_\mu(\nabla_\mu^* + \nabla_\mu) - a\frac{1}{2}\nabla_\mu^*\nabla_\mu + \underline{M_0 + ac_{\rm sw}\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}}$$

Even-odd preconditioning:

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

with diagonal part[8] $(M_0 = 4 + m_0)$

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

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

# New Wilson–Dirac operator[3]

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with exponential clover term

$$D = \tfrac{1}{2}\gamma_\mu(\nabla^*_\mu + \nabla_\mu) - a\tfrac{1}{2}\nabla^*_\mu\nabla_\mu + \underline{M_0 + a c_{\rm sw}\tfrac{\rm i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}}$$

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$$D_{\rm ee} + D_{\rm oo} = M_0 + c_{\rm sw}\tfrac{\rm i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu} \quad \sim \quad \boxed{M_0 \exp\left\{\frac{c_{\rm sw}}{M_0}\frac{\rm i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}\right\}}$$

✗ not protected from arbitrarily small eigenvalues

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

✓ Employ exponential mapping

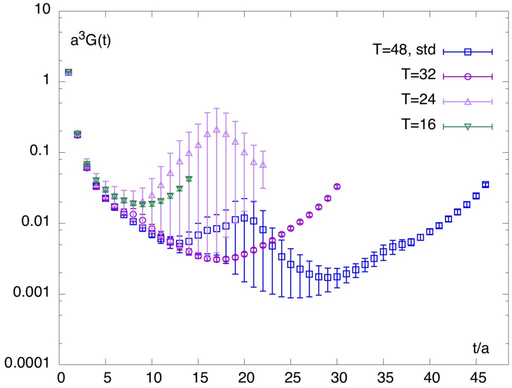
- regulates UV fluctuations
- valid Symanzik expansion/improvement
- guarantees invertibility

# New Wilson–Dirac operator

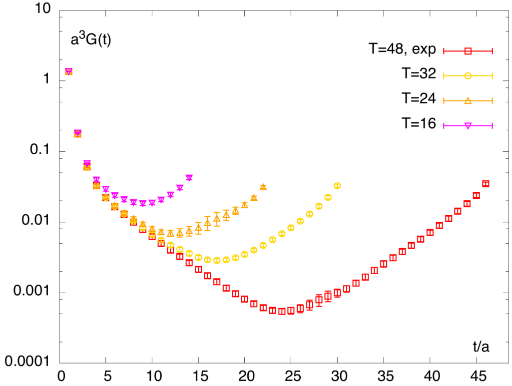
A clean comparison of fermion actions

- Impact best seen in pure gauge theory ($N_\mathrm{f} = 0$, quenched; i.e. same gauge background).
  Ill-defined theory for fermionic observables. $\Rightarrow$ exceptional problems
- Different lattices $L/a \in \{16, 24, 32, 48\}$ and same gluon action ($\beta = 6.0$, $a = 0.094\,\mathrm{fm}$).
- pion correlator $G(t) \propto e^{-m_\pi t}$ at zero momentum, $m_\pi \approx 220\,\mathrm{MeV}$

std. Wilson–Dirac operator




new Wilson–Dirac operator



# Algorithmic improvements for stability



## Stochastic Molecular Dynamics (SMD) algorithm[4–7]

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

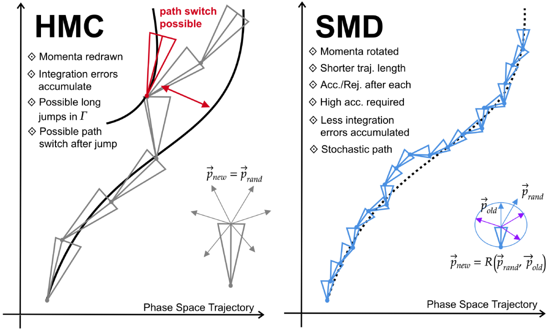
$$\pi \to c_1\pi + c_2 v\,, \qquad c_1 = e^{-\epsilon\gamma}\,,\quad c_1^2 + c_2^2 = 1\,,\qquad v(x,\mu),\eta(x) \in \mathcal{N}(0,1)$$

$$\phi \to c_1\phi + c_2 D^\dagger\eta\,,$$

($\gamma > 0$: friction parameter; $\epsilon$: MD integration time)

+ MD evolution + accept-reject step + repeat. If rejected: $\{\tilde{U},\tilde{\pi},\tilde{\phi}\} \to \{U,-\pi,\tilde{\phi}\}$

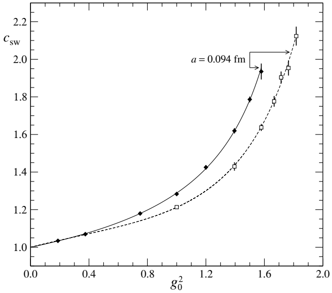
- ergodic[9] for sufficiently small $\epsilon$ (typically $\epsilon < 0.35$ vs. $\tau = 1-2$)
- exact algorithm
- significant reduction of unbounded energy violations $|\Delta H| \gg 1$
- a bit “slower“ than HMC but compensated by shorter autocorrelation times
- smooth changes in $\phi_t, U_t$ improve update of deflation subspace



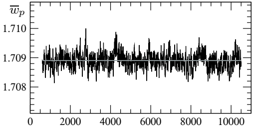
# Comparison to traditional Wilson–Clover action

e.g: $N_\mathrm{f} = 2+1$ data of Coordinated Lattice Simulations (CLS) effort[10–12]

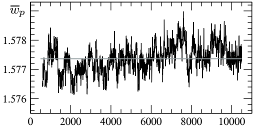
Non-perturbative improvement:




plaquette (energy density) with SMD: $a = 0.095\,\mathrm{fm}$




exp. clover $(A_1)$

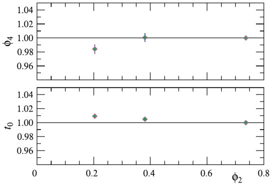



std. clover $(X_1)$

Chiral trajectory:

$$t_0 \text{ and } \phi_4 \equiv 8t_0(\tfrac{1}{2}m_\pi^2 + m_\mathrm{K}^2) = 1.11 \sim \mathrm{Tr}[M_\mathrm{q}]$$

Stabilised Wilson

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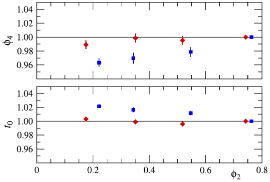
Standard Wilson




$a = 0.064, 0.086\,\mathrm{fm}$

**key observation**

- smoother fluctuations
- smaller lattice spacing effects


$N_\mathrm{f} = 2 + 1$+all stabilising measures[3]

- M. Cé, M. Bruno, J. Bulava, A. Francis, P. F., J. Green, M. Lüscher, A. Rago, M. Hansen
- $m_\pi = 270\,\mathrm{MeV} = 2m_\pi^\text{phys}$
- `openQCD-2.0`, `openQCD-2.4`[13]

# Master fields prefer the target partition function

## Reweighting of observables not available

**QCD simulations necessitate frequency-splitting methods**

- Hasenbusch (mass-)preconditioning for quark doublet $(\mu_n > \ldots > \mu_0)$

$$S_{\rm pf} = (\phi_0, \frac{1}{D^\dagger D + \mu_n^2}\phi_0) + \sum_{k=1}^{n}(\phi_k, \frac{D^\dagger D + \mu_{n-k+1}^2}{D^\dagger D + \mu_{n-k}^2}\phi_k)$$

requires mass-reweighting if regulator mass $\mu_0 \neq 0$

- rational approximation of strange (or charm) quark determinant is given by

$$\det(D_{\rm s}) = W_{\rm s}\det(R^{-1})\ , \quad R = C\prod_{k=0}^{m-1}\frac{D_{\rm s}^\dagger D_{\rm s} + \omega_k^2}{D_{\rm s}^\dagger D_{\rm s} + \nu_k^2}$$

: Zolotarev optimal rat. approx.

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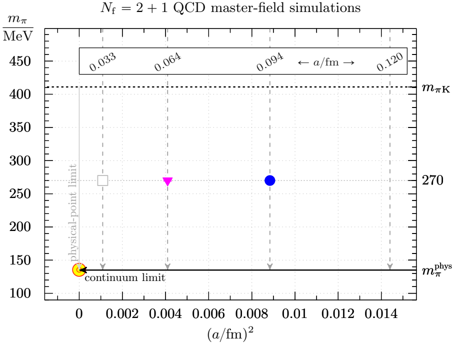
with reweighting factor $W_{\rm s} = \det(D_{\rm s}R)$ to correct approximation error ($m =$degree of $[D_{\rm s}^\dagger D_{\rm s}]^{-1/2}$) $\Rightarrow$ ✓ if approximation is sufficiently accurate

Complying with strict bound $\frac{\sigma(W_{\rm s})}{\langle W_{\rm s}\rangle} \leq 0.1$ guarantees unbiased results in all observables.

# Summary of $N_f = 2 + 1$ master-field simulations

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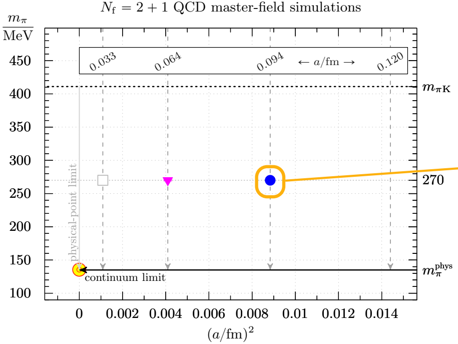


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$V = 96^4$ ($L = 9\,\mathrm{fm}$, $m_\pi L \approx 12.3$)

- $V/V_4 = 3^4 = 81$ ($N_{\mathrm{core}} = 6144$)
- *Cost:* 3 Mch (thermal.) + 0.2 Mch (add. cfg.)
- *Total memory used:* 1.8 TiB (= 309.1 MiB per core)
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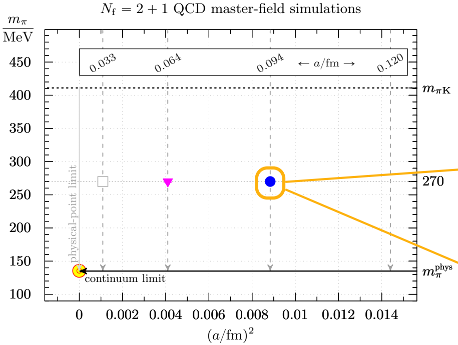


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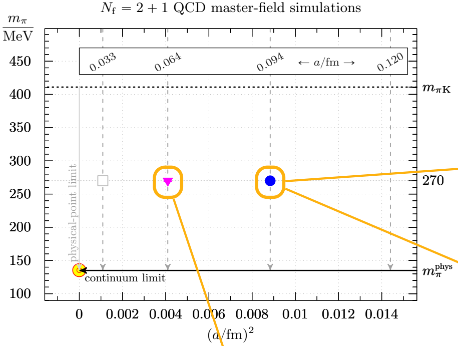


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**$V = 144^4$ ($L = 9.2\,\mathrm{fm}$, $m_\pi L \approx 12.6$)**

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- *Cost:* 20 Mch (thermal.) + 13 Mch (per add. cfg.)
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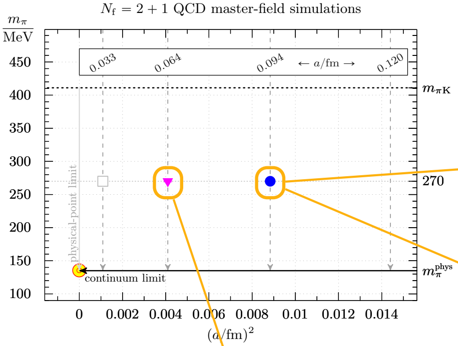


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**preparing for finer lattice spacing ($a \sim 0.033\,\mathrm{fm}$)**
**$\rightsquigarrow$ continuum limit**

# How to (efficiently) calculate hadronic observables?

**Variety of choices:**

time-momentum correlators

$$C(x_0, \mathbf{p}) = \sum\nolimits_{\mathbf{x}} \exp(-i\mathbf{p}\mathbf{x}) C(x, 0)$$

have large footprint in space for $\mathbf{p} = \mathbf{0}$
(inexact momentum projection $\rightsquigarrow$ more localized)

$\Rightarrow$ position-space correlators

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- Dirichlet b.c. on blocks[1] (induce boundary effect)
- random source (useable)
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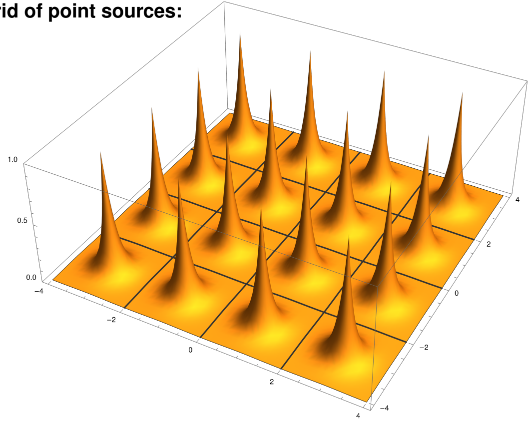
**Grid of point sources:**




2D sketch of exponential decay of „2-pt function“ with $(8a/2a)^2 = 4^2 = 16$ grid source points

Take away message

***employ techniques compatible with MF translation average for single inversion of Dirac op.***

Hadron propagators

E.g. meson 2-pt function (like pion propagator):

$$C_{\Gamma\Gamma'}(x) = -\mathrm{Tr}\{\Gamma\gamma_5 D^{-1}(x,0)\gamma_5\Gamma' D^{-1}(x,0)\}\ , \qquad ||D^{-1}(x,0)|| \sim e^{-m|x|/2}$$

with localisation range $1/m$ (not ultra-local)

- Asymptotic form of position-space correlators analytically known when $a = 0$ ($T, L = \infty$).
  For $|x| \to \infty$:

$$C_{\mathrm{PP}}(x) \to \frac{|c_{\mathrm{P}}|^2}{4\pi^2}\frac{m_{\mathrm{P}}^2}{|x|}K_1(m_{\mathrm{P}}|x|)\ ,$$

$$C_{\mathrm{NN}}(x) \to \frac{|c_{\mathrm{N}}|^2}{4\pi^2}\frac{m_{\mathrm{N}}^2}{|x|}\left[K_1(m_{\mathrm{N}}|x|) + \frac{\not{x}}{|x|}K_2(m_{\mathrm{N}}|x|)\right]$$

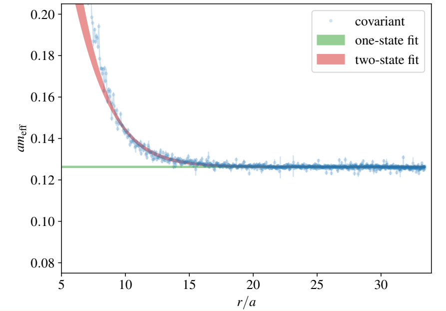
- axis/off-axis directions different cutoff effects
- correlator averaged over equivalent distances $r = |x|$:

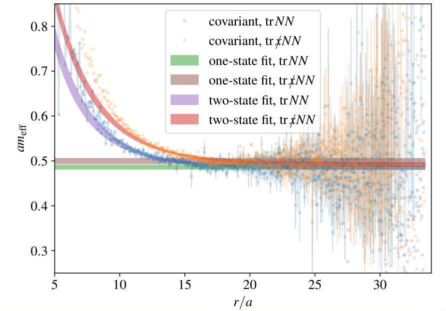
$$\overline{C}(r) = \frac{1}{\mathrm{r}_4((r/a)^2)}\sum_{|x|=r} C(x)$$

# Hadronic observables

from position-space correlators & grid-points offset $b = 48a$ ($r_{\max} = 48a/\sqrt{2} \leq 34a$)

## Effective masses of pion and nucleon ($a = 0.94\,\mathrm{fm}$) on $96^4$



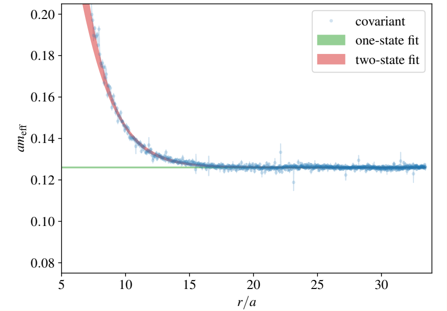

## Comments:

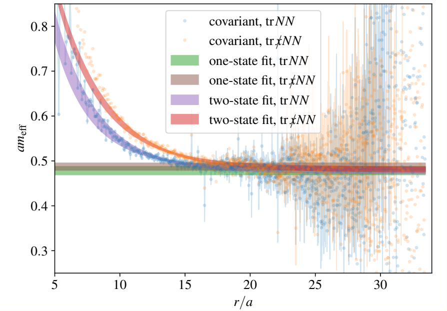
- similar statistics (4096 noise src.) and computational effort on $96^4$ ($x_{\mathrm{gs}} = 12$) and $192^4$ ($x_{\mathrm{gs}} = 24$)
- different methods for proper calculations of uncertainties available (bootstrap, $\Gamma$-method)
- using empirical ansatz for excited state effects
- no boundary effects observed

# Hadronic observables

from position-space correlators & grid-points offset $b = 48a$ ($r_{\max} = 48a/\sqrt{2} \leq 34a$)

## Effective masses of pion and nucleon ($a = 0.94\,\mathrm{fm}$) on $192^4$

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- no boundary effects observed

# You can profit from stabilising measures too

OPEN LATtice initiative

## $N_{\mathrm{f}} = 2 + 1$ Stabilised Wilson-Fermion simulations

- perform standard-sized lattice simulations
- implement <u>all</u> stabilising measures[14] (Exp-Clover action, SMD, …)
- various lattices $\{a/L, \beta, m_\pi\}$ to complement master-field simulations
- provide ensembles under open science policy
- `https://openlat1.gitlab.io`

OPEN LATtice initiative

This is an effort within the Lattice QCD community (started in 2019) for the production and sharing of dynamical gauge field ensembles to study physical phenomena of the strong interaction. We are aware that not every young researcher can be in the favourable position to belong to one of the big collaborations with access to large scale simulations to pursue new ideas. We want to close this gap by forming the present initiative centered around latest developments in the field. We offer partnership and access to (2+1)-flavour QCD

# $N_\mathrm{f} = 2 + 1$ Stabilised Wilson-Fermion simulations

*OpenLat team*

Francesca Cuteri

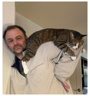
Anthony Francis

Patrick Fritzsch

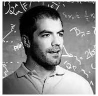
Giovanni Pederiva

Antonio Rago

Andrea Shindler

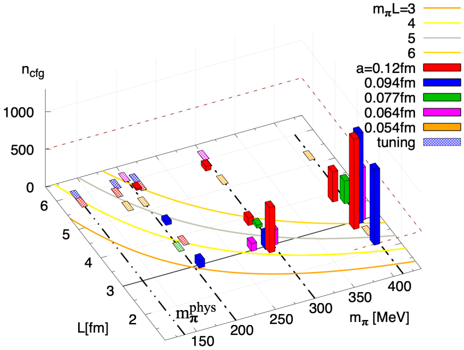


André Walker-Loud



Savvas Zafeiropoulos

*continues to explore the behaviour of StabWF*



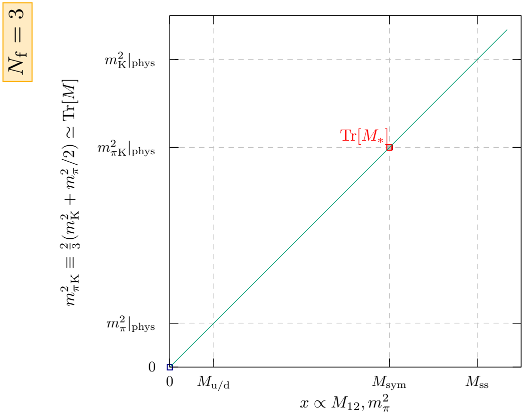

- approaching physical points at coarse lattice spacings $a = 0.094, 0.12\,\mathrm{fm}$
- 5 lattice spacings at $SU(3)$-flavour-symmetric point + future $a \simeq 0.033\,\mathrm{fm}$
- no negative eigenvalues of $D_\mathrm{s}$ observed so far

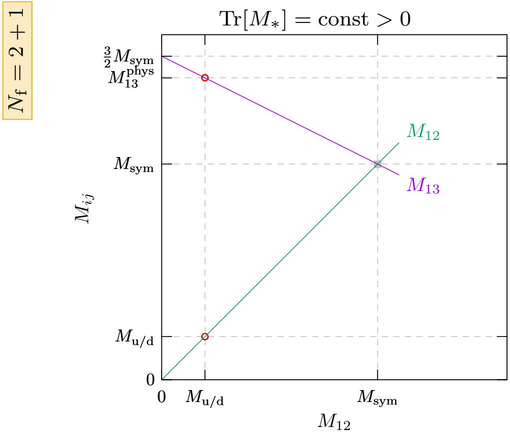
# $N_\mathrm{f} = 2 + 1$ Stabilised Wilson-Fermion simulations

Tuning follows previous $2+1$-flavour UKQCD & CLS strategy ($\mathrm{Tr}[M] = \mathrm{const}$)

Reason: more complicated renormalisation and improvement pattern (unknown $a\mathrm{Tr}[M]$ counter-terms)

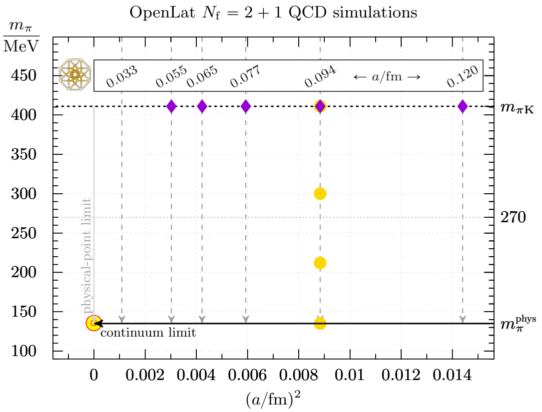
Idealised tuning of physical run parameters for Wilson fermions in hadronic scheme: *flavour-averaged meson mass*



# $N_\mathrm{f} = 2 + 1$ Stabilised Wilson-Fermion simulations

Tuning follows previous $2 + 1$-flavour UKQCD & CLS strategy ($\mathrm{Tr}[M] = \mathrm{const}$)




$\phi_4 = 8t_0 \frac{3}{2} m_{\pi K} = 1.115$ , $m_{\pi K} = 410.9(2)$ MeV

$m_{\pi K} = \frac{2}{3}(m_K^2 + m_\pi^2/2)$ , $\sqrt{8t_0} = 0.414(5)$ fm

symmetric point ensembles

| $\beta$ | g.b.c. | $T/a$ | $L/a$ | $a/\mathrm{fm}$ | $L/\mathrm{fm}$ | $Lm_{\pi K}$ |
|---|---|---|---|---|---|---|
| 4.1 | O | 128 | 64 | 0.055 | 3.5 | 7.3 |
| 4.0 | P | 96 | 48 | 0.065 | 3.1 | 6.5 |
| 3.9 | P | 96 | 48 | 0.077 | 3.7 | 7.7 |
| 3.8 | P | 96 | 32 | 0.095 | 3.0 | 6.3 |
| 3.685 | P | 96 | 24 | 0.120 | 3.8 | 8.0 |

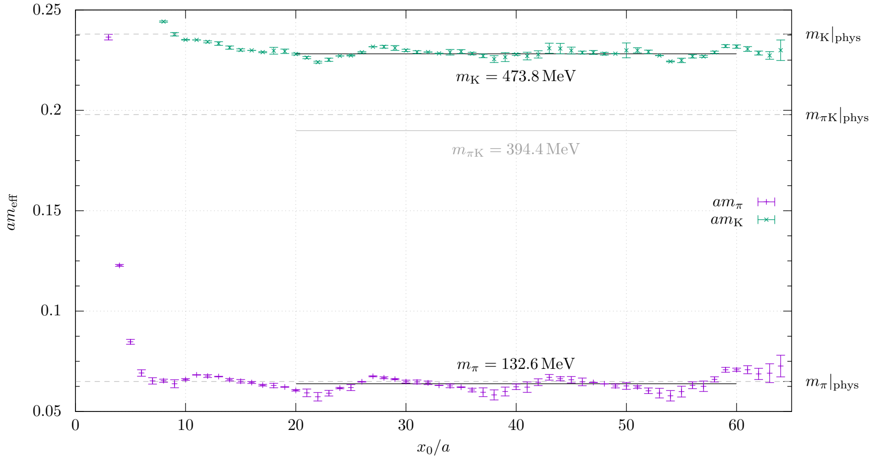
chiral trajectory at $a = 0.095$ fm
($\beta = 3.8, \mathrm{Tr}[M_0] = -1.205759$)

preliminary

| $T/a$ | $L/a$ | $\frac{L}{\mathrm{fm}}$ | $\frac{m_\mathrm{PS}}{\mathrm{MeV}}$ | $Lm_\mathrm{PS}$ |
|---|---|---|---|---|
| 96 | 32 | 3.04 | 410 | 6.32 |
| 96 | 32 | 3.04 | 300 | 4.62 |
| 128 | 48 | 4.56 | 212 | 4.90 |
| 128 | 72 | 6.84 | 135 | 4.68 |

**Tuning** physical pion simulation at $a = 0.095\,\mathrm{fm}$ and $128 \times 72^3$ lattice

effective masses:

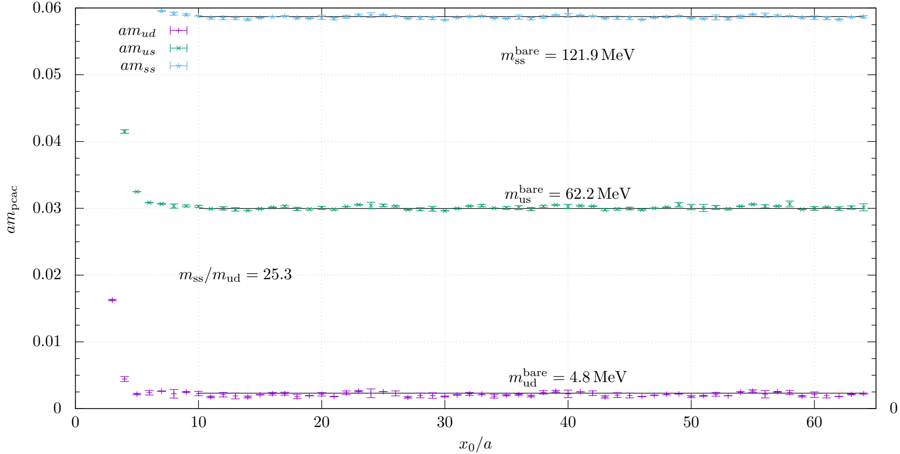


# $N_\mathrm{f} = 2+1$ Stabilised Wilson-Fermion simulations

## Towards physical pion mass

**Tuning** physical pion simulation at $a = 0.095\,\mathrm{fm}$ and $128 \times 72^3$ lattice

current quark masses:

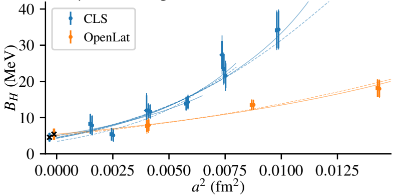


**StabWF simulations:**

- less problematic to simulate
- simpler tuning
- smaller cutoff effects
- renormalisation factors closer to PT
- physical pions possible also at coarse lattice spacing
- $\mathrm{Tr}[M] = \mathrm{const}$ needs additional tuning for phys. mass (reason: LO $\chi$PT & mass counter-terms)
- …

*H* dibaryon: *a* → 0 universality (PRELIMINARY)

BaSc: Baryon Scattering collaboration — combined effort of “Mainz” and sLapHnn




Three exp-clover ensembles with $L \approx 3$ fm.

Second action at SU(3) point: exponentiated clover / stabilized Wilson (OpenLat). Smaller lattice artifacts than standard clover (CLS).

**Open (related) questions:**

- cost figure
- size of auto-correlations (HMC vs. SMD)
- performance of other actions at physical point
- …

# Summary

Master-fields require stabilising measures

- modified fermion action (improvement term)
- stochastic Molecular dynamics (SMD) algorithm
- uniform norm & quadruple precision
- multilevel deflation

So far:

- stabilising measures (action, SMD, …) work excellent, especially at coarse lattice spacing ✓
- $96^4$, $192^4$ ($a = 0.095\,\mathrm{fm}$) and $144^4$ ($a = 0.065\,\mathrm{fm}$) master-field ready for physics applications ✓
- master-field prefers traget partition function ✓
- very large volumes like $(18\,\mathrm{fm})^4$ still challenging but doable (or $m_\pi^{\mathrm{phys}}$) ✓
- position-space correlators $\rightsquigarrow$ hadron masses, decay constants, …

Ongoing:

- exploration of physical calculations & benchmarking
- continuum limit scaling behaviour
- master-fields: natural setup to study spectral reconstruction
- complementary large-scale lattice simulations (OpenLat)

We just start to uncover new possibilities.

Backup slides

# Exponential clover implementation

Apply **Cayley–Hamilton theorem** for $6 \times 6$ hermitean matrices.

$$\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}(x) = \begin{pmatrix} A_+(x) & 0 \\ 0 & A_-(x) \end{pmatrix} ,$$

$$\mathrm{tr}\{A\} = 0 \quad \Rightarrow \quad A^6 = \sum_{k=0}^{4} p_k A^k$$

Expansion coefficients ($p_k \in \mathbb{R}$)

$$p_0 = \frac{1}{6}\mathrm{tr}\{A^6\} - \frac{1}{8}\mathrm{tr}\{A^4\}\mathrm{tr}\{A^2\} - \frac{1}{18}\mathrm{tr}\{A^3\}^2 + \frac{1}{48}\mathrm{tr}\{A^2\}^3$$
$$p_1 = \frac{1}{5}\mathrm{tr}\{A^5\} - \frac{1}{6}\mathrm{tr}\{A^3\}\mathrm{tr}\{A^2\} ,$$
$$p_2 = \frac{1}{4}\mathrm{tr}\{A^4\} - \frac{1}{8}\mathrm{tr}\{A^2\}^2 ,$$
$$p_3 = \frac{1}{3}\mathrm{tr}\{A^3\} ,$$
$$p_4 = \frac{1}{2}\mathrm{tr}\{A^2\} ,$$

Any polynomial in $A$ of degree $N \geq 6$ can be reduced to

$$\sum_{k=0}^{5} q_k A^k ,$$

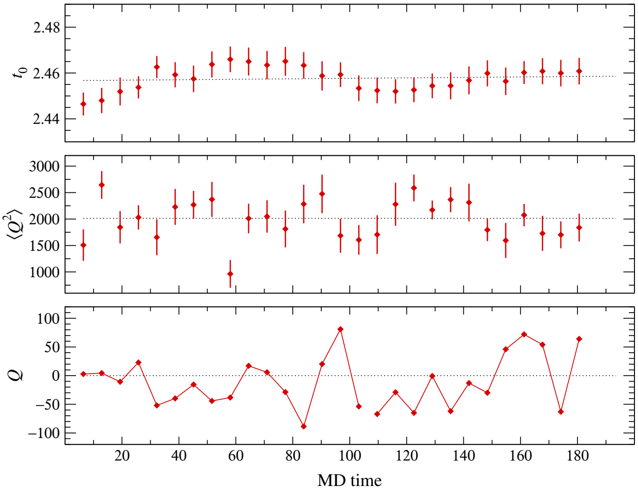
with $A$-dependent coefficients $q_k$, calculated recursively.

$$\exp(A) = \sum_{k=0}^{N} \frac{A^k}{k!} + r_N(A)$$ converges rapidly with bound $$||r_N(A)|| \leq \frac{||A||^{N+1}}{(N+1)!}\exp(||A||)$$

$\Rightarrow \exp\left(\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}(x)\right)$ easily obstained to machine precision.

# Monitoring observables (thermalisation)

$96^4$ : $a = 0.095\,\mathrm{fm}$, $m_\pi = 270\,\mathrm{MeV}$, $Lm_\pi = 12.5$ ($L = 9\,\mathrm{fm}$)




Simulations without TM-reweighting:

- no spikes in $\Delta H$
- $\langle e^{-\Delta H} \rangle = 1$ within errors
- acceptance rate 98% or higher
- checked that $\sigma(\hat{D}_s) \in [r_a, r_b]$ of Zolotarev rational approximation
- adapt solver tolerances to exclude statistically relevant effects of numerical inaccuracies
- autocorrelation times: 20-30 MDU

# Master-field simulations

Thermalising $192^4$ ($a = 0.094\,\mathrm{fm}$, $m_\pi = 270\,\mathrm{MeV}$) at LRZ using 768 nodes (36864 cores)

openQCD-2.0.2: multilevel DFL solver (full double prec.)

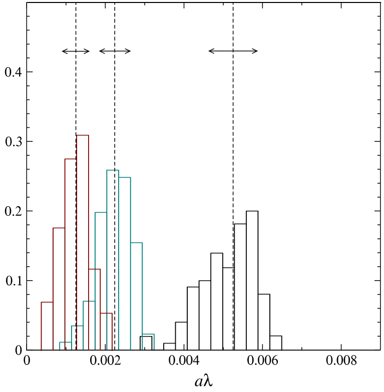
```
SMD parameters:
actions = 0 1 2 3 4 5 6 7 8
npf = 8
mu = 0.0 0.0012 0.012 0.12 1.2
nlv = 2
gamma = 0.3
eps = 0.137
iacc = 1

...

Rational 0:
degree = 12
range = [0.012,8.1]

Level 0:
4th order OMF integrator
Number of steps = 1
Forces = 0

Level 1:
4th order OMF integrator
Number of steps = 2
Forces = 1 2 3 4 5 6 7 8
```

```
Update cycle no 48
dH = -1.4e-02, iac = 1
Average plaquette = 1.708999
Action  1: <status> = 0
Action  2: <status> = 0 [0,0|0,0]
Action  3: <status> = 0 [0,0|0,0]
Action  4: <status> = 0 [0,0|0,0]
Action  5: <status> = 2 [5,2|7,6]
Action  6: <status> = 271
Action  7: <status> = 21 [3,2|5,3]
Action  8: <status> = 22 [3,2|5,3]
Field   1: <status> = 139
Field   2: <status> = 31 [3,2|6,4]
Field   3: <status> = 38 [5,3|8,7]
Field   4: <status> = 33 [5,2|7,6]
Field   5: <status> = 267
Field   6: <status> = 26 [3,2|5,3]
Field   7: <status> = 24 [3,2|5,3]
Force   1: <status> = 91
Force   2: <status> = 22 [3,2|6,4];23 [3,2|5,4]
Force   3: <status> = 28 [5,3|7,6];30 [5,3|7,6]
Force   4: <status> = 29 [5,2|7,6];32 [5,2|7,6]
Force   5: <status> = 28 [5,2|7,5];30 [5,2|7,6]
Force   6: <status> = 303
Force   7: <status> = 22 [3,2|5,3];23 [3,2|5,3]
Force   8: <status> = 23 [3,2|5,3];26 [3,2|5,3]
Modes   0: <status> = 0,0|0,0
Modes   1: <status> = 4,2|5,5 (no of updates = 4)
Acceptance rate = 1.000000
Time per update cycle = 4.34e+03 sec (average = 4.38e+03 sec)
```

# Towards large scale simulations

How does the lowest eigenvalue distribution scale with quark mass?

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




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

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

$m_\pi = 220\,\mathrm{MeV},\ m_\pi L = 3.4$

(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 $\sigma$ decreases with $m$
- somewhat similar to $N_\mathrm{f} = 2$ case[15] (unimproved Wilson)
- (non-)Gaussian ?
- empirical:[15] $\sigma \simeq a/\sqrt{V}$

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