

Master-field simulations of QCD and the exponential clover action

Patrick Fritzsch



Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin



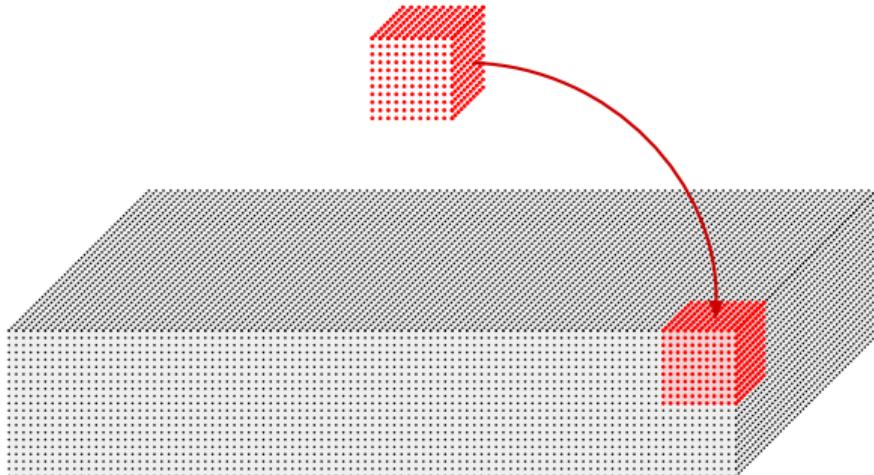
Comput.Phys.Commun. 255 (2020) 107355
e-Print: 1911.04533 [hep-lat]

in collaboration with

M. Cè, M. Bruno, J. Bulava, A. Francis, J. Green, M. Hansen, M. Lüscher, A. Rago
and
F. Cuteri, G. Pederiva, A. Shindler, A. Walker-Loud, S. Zafeiropoulos

Master fields?
What's that?
Why?

Master fields?
What's that?
Why?



- *negligible finite-volume effects*
- *absence of 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

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[U] \mathcal{O} e^{-S_G[U] - S_{\text{eff}}[U]}$$

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

with Wilson–Dirac operator Q and

$$e^{-S_{\text{eff}}} \simeq \prod_f \det(Q_f), \quad f \in \{u, d, s, \dots\}$$

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

- with importance sampling
- draw conjugate momenta π & integrate molecular dynamics (MD) equations
- made exact by (global) Metropolis accept-reject step ($\Delta H = \Delta S$)
- ergodicity maintained by redrawing the momenta and **advanced techniques to solve large linear systems**:

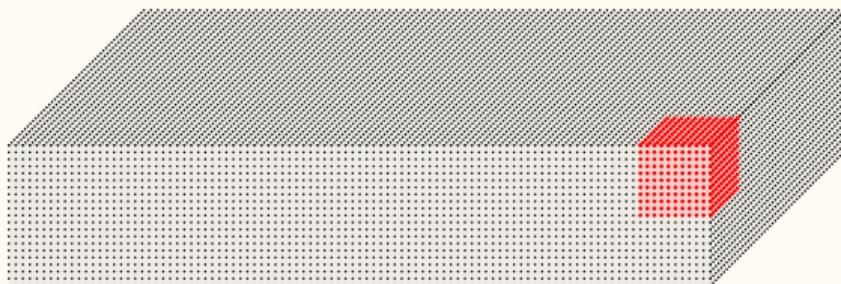
- various (Krylov) solvers
- precondition techniques (eo, det-splitting, ...)
- mixed-precision arithmetic
- symplectic integrators w/ multiple time-scales
- architecture dependent optimisations
- ...

The master-field approach^[1]

Master-field lattice

single master-field replaces classical (Markov chain) ensemble

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



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

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

$$\langle\langle \mathcal{O}(x) \rangle\rangle = \frac{1}{N_V} \sum_z \mathcal{O}(x+z)$$

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 simulation cost and reliability of a simulation.

Discretisation aspects

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

Algorithmic aspects

- 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)
- solver parameters (stability & performance)

Physical aspects

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

Large potential for algorithmic instabilities and precision issues.



Additional stability measures required.^[3]



include ...

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

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

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

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

$\|\eta\|_\infty$ for all forces (res_F = 10⁻¹² … 10⁻¹⁰) and some actions (res_φ = 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, …



with exponential clover term

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

Even-odd preconditioning:

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

with diagonal part^[8]

$$(M_0 = 4 + m_0)$$

$$D_{ee} + \textcolor{brown}{D}_{oo} = M_0 + c_{\text{sw}} \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu} \sim$$

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

X not protected from arbitrarily small eigenvalues

small mass, rough gauge field, large lattice promote instabilities in $(\textcolor{brown}{D}_{oo})^{-1}$

✓ Employ exponential mapping

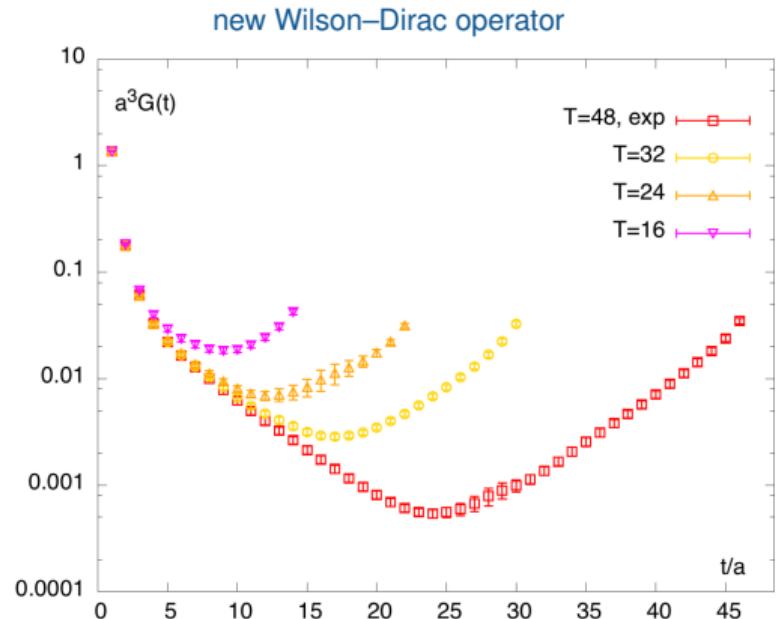
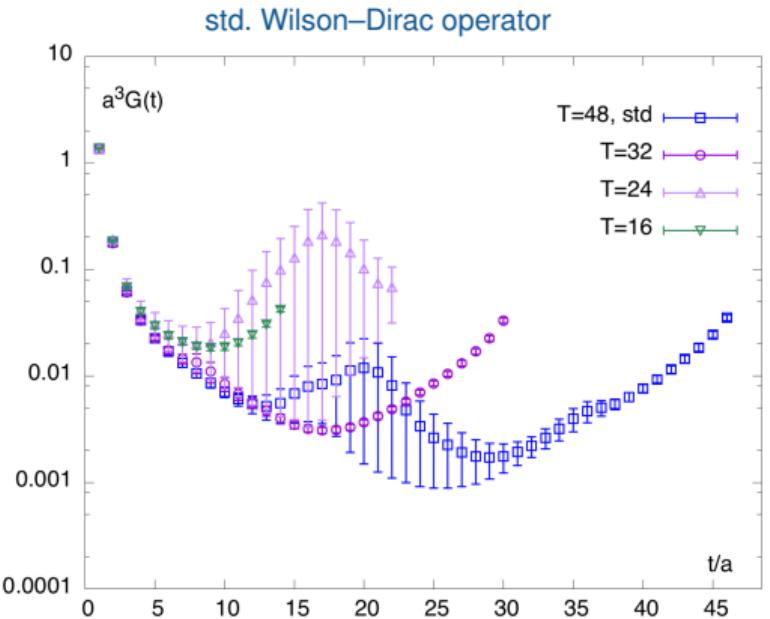


- regulates UV fluctuations
- valid Symanzik expansion/improvement
- guarantees invertibility

New Wilson–Dirac operator

A clean comparison of fermion actions

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





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

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

$$\pi \rightarrow c_1\pi + c_2v,$$

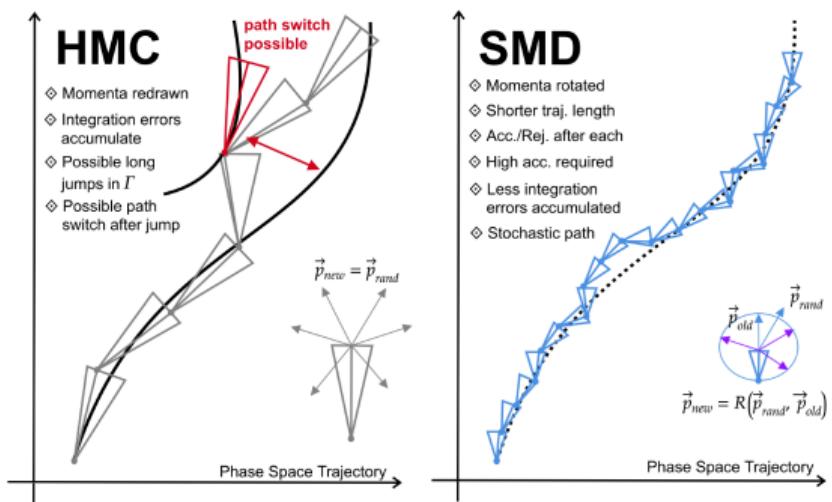
$$c_1 = e^{-\epsilon\gamma}, \quad c_1^2 + c_2^2 = 1, \quad v(x, \mu), \eta(x) \in \mathcal{N}(0, 1)$$

$$\phi \rightarrow c_1\phi + c_2D^\dagger\eta,$$

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

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

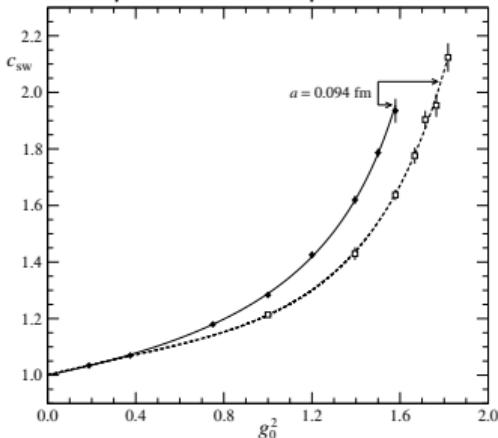
- ergodic^[9] for sufficiently small ϵ
(typically $\epsilon < 0.35$ vs. $\tau = 1 - 2$)
- exact algorithm
- significant reduction of unbounded energy violations
 $|\Delta H| \gg 1$
- a bit “slower” than HMC but compensated by shorter autocorrelation times
- smooth changes in ϕ_t, U_t improve update of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



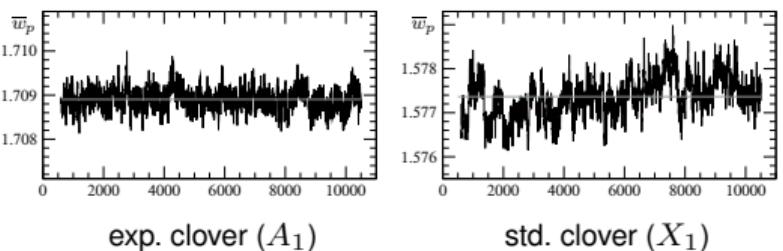
Comparison to traditional Wilson–Clover action

e.g. $N_f = 2 + 1$ data of Coordinated Lattice Simulations (CLS) effort^[10–12]

Non-perturbative improvement:



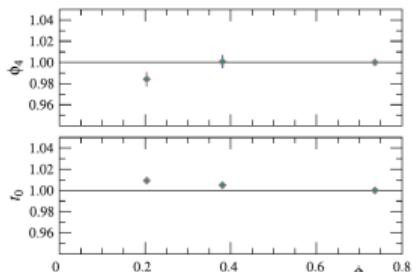
plaquette (energy density) with SMD: $a = 0.095 \text{ fm}$



Chiral trajectory:

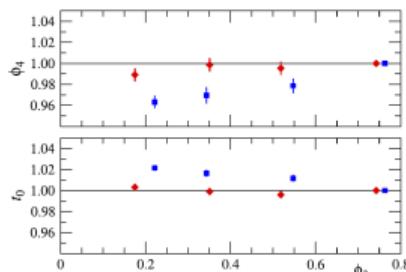
$$t_0 \text{ and } \phi_4 \equiv 8t_0\left(\frac{1}{2}m_\pi^2 + m_K^2\right) = 1.11 \sim \text{Tr}[M_q]$$

Stabilised Wilson



$a = 0.095 \text{ fm}$

Standard Wilson



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

key observation

- smoother fluctuations
- smaller lattice spacing effects



$N_f = 2 + 1 + \text{all stabilising measures}^{[3]}$

- M. Cé, M. Bruno, J. Bulava, A. Francis, P. F.,
J. Green, M. Lüscher, A. Rago, M. Hansen
- $m_\pi = 270 \text{ MeV} = 2m_\pi^{\text{phys}}$
- 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 ($\mu_n > \dots > \mu_0$)

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

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

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

$$\det(D_s) = W_s \det(R^{-1}), \quad R = C \prod_{k=0}^{m-1} \frac{D_s^\dagger D_s + \omega_k^2}{D_s^\dagger D_s + \nu_k^2} \quad : \text{Zolotarev optimal rat. approx.}$$

with reweighting factor $W_s = \det(D_s R)$ to
correct approximation error ($m = \text{degree of } [D_s^\dagger D_s]^{-1/2}$)

Master fields prefer the target partition function

Reweighting of observables not available

QCD simulations necessitate frequency-splitting methods

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

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

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

$\Rightarrow \checkmark$ if $\mu_0 = 0$

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

$$\det(D_s) = W_s \det(R^{-1}), \quad R = C \prod_{k=0}^{m-1} \frac{D_s^\dagger D_s + \omega_k^2}{D_s^\dagger D_s + \nu_k^2} \quad : \text{Zolotarev optimal rat. approx.}$$

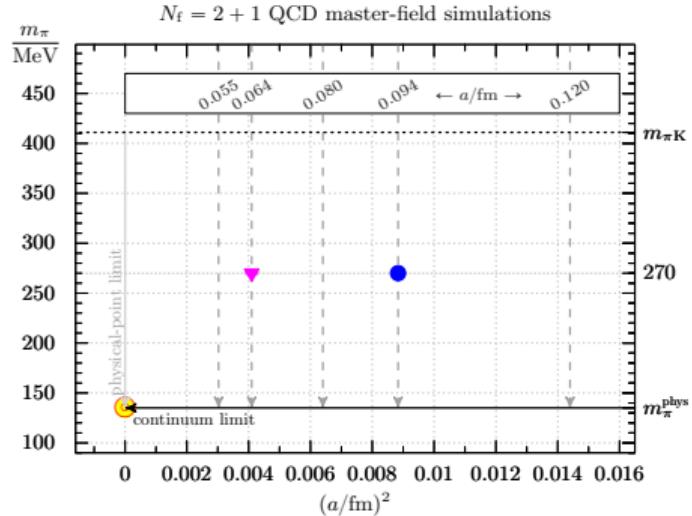
with reweighting factor $W_s = \det(D_s R)$ to

correct approximation error ($m = \text{degree of } [D_s^\dagger D_s]^{-1/2}$)

$\Rightarrow \checkmark$ if approximation is sufficiently accurate

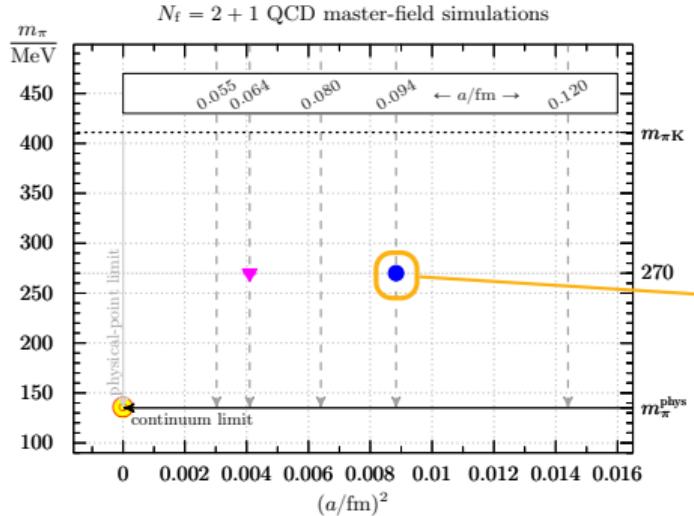
Complying with strict bound $\frac{\sigma(W_s)}{\langle W_s \rangle} \leq 0.1$ guarantees unbiased results in all observables.

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



Std. lattice: $m_\pi = 270$ MeV, $V_4 = 32^4$, $L = 3$ fm, $m_\pi L = 4.1$

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

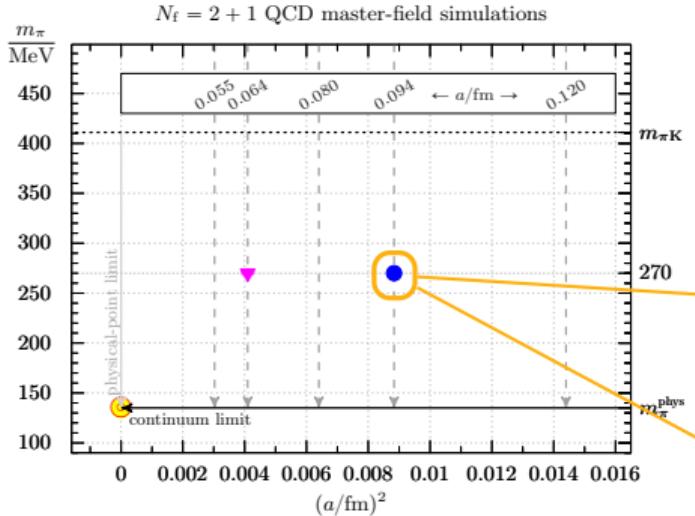


Std. lattice: $m_\pi = 270$ MeV, $V_4 = 32^4$, $L = 3$ fm, $m_\pi L = 4.1$

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

- $V/V_4 = 3^4 = 81$ ($N_{\text{core}} = 6144$)
- Cost: 3 Mch (thermal.) + 0.2 Mch (add. cfg.)
- Total memory used: 1.8 TiB (= 309.1 MiB per core)
- On disc: 132 GiB (= 46 GiB U + 61 GiB ϕ + 20 GiB π)

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



Std. lattice: $m_\pi = 270$ MeV, $V_4 = 32^4$, $L = 3$ fm, $m_\pi L = 4.1$

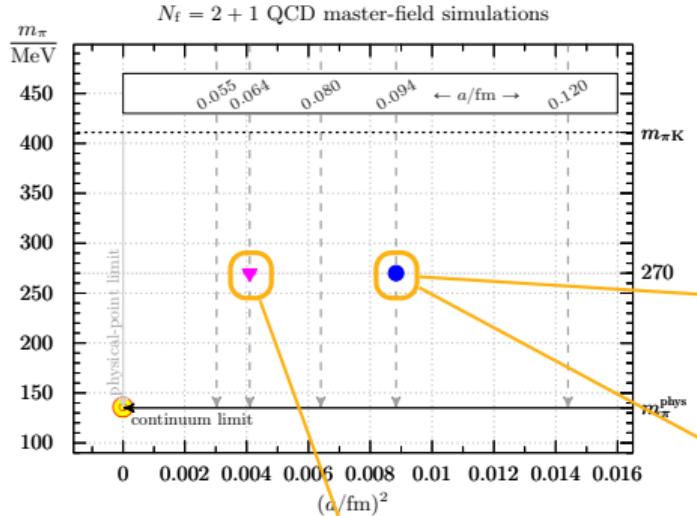
$V = 96^4$ ($L = 9$ fm, $m_\pi L \approx 12.3$)

- $V/V_4 = 3^4 = 81$ ($N_{\text{core}} = 6144$)
- Cost: 3 Mch (thermal.) + 0.2 Mch (add. cfg.)
- $\text{Total memory used:}$ 1.8 TiB (= 309.1 MiB per core)
- On disc: 132 GiB (= 46 GiB U + 61 GiB ϕ + 20 GiB π)

$V = 192^4$ ($L = 18$ fm, $m_\pi L \approx 24.7$)

- $V/V_4 = 6^4 = 1296$ ($N_{\text{core}} = 36864$)
- Cost: 45 Mch (thermal.) + 9 Mch (add. cfg.)
- $\text{Total memory used:}$ 35.9 TiB (= 1019.8 MiB per core)
- On disc: 2 TiB (= 729 GiB U + 972 GiB ϕ + 324 GiB π)

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



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

- $V/V_4 = (144/48)^3 = 81$ ($N_{\text{core}} = 10368$)
- **Cost:** 20 Mch (thermal.) + 13 Mch (per add. cfg.)
- **Total memory used:** 11.1 TiB (= 1.1 GiB per core)
- **On disc:** 642 GiB (= 231 GiB U + 308 GiB ϕ + 103 GiB π)

Std. lattice: $m_\pi = 270$ MeV, $V_4 = 32^4$, $L = 3$ fm, $m_\pi L = 4.1$

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

- $V/V_4 = 3^4 = 81$ ($N_{\text{core}} = 6144$)
- **Cost:** 3 Mch (thermal.) + 0.2 Mch (add. cfg.)
- **Total memory used:** 1.8 TiB (= 309.1 MiB per core)
- **On disc:** 132 GiB (= 46 GiB U + 61 GiB ϕ + 20 GiB π)

$V = 192^4$ ($L = 18$ fm, $m_\pi L \approx 24.7$)

- $V/V_4 = 6^4 = 1296$ ($N_{\text{core}} = 36864$)
- **Cost:** 45 Mch (thermal.) + 9 Mch (add. cfg.)
- **Total memory used:** 35.9 TiB (= 1019.8 MiB per core)
- **On disc:** 2 TiB (= 729 GiB U + 972 GiB ϕ + 324 GiB π)

How to (efficiently) calculate hadronic observables?

Variety of choices:

time-momentum correlators

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

have large footprint in space for $\mathbf{p} = 0$

(inexact momentum projection \rightsquigarrow more localized)

\Rightarrow position-space correlators

- single point source (inefficient)
- Dirichlet b.c. on blocks^[1] (induce boundary effect)
- random source (useable)
- ...



How to (efficiently) calculate hadronic observables?

Variety of choices:

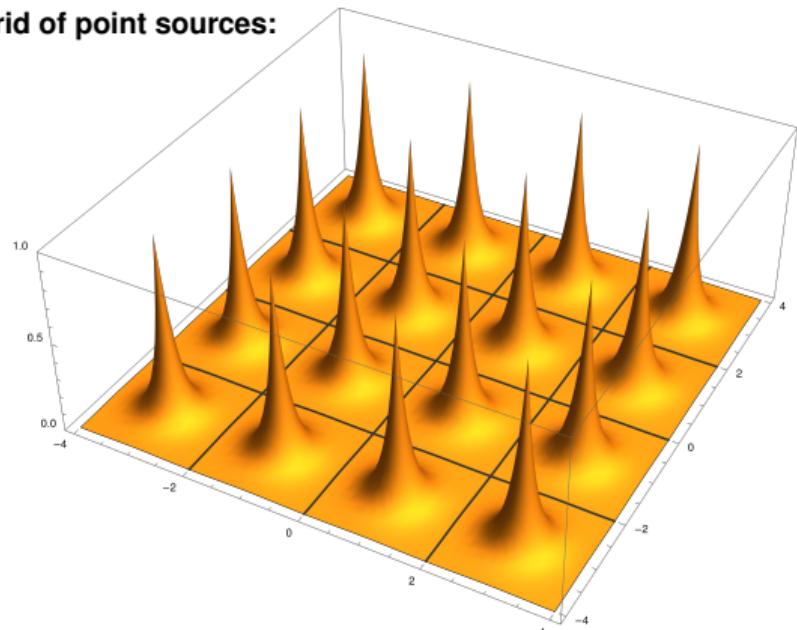
time-momentum correlators

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

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

\Rightarrow position-space correlators

- single point source (inefficient)
- Dirichlet b.c. on blocks^[1] (induce boundary effect)
- random source (useable)
- ...



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.

Hadronic observables

in position space

Hadron propagators

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

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

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

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

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

$$C_{\text{NN}}(x) \rightarrow \frac{|c_{\text{N}}|^2}{4\pi^2} \frac{m_{\text{N}}^2}{|x|} \left[K_1(m_{\text{N}}|x|) + \frac{f}{|x|} K_2(m_{\text{N}}|x|) \right]$$

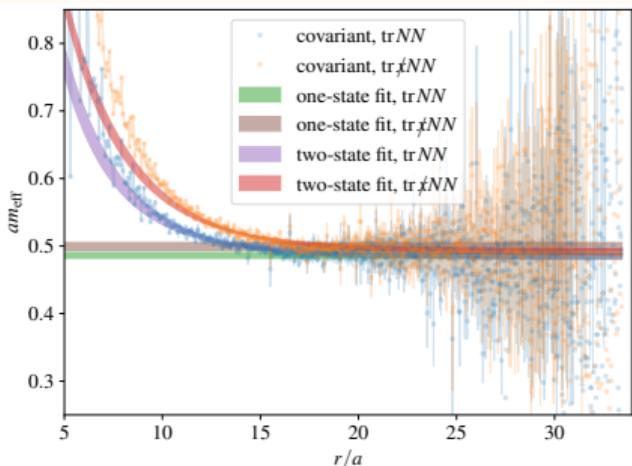
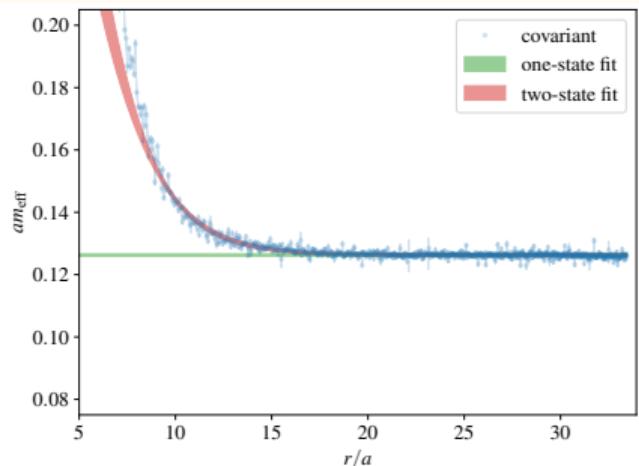
- axis/off-axis directions different cutoff effects
- correlator averaged over equivalent distances $r = |x|$:

$$\overline{C}(r) = \frac{1}{r_4((r/a)^2)} \sum_{|x|=r} C(x)$$

Hadronic observables

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

Effective masses of pion and nucleon ($a = 0.94$ fm) on 96^4



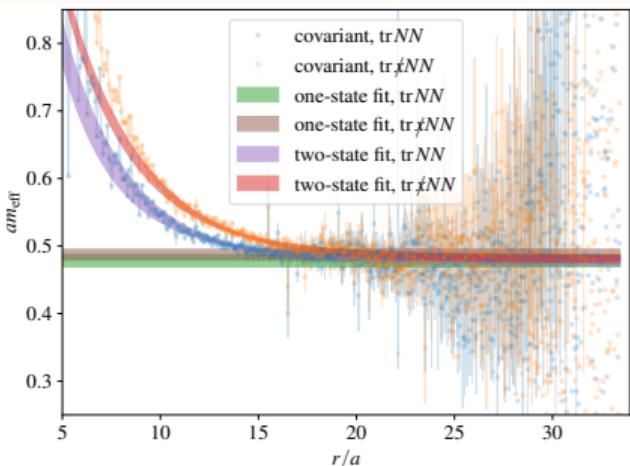
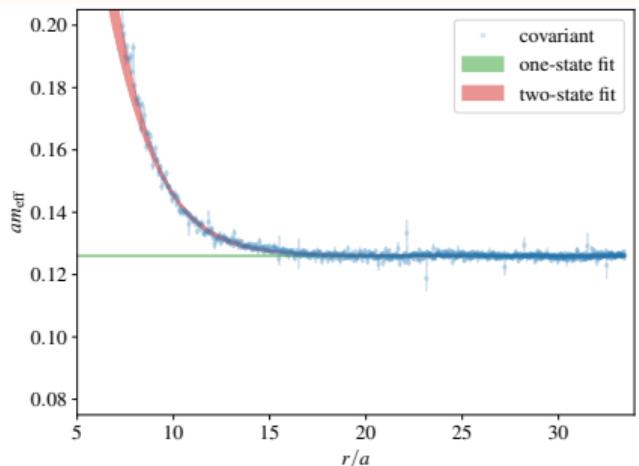
Comments:

- similar statistics (4096 noise src.) and computational effort on 96^4 ($x_{\text{gs}} = 12$) and 192^4 ($x_{\text{gs}} = 24$)
- different methods for proper calculations of uncertainties available (bootstrap, Γ -method)
- using empirical ansatz for excited state effects
- no boundary effects observed
- presented by M. Cè (Aug 11, 11:50)

Hadronic observables

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

Effective masses of pion and nucleon ($a = 0.94$ fm) on 192^4



Comments:

- similar statistics (4096 noise src.) and computational effort on 96^4 ($x_{\text{gs}} = 12$) and 192^4 ($x_{\text{gs}} = 24$)
- different methods for proper calculations of uncertainties available (bootstrap, Γ -method)
- using empirical ansatz for excited state effects
- no boundary effects observed
- presented by M. Cè (Aug 11, 11:50)



$N_f = 2 + 1$ Stabilised Wilson-Fermion simulations

- perform standard-sized lattice simulations
- implement all 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>

$N_f = 2 + 1$ Stabilised Wilson-Fermion simulations



Current OPENLAT team:



Francesca
Cuteri



Anthony
Francis



Patrick
Fritzsch



Giovanni
Pederiva



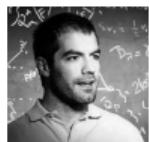
Antonio
Rago



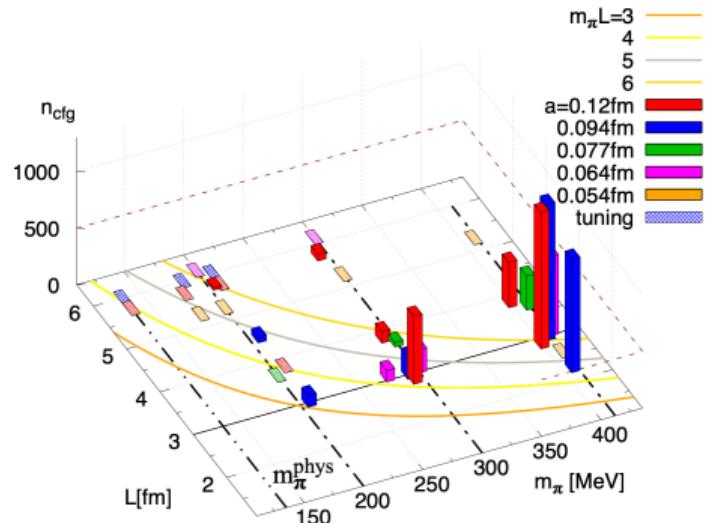
Andrea
Shindler



André
Walker-Loud



Savvas
Zafeiropoulos



■ more information on policies & status:

A. Francis (Aug 9, 14:30), *Lattice Data session, 461*
„OpenLat“

■ first results of spectroscopic calculations:

G. Pederiva (Aug 9, 16:50), *Hadron Spec. & Int., 433*
„Benchmark Continuum Limit Results for Spectroscopy with StabWF“

■ continue to explore the behaviour of StabWF with colleagues from CLS

- approaching physical points at coarse lattice spacings $a = 0.094, 0.12$ fm
- 5 lattice spacings at $SU(3)$ -flavour-symmetric point
- no negative eigenvalues of D_s observed so far



$N_f = 2 + 1$ Stabilised Wilson-Fermions @Lattice22

Growing interest reflected in this year's contributions

Traditional simulations:

- J. Kuhlmann (Aug 9, 20:00), Poster session, 302
„On improvement and renormalisation of quark currents with StabWF“
- R.F. Basta (Aug 9, 20:00), Poster session, 381
„QCD Thermodynamics with StabWF“
- F. Joswig (Aug 11, 12:10), Hadron Spec. & Int., 189
„Exploring distillation at the SU(3) flavour symmetric point“
- J. Green (Aug 11, 12:10), Nuclear Physics, 215
„Nucleon-nucleon scattering from distillation“

Topics covered:

- Renormalisation & Symanzik improvement
- Thermodynamics
- Hadron spectrum calculations
- Nuclear physics & scattering amplitudes
- Spectral reconstruction

Master-field simulations:

- A. Francis (Aug 8, 14:40), Theoretical Dev., 209
„Translating topological benefits in very cold master-field simulations“
- J. Bulava (Aug 9, 9:20), Plenary session, 278
„The spectral reconstruction of inclusive rates“
- M. Cè (Aug 11, 11:50), Hadron Spec. & Int., 356
„Hadronic observables from master-field simulations“

$N_f = 2 + 1$ Stabilised Wilson-Fermions @Lattice22

Growing interest reflected in this year's contributions

Traditional simulations:

- J. Kuhlmann (Aug 9, 20:00), Poster session, 302
„On improvement and renormalisation of quark currents with StabWF“
- R.F. Basta (Aug 9, 20:00), Poster session, 381
„QCD Thermodynamics with StabWF“
- F. Joswig (Aug 11, 12:10), Hadron Spec. & Int., 189
„Exploring distillation at the SU(3) flavour symmetric point“
- J. Green (Aug 11, 12:10), Nuclear Physics, 215
„Nucleon-nucleon scattering from distillation“

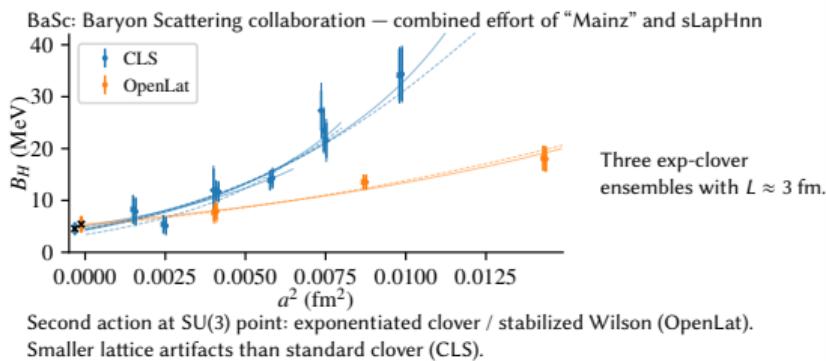
Master-field simulations:

- A. Francis (Aug 8, 14:40), Theoretical Dev., 209
„Translating topological benefits in very cold master-field simulations“
- J. Bulava (Aug 9, 9:20), Plenary session, 278
„The spectral reconstruction of inclusive rates“
- M. Cè (Aug 11, 11:50), Hadron Spec. & Int., 356
„Hadronic observables from master-field simulations“

Topics covered:

- Renormalisation & Symanzik improvement
- Thermodynamics
- Hadron spectrum calculations
- Nuclear physics & scattering amplitudes
- Spectral reconstruction

H dibaryon: $a \rightarrow 0$ universality (PRELIMINARY)



The future of master fields & StabWF

My personal opinion

- Growing evidence for smaller cutoff effects with StabWF
- Physical point simulations become available
- Increasing user base for StabWF
- Exascale machines may turn out to be particularly suitable for MF simulations
- Master field at *another lattice spacing*, then shift focus *towards physical point* master fields
- Master field simulations may have a political dimension:
 - Much larger computing resources required
 - Probe performance of HPC facilities (landmark sim.)
 - Community-driven effort (within EuroLat, ...?)
 - + General purpose
 - + Open access
 - + Computing time for smaller groups?

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 ✓
- $96^4, 192^4$ ($a = 0.095 \text{ fm}$) and 144^4 ($a = 0.065 \text{ fm}$) master-field ready for physics applications ✓
- master-field prefers target partition function ✓
- very large volumes like $(18 \text{ fm})^4$ still challenging but doable (or m_π^{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 6×6 hermitean matrices.

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

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

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.

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

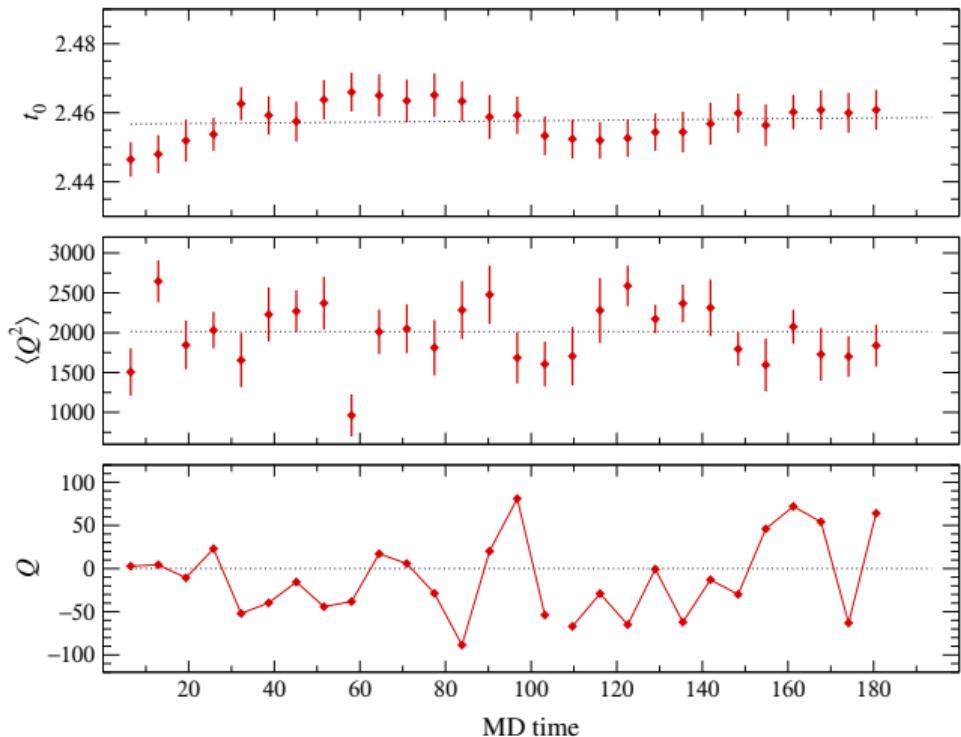
$$\begin{aligned} p_0 &= \frac{1}{6}\text{tr}\{A^6\} - \frac{1}{8}\text{tr}\{A^4\}\text{tr}\{A^2\} - \frac{1}{18}\text{tr}\{A^3\}^2 + \frac{1}{48}\text{tr}\{A^2\}^3 \\ p_1 &= \frac{1}{5}\text{tr}\{A^5\} - \frac{1}{6}\text{tr}\{A^3\}\text{tr}\{A^2\}, \\ p_2 &= \frac{1}{4}\text{tr}\{A^4\} - \frac{1}{8}\text{tr}\{A^2\}^2,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

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

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

Monitoring observables (thermalisation)

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



Simulations without TM-reweighting:

- no spikes in ΔH
- $\langle e^{-\Delta H} \rangle = 1$ 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 ($a = 0.094$ fm, $m_\pi = 270$ MeV) at LRZ using 768 nodes (36864 cores)

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

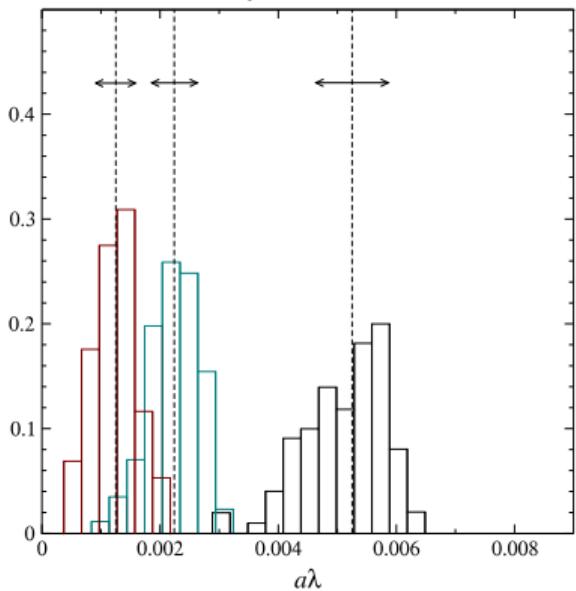
```
SMD parameters:  
actions = 0 1 2 3 4 5 6 7 8  
npf = 8  
mu = 0.0 0.0012 0.012 0.12 1.2  
nlv = 2  
gamma = 0.3  
eps = 0.137  
iacc = 1  
  
...  
  
Rational 0:  
degree = 12  
range = [0.012,8.1]  
  
Level 0:  
4th order OMF integrator  
Number of steps = 1  
Forces = 0  
  
Level 1:  
4th order 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?

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



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

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

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

(historical data missing for detailed comparison)

Overall behaviour of smallest eigenvalue

- $a\lambda = \min \left\{ \text{spec}(D_u^\dagger D_u)^{1/2} \right\}$
 $(a\lambda = 0.001 \sim 2 \text{ MeV})$
 - median $\mu \propto Zm$
 - width σ decreases with m
 - somewhat similar to $N_f = 2$ case^[15]
(unimproved Wilson)
 - (non-)Gaussian ?
 - empirical:^[15] $\sigma \simeq a/\sqrt{V}$



Bibliography I

- [1] M. Lüscher, *Stochastic locality and master-field simulations of very large lattices*, EPJ Web Conf. **175** (2018) 01002, [1707.09758].
- [2] L. Giusti and M. Lüscher, *Topological susceptibility at $T > T_c$ from master-field simulations of the $SU(3)$ gauge theory*, Eur. Phys. J. C **79** (2019) 207, [1812.02062].
- [3] A. Francis, P. Fritzsch, M. Lüscher and A. Rago, *Master-field simulations of $O(a)$ -improved lattice QCD: Algorithms, stability and exactness*, Comput. Phys. Commun. **255** (2020) 107355, [1911.04533].
- [4] A. M. Horowitz, *Stochastic Quantization in Phase Space*, Phys. Lett. **156B** (1985) 89.
- [5] A. M. Horowitz, *The Second Order Langevin Equation and Numerical Simulations*, Nucl. Phys. **B280** (1987) 510.
- [6] A. M. Horowitz, *A Generalized guided Monte Carlo algorithm*, Phys. Lett. **B268** (1991) 247–252.
- [7] K. Jansen and C. Liu, *Kramers equation algorithm for simulations of QCD with two flavors of Wilson fermions and gauge group $SU(2)$* , Nucl. Phys. **B453** (1995) 375–394, [hep-lat/9506020]. [Erratum: Nucl. Phys.B459,437(1996)].
- [8] B. Sheikholeslami and R. Wohlert, *Improved Continuum Limit Lattice Action for QCD with Wilson Fermions*, Nucl. Phys. **B259** (1985) 572.
- [9] M. Lüscher, *Ergodicity of the SMD algorithm in lattice QCD*, unpublished notes (2017) .
<http://luscher.web.cern.ch/luscher/notes/smd-ergodicity.pdf>.
- [10] M. Bruno, D. Djukanovic, G. P. Engel, A. Francis, G. Herdoíza et al., *Simulation of QCD with $N_f = 2 + 1$ flavors of non-perturbatively improved Wilson fermions*, JHEP **1502** (2015) 043, [1411.3982].
- [11] G. S. Bali, E. E. Scholz, J. Simeth and W. Söldner, *Lattice simulations with $N_f = 2 + 1$ improved Wilson fermions at a fixed strange quark mass*, Phys. Rev. **D94** (2016) 074501, [1606.09039].
- [12] M. Bruno, T. Korzec and S. Schaefer, *Setting the scale for the CLS $2 + 1$ flavor ensembles*, Phys. Rev. **D95** (2017) 074504, [1608.08900].
- [13] M. Lüscher, *openQCD*, . <https://luscher.web.cern.ch/luscher/openQCD/index.html>.
- [14] F. Cuteri, A. Francis, P. Fritzsch, G. Pederiva, A. Rago, A. Shindler et al., *Properties, ensembles and hadron spectra with Stabilised Wilson Fermions*, in *38th International Symposium on Lattice Field Theory*, 1, 2022. 2201.03874.
- [15] L. Del Debbio, L. Giusti, M. Lüscher, R. Petronzio and N. Tantalo, *QCD with light Wilson quarks on fine lattices. II. DD-HMC simulations and data analysis*, JHEP **0702** (2007) 082, [hep-lat/0701009].