Master-fields in lattice QCD

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Lattice QCD on a slide

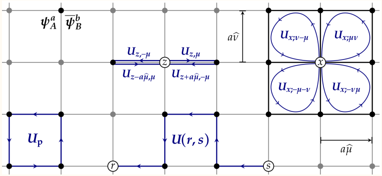
4D Euclidean space with gauge group $\mathrm{SU}(3)$ and N_f quark flavours:

$$\mathcal{L}^{\mathrm{QCD}} = -\frac{1}{2g^2}\mathrm{Tr}[F_{\mu\nu}F_{\mu\nu}] + \sum_{i=1}^{N_\mathrm{f}} \overline{\psi}_i[\gamma_\mu D_\mu + m_i]\psi_i$$

- gauge invariant
- $N_\mathrm{f}+1$ free parameters $\left\{ \begin{array}{ll} \text{strong coupling} & g^2 \\ \text{quark masses} & m_i, i=1,\dots,N_\mathrm{f} \end{array} \right\}$ require physical input

Lattice regularization

- lattice spacing (a) and physical volume ($V_4 = L^4$) $\rightarrow$ finite lattice Λ
- fermions $\psi, \overline{\psi}$ on lattice sites $x \in \Lambda$
- gluons $U(x + a\hat{\mu}, x)$ on lattice links
- a variety of lattice actions $\mathcal{S} = \mathcal{S}_\mathrm{G} + \mathcal{S}_\mathrm{F}$
- E.g. Wilson fermion action in its improved form:

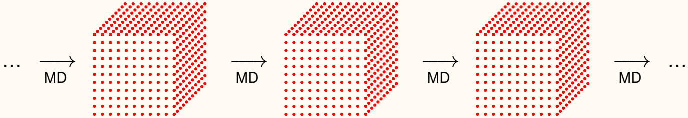


$$\mathcal{S}_\mathrm{W} \equiv a^4 \sum_{x\in\Lambda} \overline{\psi}_x Q \psi_x \,, \qquad Q = \tfrac{1}{2}\gamma_\mu(\nabla^*_\mu + \nabla_\mu) - a\tfrac{1}{2}\nabla^*_\mu\nabla_\mu + M_0 + a c_\mathrm{sw}\,\tfrac{\mathrm{i}}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}$$

The standard lattice QCD approach

Markov Chain Monte Carlo simulations of QCD

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



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

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[U]\, \mathcal{O}\, e^{-\mathcal{S}_{\mathrm{G}}[U] - \mathcal{S}_{\mathrm{eff}}[U]} \approx \frac{1}{N_U} \sum_{i=1}^{N_U} \mathcal{O}[U_i]\,, \qquad e^{-\mathcal{S}_{\mathrm{eff}}} \simeq \det(Q)^{N_{\mathrm{f}}}$$

Hybrid Monte-Carlo algorithm

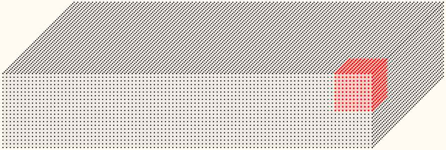
- employs importance sampling
- draw conj. momenta π & integrate molecular dynamics (MD) equations (symplectic integrators)
- made exact by (global) Metropolis accept-reject step ($\Delta H = \Delta \mathcal{S}$)
- ergodicity maintained by redrawing the momenta

+ various (Krylov) solvers, precondition techniques (eo, det-splitting, …), multiple time-scales, …

The master-field approach[1]

Master-field lattice

a single master-field to replace classical (Markov chain) ensemble



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

„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.)
- field-theoretical expectation value $\langle \mathcal{O} \rangle$ from translation averages $\langle\langle \mathcal{O} \rangle\rangle$ of observables

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

provided localisation range of $\mathcal{O} \ll L$ (lattice extent)

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

Are we well prepared for very large simulations of QCD?

Critical aspects of lattice QCD simulations

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

Algorithmic aspects

- update algorithm: Hybrid Monte-Carlo (exploration of phase space)
- integration schemes and length (symplectic)
- numerical precision, e.g. in global sums (Metropolis step) (double precision)
- solver parameters (stability & performance)

Physical aspects

- coarse lattice spacings a promote large fluctuations of gauge field (roughness of fields U_i)
- small quark masses $m_{\rm ud}$ result in small eigenvalues of lattice Dirac operator ($\lambda_{\rm min}(m_{\rm ud})$)
- large number of sites $(L/a)^4$ increases risk for exceptional behaviour (e.g. from MD force)

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

Stabilising measures for QCD[3]

A.Francis, P.F., M.Lüscher, A.Rago, Comput.Phys.Commun. 255 (2020) 107355

- new Wilson–Dirac operator
- stochastic molecular dynamics (SMD) algorithm[4–7]
- solver stopping criteria

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

✓ 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

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

…

New Wilson–Dirac operator

A.Francis, P.F., M.Lüscher, A.Rago, Comput.Phys.Commun. 255 (2020) 107355

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

Even-odd preconditioning:

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

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

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

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

✓ Employ bounded counterterm operator

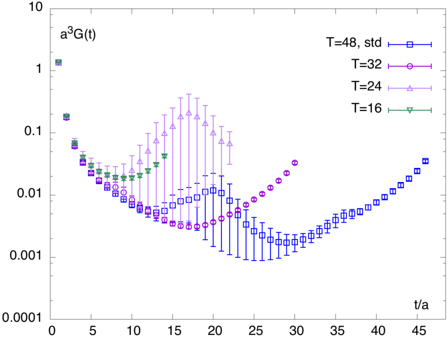
- valid Symanzik improvement
- guarantees invertibility

New Wilson–Dirac operator

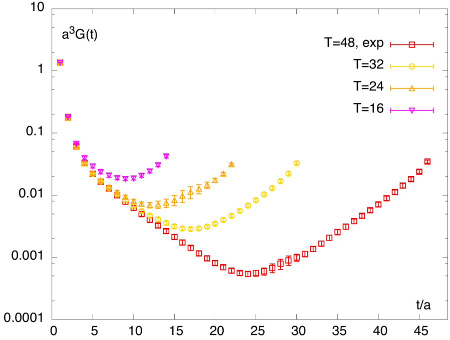
A clean comparison of fermion actions

- Impact best seen in pure gauge theory ($N_\mathrm{f} = 0$, quenched).
  Ill-defined theory for fermionic observables. $\Rightarrow$ exceptional problems
- Different lattices $L/a \in \{16, 24, 32, 48\}$ and same gluon action ($\beta = 6.0$).
- 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

A.Francis, P.F., M.Lüscher, A.Rago, Comput.Phys.Commun. 255 (2020) 107355

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

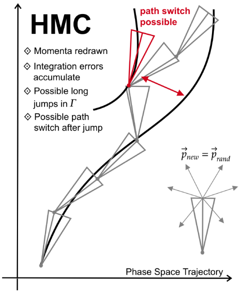
Refresh $\pi(x,\mu)$, $\phi(x)$ by random field rotation

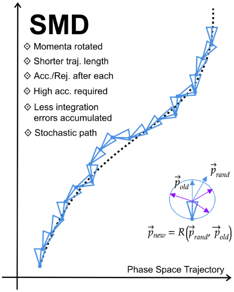
$$\pi \to c_1\pi + c_2 v\,, \qquad c_1 = e^{-\epsilon\gamma}\,, \quad c_1^2 + c_2^2 = 1\,, \qquad v(x,\mu), \eta(x) \in \mathcal{N}(0,1)$$

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

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

- ergodic[8] 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

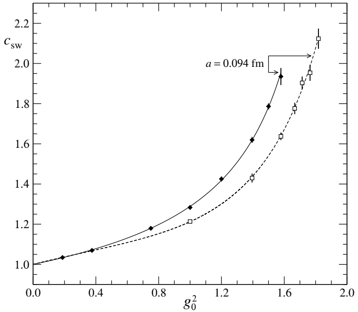




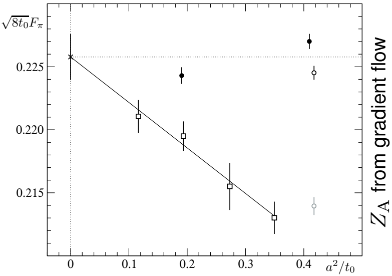
Check against standard Wilson action (CLS[9–11])

$N_\mathrm{f} = 2+1$ published in [3]

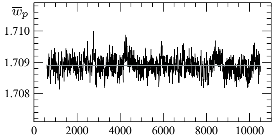
Non-perturbative improvement:



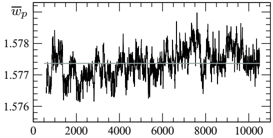
$$\phi_4 \equiv 8t_0(\tfrac{1}{2}m_\pi^2 + m_\mathrm{K}^2) = 1.11 \sim \mathrm{Tr}[M_\mathrm{q}]$$



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



exp. clover (A_1)



std. clover (X_1)

$N_\mathrm{f} = 2+1$ published in [3]

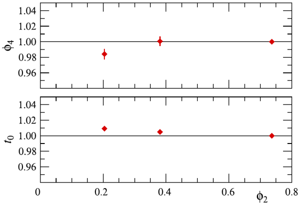
Using set of normal-sized lattices:

ID	a/fm	β	$T \cdot L^3$	$\frac{m_\pi}{\mathrm{MeV}}$	$\frac{m_\mathrm{K}}{\mathrm{MeV}}$	Lm_π	b.c.	status	$\langle P_\mathrm{acc} \rangle$	$R_\mathrm{spk}[\%]$
A_1	0.095	3.8	$96 \cdot 32^3$	410	410	6.3	P	✓	97.5%	0.19(10)
A_2			$96 \cdot 32^3$	294	458	4.5	P	✓	98.6%	0.19(10)
A_3			$96 \cdot 32^3$	220	478	3.4	P	✓	98.1%	0.10(7)
B_1	0.064	4.0	$96 \cdot 48^3$	410	410	6.4	P	✓	98.8%	0.0
C_1	0.055	4.1	$96 \cdot 48^3$	410	410	5.5	O	✓	98.7%	0.0

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

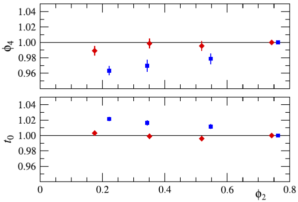
Chiral trajectory of ϕ_4, t_0:

Stabilised Wilson



$a = 0.095\,\mathrm{fm}$

Standard Wilson



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

1st dynamical master-field simulations

- M. Cé, M. Bruno, J. Bulava, A. Francis, P. F, J. Green, M. Lüscher, A. Rago, M. Hansen.
- $N_\mathrm{f} = 2 + 1$+stabilising measures[3]
- $a = 0.095\,\mathrm{fm}$, $m_\pi = 270\,\mathrm{MeV}$
- `openQCD-2.0`[12]
  60 Mch on superMUC-NG (PRACE)

1^{st} dynamical master-field simulations

on superMUC-NG @ LRZ, Munich

Goal: show viability of master-field approach

2 master-field lattices at coarse lattice spacing $a = 0.095\,\text{fm}$

- 96^4 ($L = \ 9\,\text{fm}$) at $m_\pi = 270\,\text{MeV} = 2m_\pi^{\text{phys}}$
- 192^4 ($L = 18\,\text{fm}$) at $m_\pi \leq 270\,\text{MeV}$

Follow well-established thermalisation strategy:

- start from smaller lattices + periodically extend one direction at a time
- adapt algorithmic parameters as needed
- iterate

starting from A_2 lattice ($m_\pi = 294\,\text{MeV}$):

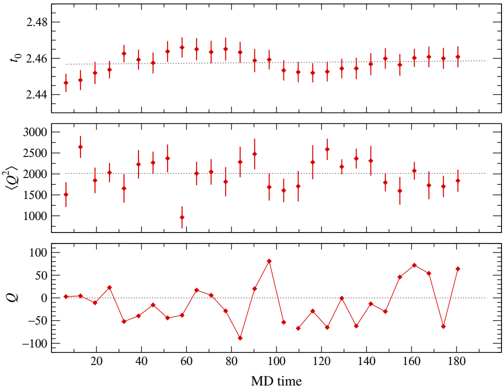
- change hopping parameter to target and twisted-mass $\mu_0 = 0$

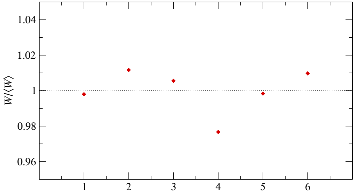
Thermalisation cost for 1st master-field:

lattice	#cores	$t_{\text{SMD}}\,[\text{sec}]$	$t_{\text{MDU}}\,[\text{sec}]$	Mcore-h	MDU
96×32^3	$16 \cdot 48$	246	794	0.03	155
$96^2 \times 32^2$	$48 \cdot 48$	277	1108	0.09	125
$96^3 \times 32$	$64 \cdot 48$	672	2800	0.42	176
96^4	$128 \cdot 48$	1080	5020	1.77	206
total:				2.31	662

Monitoring observables (thermalisation)

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





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
- std.-deviation σ_W of strange-quark „reweighting factors“ within strict bound

$$\frac{\sigma_W}{\langle W \rangle} \leq 0.1$$

to guarantee unbiased results

1[st] dynamical master-field simulations

192^4 : $a = 0.095\,\mathrm{fm}$, $m_\pi = 270\,\mathrm{MeV}$, $Lm_\pi = 25$ ($L = 18\,\mathrm{fm}$)

Obstacle:

> very large physical volumes (periodic b.c.) still promote issues
> (at least at coarse lattice spacing)
> they could always be solved through restarts so far

We observe

- deflated solver fails occasionally for the little Dirac op.
- spikes in ΔH
- no. of such events increases with larger V and smaller m_π
- origin unknown (multiple sources?)

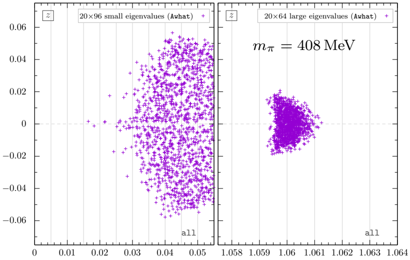
Mitigation strategy?

- require better understanding of the problem (algorithmic and/or physical origin?)
- use fallback-solver (less performat)
- …

Master-field simulations

Study deflation subspace ($a = 0.095\,\mathrm{fm}$)

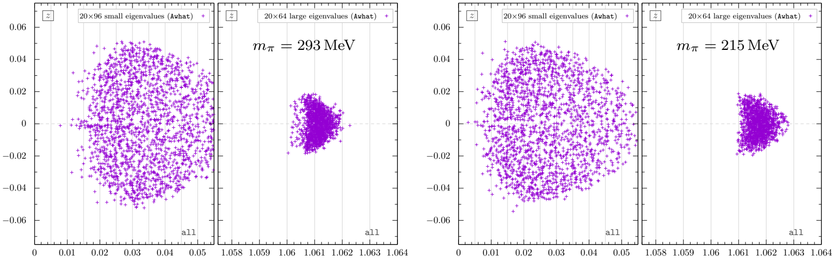
Small/Large eigenvalue spectrum of eo-preconditioned DFL operator **Awhat** on A-lattices (96×32^3):



Deflation subspace ⇔ „low-modes“ $\{\psi_1, \cdots, \psi_{N_s}\}$

$$A_w = P_0 D P_0 \qquad \text{: restricted Dirac op.}$$

P_0: orthogonal projector to DFL subspace



Upgrade of openQCD

to support multilevel deflation in version 2.0.2

Solution: Multilevel deflation

- effectively results in a preconditioning of the std. little Dirac op.
- introduce stack of deflation subspaces (block grid levels $0 \leq k \leq k_{\max}$)
- little Dirac ops. at block-level k: $A_k = P_k A_{k-1} P_k = P_k D P_k$
- derived from the same set of global low modes $\{\psi_1, \cdots, \psi_{N_s}\}$ (at top level, $k_{\max}$)
- especially large lattices profit from additional levels (smaller cost)
- projection/lifting now implemented in double precision for stability (larger cost)

Thermalisation cost:

lattice	#cores	$\bar{t}_{\mathrm{SMD}}[\mathrm{sec}]$	$\bar{t}_{\mathrm{MDU}}[\mathrm{h}]$	Mcore-h	MDU
192×96^3	$128 \cdot 48$	2740	794	2.32	95
$192^2 \times 96^2$	$256 \cdot 48$	3080	4.73	2.54	45
$192^3 \times 96$	$512 \cdot 48$	3190	5.34	4.49	35
192^4	$768 \cdot 48$	4789	9.71	35.12	102
total:				44.47	277

Hadronic observables

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 $1/m$

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

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

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

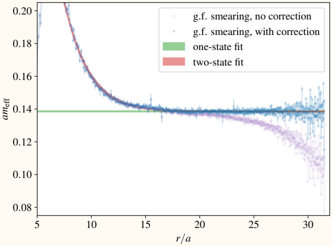
- axis/off-axis directions will have different cutoff effects
- consider the correlator averaged over 4D spheres of radius $r=|x|$:

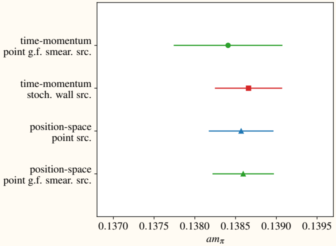
$$\overline{C}(r) = \frac{1}{\mathrm{r}_4((r/a)^2)}\sum\nolimits_{|x|=r} C(x)$$

Hadronic observables

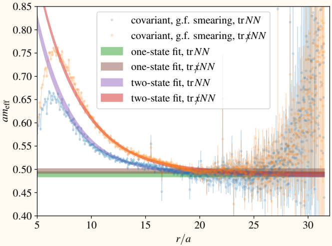
On test-ensemble 96×64^3, $a = 0.095\,\mathrm{fm}$

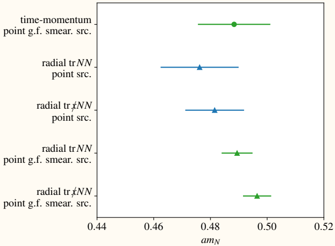
Pion: $m_\pi = 290.5(8)\,\mathrm{MeV}$





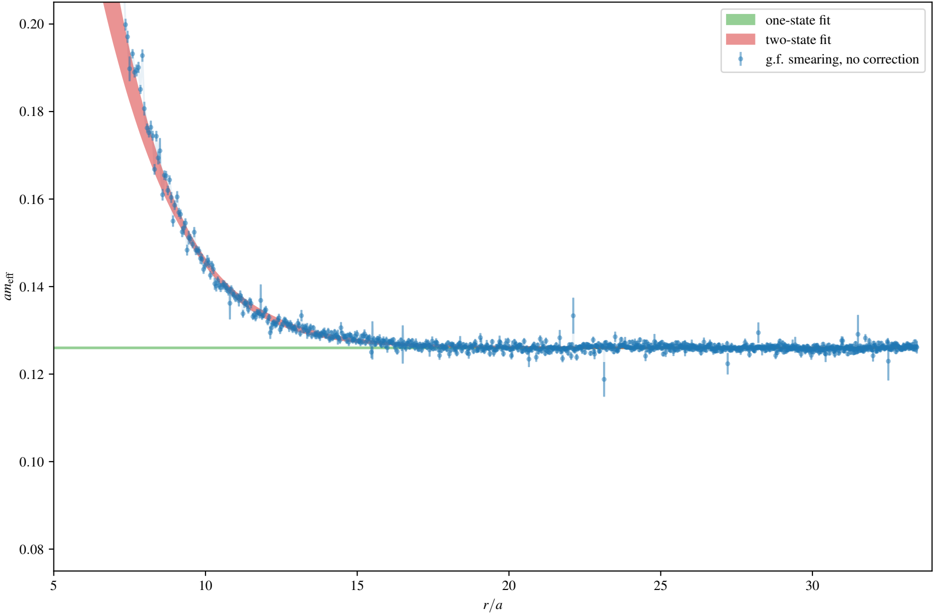
Nucleon: $m_N = 1025(10)\,\mathrm{MeV}$





Hadronic observables

Hot off the press: master-field 192^4, $a = 0.095\,\mathrm{fm}$



OPEN
LATtice
initiative

$N_\mathrm{f} = 2+1$ Stabilised WF for physics

- core team: F.Cuteri, A. Francis, P. F, K. Orginos, A. Rago, A. Shindler, A. Walker-Loud, *S. Zafeiropoulos*
- implements new action & stabilising measures[13]
- various lattices $\{a/L, \beta, m_\pi\}$ to complement master-field simulations
- to be shared

Summary & perspectives

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 approach not compatible with reweighting techniques ✗
- very large volumes like $(18\,\mathrm{fm})^4$ still challenging but doable (or m_π^{phys}) ✓
- position-space correlators can be used to extract hadron masses

Ongoing:

We just start to uncover new possibilities.

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

Backup slides

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
```

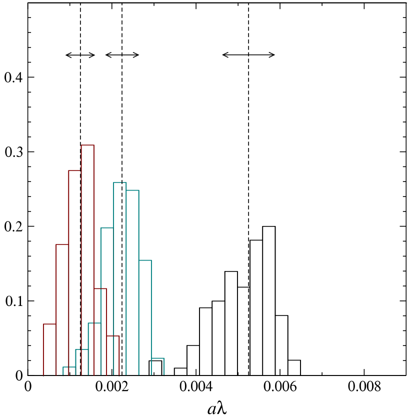
```
Update cycle no 48
dH = -1.4e-02, iac = 1
Average plaquette = 1.708999
Action  1: <status> = 0
Action  2: <status> = 0 [0,0|0,0]
Action  3: <status> = 0 [0,0|0,0]
Action  4: <status> = 0 [0,0|0,0]
Action  5: <status> = 2 [5,2|7,6]
Action  6: <status> = 271
Action  7: <status> = 21 [3,2|5,3]
Action  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)
```

Cost: 0.33 Mch / MDU => 10 Mch / indep. cnfg => 30 Mch / 3 indep. master-fields

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 $N_\text{f} = 2$ case[14] (unimproved Wilson)
- (non-)Gaussian ?
- empirical:[14] $\sigma \simeq a/\sqrt{V}$

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