Master-field simulations of QCD

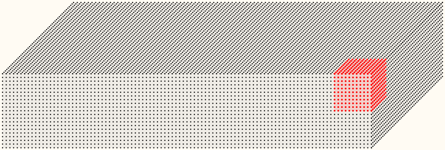
Patrick Fritzsch

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

in collaboration with
M. Cè, M. Bruno, J. Bulava, A. Francis, J. Green, M. Hansen, M. Lüscher, A. Rago

The master-field approach[1]

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



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

„Stochastic locality“

- QCD field variables in distant regions fluctuate largely independent
- their distribution is everywhere the same (with periodic bc.)
- translation averages of observables $\langle\langle \mathcal{O}(x) \rangle\rangle = V^{-1}\sum_z \mathcal{O}(x+z)$ coincide with their field-theoretical expectation values up to $O(V^{-1/2})$ corrections, provided localisation range of $\mathcal{O} \ll$ lattice extent

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

QCD with Wilson fermions requires additional stability measures.[3]

Stabilising measures for QCD[3]

- Stochastic Molecular Dynamics (SMD) algorithm[4–7]
- solver stopping criteria ✓ uniform norm $\|\eta\|_\infty = \sup_x \|\eta(x)\|_2$ V-independent
- global accept-reject step ✓ quadruple precision in global sums
- new clover-term in Wilson–Dirac operator ✓ guarantees invertibility

$$D = \tfrac{1}{2}\{\gamma_\mu(\nabla_\mu^* + \nabla_\mu) - a\nabla_\mu^*\nabla_\mu\} + \delta D_{\rm v} + m_0$$

uses exponential variant in diagonal part $(M_0 = 4 + m_0)$

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

of even-odd preconditioned operator ($\hat{D} = D_{\rm ee} - D_{\rm eo}(D_{\rm oo})^{-1}D_{\rm oe}$)

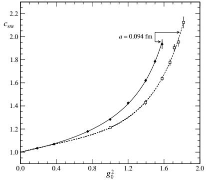
- …together with well-established techniques

✓ SAP, local deflation, mass-preconditioning, multiple time-scales, …

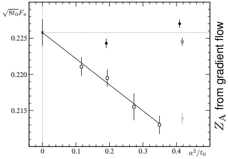
Multiple checks against std SW-improved action[8–10]

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

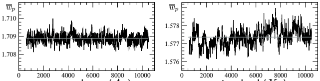
Non-perturbative improvement:



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

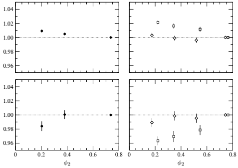


plaquette test with SMD: $a = 0.095$ fm



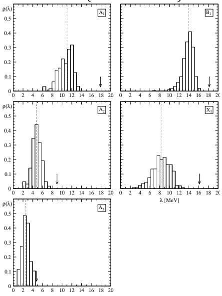
exp. clover (A_1) standard (X_1)

Quark mass dependence of t_0 and ϕ_4



exp. clover standard

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



ID	a/fm	β	$T \cdot L^3$	$\frac{m_\pi}{\rm MeV}$	$\frac{m_{\rm K}}{\rm MeV}$	Lm_π	b.c.	status	$\langle P_{\rm acc}\rangle$	$R_{\rm spk}[\%]$
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-lvOMF-4, $N_{\rm pf} \leq 8$, $R_{\rm deg} \leq 10$)

Progress

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]
- $a = 0.095\,\mathrm{fm}$, $m_\pi = 270\,\mathrm{MeV}$
- using `openQCD-2.0`[11] and 60 Mch from PRACE

1^{st} dynamical master-field simulations

running on superMUC-NG @ LRZ, Munich

Goal: show viability of master-field approach

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

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

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 ($m_\pi = 294\,\mathrm{MeV}$):

- change hopping parameter to target <u>and</u> twisted-mass $\mu_0 = 0$
- $96 \times 32^3 \quad \to \quad 96^2 \times 32^2 \quad \to \quad 96^3 \times 32 \quad \to \quad 96^4$

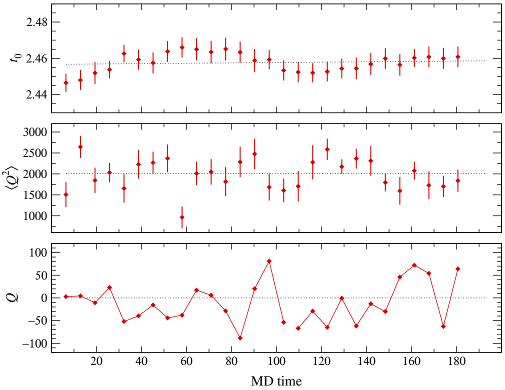
Thermalisation cost for 1st master-field:

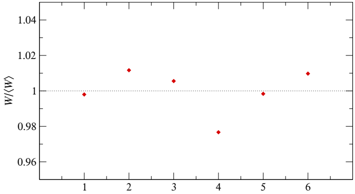
lattice	#cores	$t_{\mathrm{SMD}}\,[\mathrm{sec}]$	$t_{\mathrm{MDU}}\,[\mathrm{sec}]$	Mcore-h	MDU
96×32^3	$16 \cdot 48$	246	794	0.03	155
$96^2 \times 32^2$	$48 \cdot 48$	277	1108	0.09	125
$96^3 \times 32$	$64 \cdot 48$	672	2800	0.42	176
96^4	$128 \cdot 48$	1080	5020	1.77	206
total:				2.31	662

subsequently $96^4 \to 192^4$ with gradually changed pion mass

Monitoring observables

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 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

Thermalisation towards 192^4

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?)

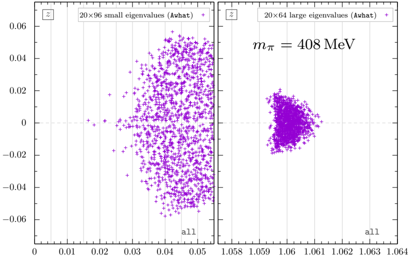
Mitigation strategy?

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

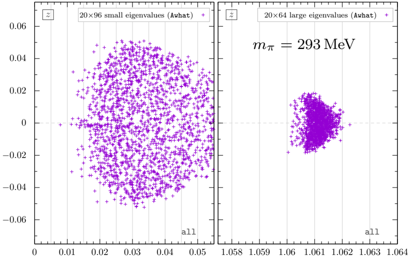
Master-field simulations

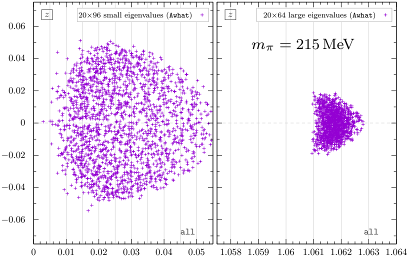
Study deflation subspace

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



> Deflation subspace ⇔ „low-modes“ $\{\psi_1, \cdots, \psi_{N_s}\}$
>
> $A_w = P_0 D P_0$: restricted Dirac op.
>
> P_0: orthogonal projector to DFL subspace





Upgrade of openQCD

to support multilevel deflation in version 2.0.2

Possible solution: Multilevel deflation

- effectively results in a preconditioning of the std. little Dirac op.
- introduce stack of deflation subspaces (block grid levels $0 \leq k \leq k_{\mathrm{max}}$)
- 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

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

Master-field simulations of QCD

Summary

192^4 runs mostly smoothly at $m_\pi = 270\,\mathrm{MeV}$, $a = 0.095\,\mathrm{fm}$ $(\mu_0 = 0)$

- 96^4 + 192^4 master-field lattice ready for physics applications ✓
- master-field approach not compatible with reweighting techniques ✗
- stabilising measures with exponential clover improve our ability to simulate coarse lattice spacings ✓
- very large volumes (or m_π^{phys}), like $(18\,\mathrm{fm})^4$, still challenging but doable ✓
- No Free Lunch theorem confirmed: stability & accuracy have a cost
- observed issues will be further investigated & reported
- we move on: smaller lattice spacing, lighter pion masses
- …

stay tuned: next talk (M. Cè) provides 1st physics calculations on master-fields

Backup slides

Algorithmic improvements for stability

General caveats: volume dependence, sampling, reversibility, … $\rightarrow$ Suggestion:

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

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

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

$$\phi \rightarrow c_1\phi + c_2 D^\dagger \eta\,,$$ ($\gamma > 0$: friction parameter; ϵ: MD integration time)

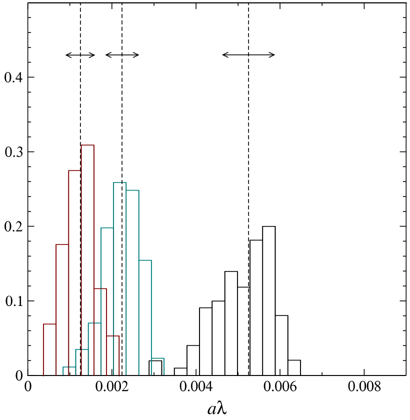
+ MD evolution + accept-reject step + repeat

- ergodic[12] 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

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 σ decreases with m
- somewhat similar to $N_\mathrm{f} = 2$ case[13] (unimproved Wilson)
- (non-)Gaussian ?
- empirical:[13] $\sigma \simeq a/\sqrt{V}$

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