Ensemble Generation of the Extended Twisted Mass Collaboration

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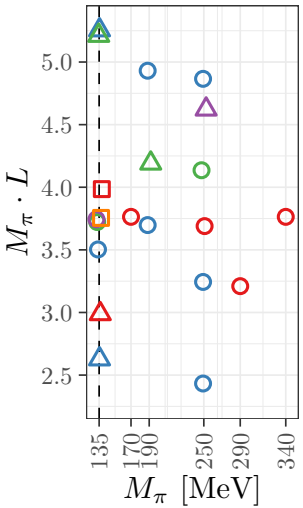
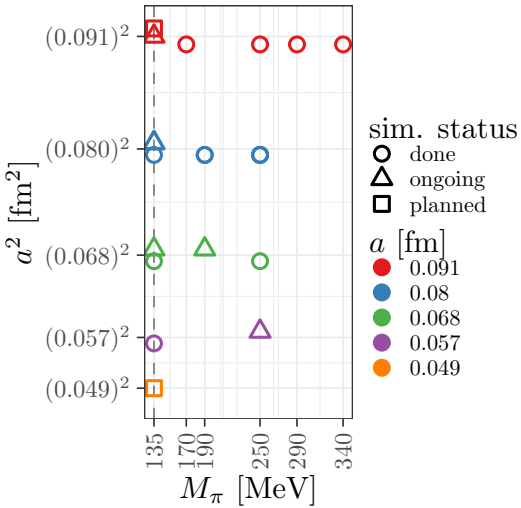
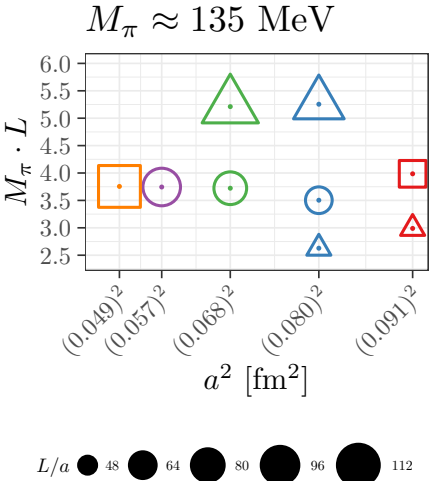
Ensemble Overview

$N_f = 2+1+1$ twisted-clover





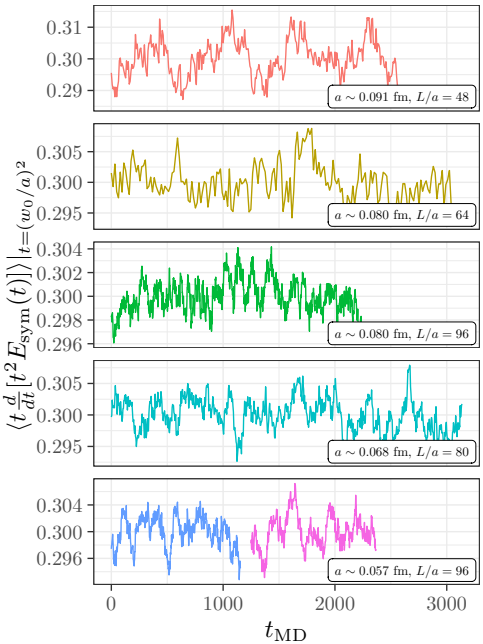


- $N_f = 2+1+1$ twisted-clover with $c_{\mathrm{SW}} \sim 1 + 0.113(3)\dfrac{g_0^2}{\langle P \rangle}$ and strange and charm quark masses tuned to within a % of the physical point. [Phys.Rev.D 98 (2018) 5, 054518, arXiv:2201.02551]
- $S_g = \frac{\beta}{3} \sum_{x;P} \left[b_0\{1 - \mathrm{ReTr}P^{1\times1}(x)\} + b_1\{1 - \mathrm{ReTr}P^{1\times2}(x)\} \right]$ with $b_0 = 1 - 8b_1$, $b_1 = -0.331$ [Iwasaki; 1983]

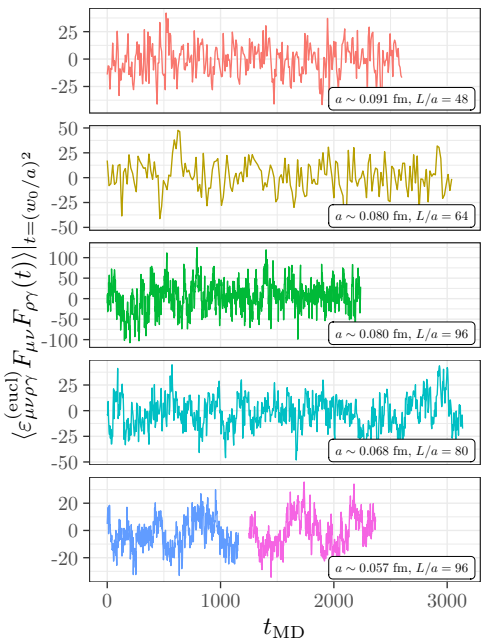
Statistical Properties of Gradient Flowed Observables

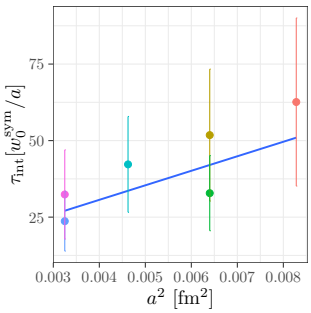
at or close to $M_\pi \sim 135$ MeV

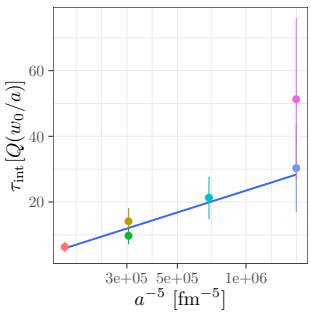
w_0/a



Q @ w_0/a







HMC Implementation and Algorithmic Choices

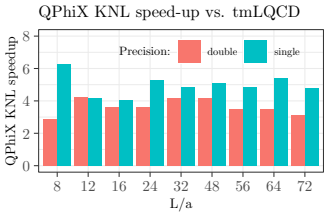
- tmLQCD software suite[a]
- HMC with 3 to 4 time scales
- 2MN or 2MNFG integrator (depending on volume)

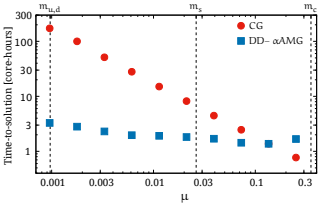
[a] https://github.com/etmc/tmlqcd

Light doublet

$$S_\ell = \sum_x \bar{\chi}(x)\left[D_W(U)+m_0+i\mu\gamma^5\tau^3+\frac{i}{4}c_{\rm SW}\sigma^{\mu\nu}\mathcal{F}^{\mu\nu}(U)\right]\chi(x)$$

- 3 to 4 ratios to mass-precondition light determinant
- large shifts → QPhiX[a] [10.1007/978-3-319-46079-6_30]
- smallest shifts → DD-αAMG[b] [10.1103/PhysRevD.94.114509]



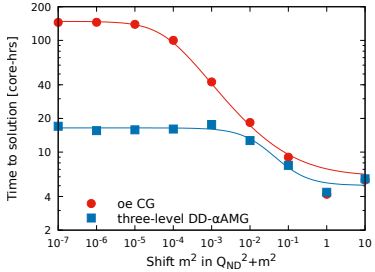


[a] https://github.com/JeffersonLab/QPhiX
[b] https://github.com/sbacchio/ddalphaamg

Heavy doublet

$$S_h = \sum_x \bar{\chi}_h(x)\left[D_W(U)+m_0+i\mu_\sigma\gamma^5\tau^3-\mu_\delta\tau^1+\frac{i}{4}c_{\rm SW}\sigma^{\mu\nu}\mathcal{F}^{\mu\nu}(U)\right]\chi_h(x)$$

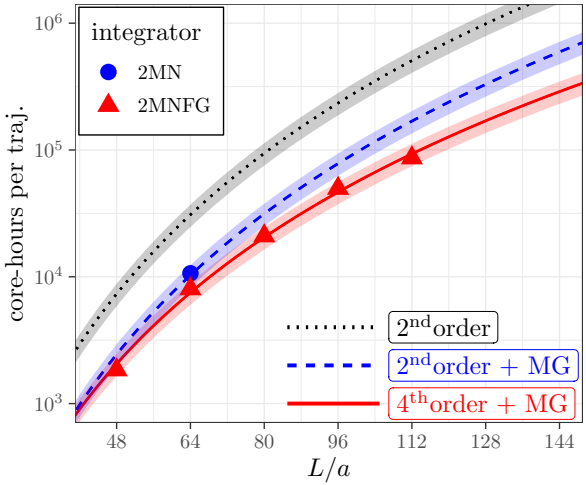
- rational approximation of order ≈ 10 [10.48550/arXiv.1002.4232, 10.1103/PhysRevD.75.011502]
- correction factor at ACC step [10.48550/arXiv.1002.4232]
- largest shifts → QPhiX multi-shift CG
- multi-shift CG with DD-αAMG refinement of 2 to 4 smallest shifts [10.1016/j.cpc.2018.10.013]

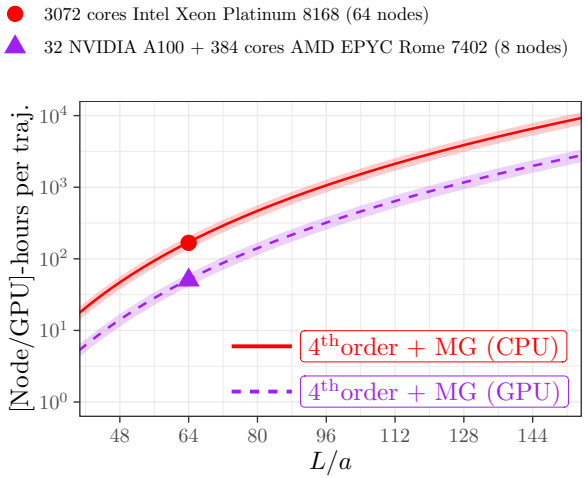


- in HMC: speedup ≈ 2 to 3 vs. QPhiX mshift solver

More details on algorithmic setup in appendix of [10.1103/PhysRevD.104.074520]

Integrators and GPU Port





- timings from real production runs, similar acceptance
  - roughly comparable, but from different machines!
  - errorband basically "invented"
- 2MN: cost $\propto c_2 L^5$
- 2MNFG: cost $\propto c_4 L^{9/2}$
- breakeven for us apparently around $L/a \approx 48$

- QUDA solvers + gauge derivative (for now)
- improvement in energy cost / trajectory > 3
- improvement in achieveable wall clock time > 2
- expect another factor 2 to 2.5 when complete
- more details: **BK**, *Software development and Machines*, Mon @ 15:00

Data Management Strategy

Configuration and Meta-data storage

- ILDG format with some meta-data (see right)
- exact provenance not tracked in detail (sometimes an issue for acknowledgements...)
  - online measurements, (most) logs and basic observables preserved
  - should at least store exact git commit & machine on which configs were generated
- total storage (expected): $\sim$ 2.5 PB for all configurations and related data

```
plaquette = 0.540826306713
trajectory nr = 121
beta = 1.726000000000, kappa = 0.140064500000,
mu = 0.001200000000, c2_rec = -0.331000
time = 1657266799
hmcversion = 5.2.0
mubar = 0.140800000000
epsilonbar = 0.152100000000
date = Fri Jul  8 09:53:19 2022
```

Collaboration-internal configuration storage

- two *data projects* at Juelich Supercomputing Center
- Collaboration Wiki to document ensembles and storage locations and, ideally, to store input files at an easily accessible location

Publication strategy

- *Plan* to make $N_f = 2$ physical point configs public as soon as ILDG useable again
- *Intent* in principle to make $N_f = 2 + 1 + 1$ configs available *at some point*

Looking into the Future / Collaboration Potential

- Completion of QUDA interface and usage for HMC on future machines (LUMI-G, Leonardo, ...)
- Need larger volumes, higher statistics in some places
- In principle openness to collaboration on various physics projects under conditions to be decided
- At present no clear plan or defined policy to make configurations available to people outside the ETMC

Thanks for your attention!