CLS 2+1 flavor simulations at physical light- and strange-quark masses

Daniel Mohler

Granada,
June 20th, 2017

Representing the CLS effort
Together with Stefan Schaefer and Jakob Simeth

Outline

The CLS 2+1 flavor ensembles – Key features

- Open boundary conditions to avoid topological freezing for $a \to 0$
- Twisted mass reweighting (for the light quarks)
- Simulation along trajectory with fixed $Tr(M)$
- Additional simulations along trajectories with fixed strange quark mass $m_s = $ const. and with $m_s = m_l$
- Flexible simulations with OpenQCD

  http://luscher.web.cern.ch/luscher/openQCD/

  - Nested hierarchical integrators
  - Hasenbusch-style mass preconditioning with an arbitrary number of pseudofermion pairs
  - Rational approximation (+ reweighting) for the strange quark
  - Deflation acceleration and chronological solver
 - A number of solvers

CLS 2+1 flavor ensembles: Overview
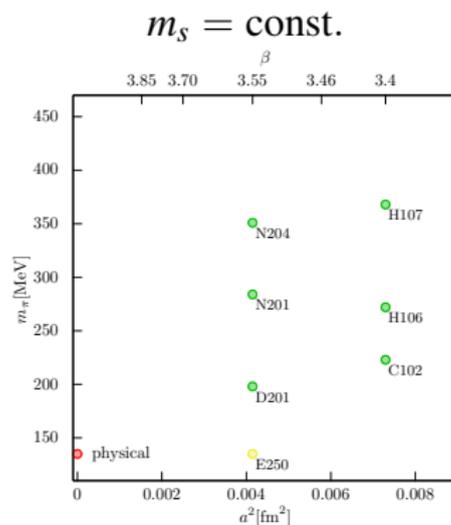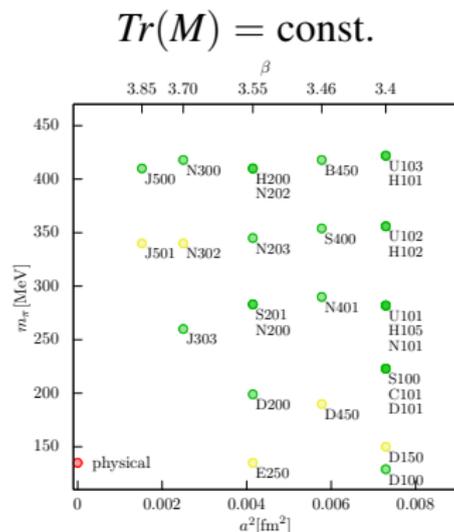
plots by Jakob Simeth, RQCD

- Letters in the name denote the aspect ratio T/L; First digit encodes β
- Ensembles at 5 lattice spacings and with a range of $M_\pi \leq 420\text{MeV}$
- Ensembles to control (or exploit) finite volume effects

CLS 2+1 flavor ensembles: Statistics – area $\propto$ MDU

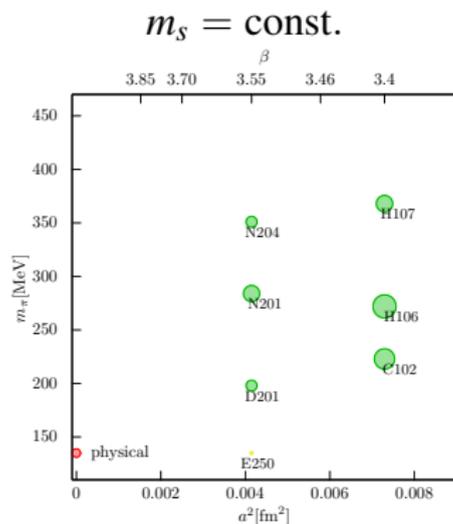Bruno *et al.* JHEP 1502 043 (2015); Bali *et al.* PRD 94 074501 (2016)
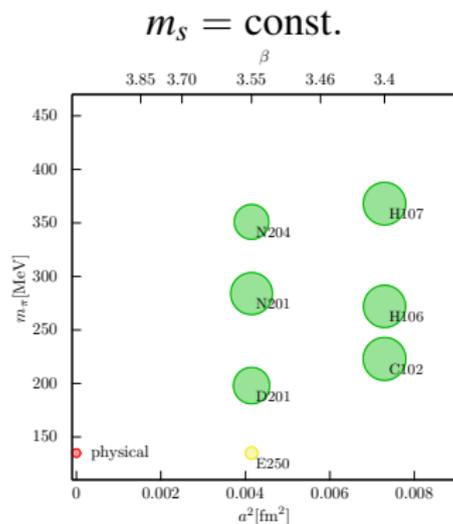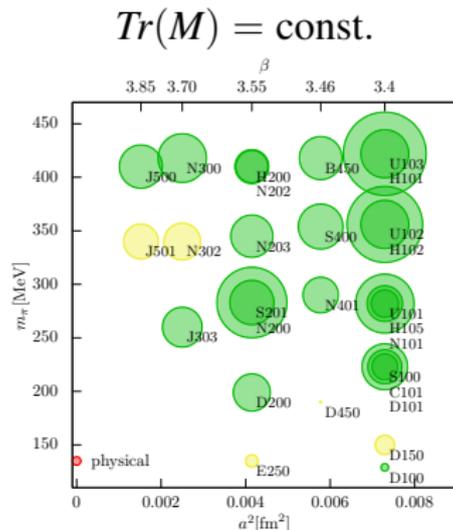
$Tr(M) = $ const.

$m_s = $ const.

plots by Jakob Simeth, RQCD

- > 4000 MDU for many ensembles
  Typically save 1 configuration every 4 MDU
- target statistics chosen considering largest τ_{int} (often YM action density)

CLS 2+1 flavor ensembles: Statistics – area $\propto$ MDU$/\tau_{\rm int}$

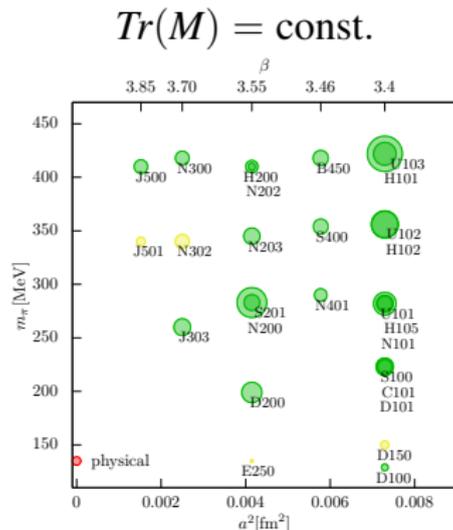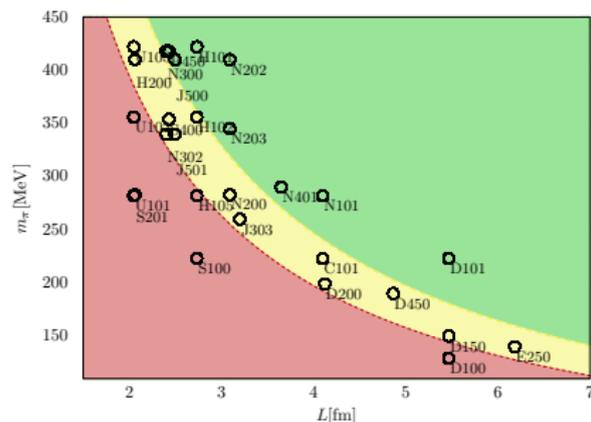Bruno *et al.* JHEP 1502 043 (2015); Bali *et al.* PRD 94 074501 (2016)

plots by Jakob Simeth, RQCD

- > 4000 MDU for many ensembles
  Typically save 1 configuration every 4 MDU
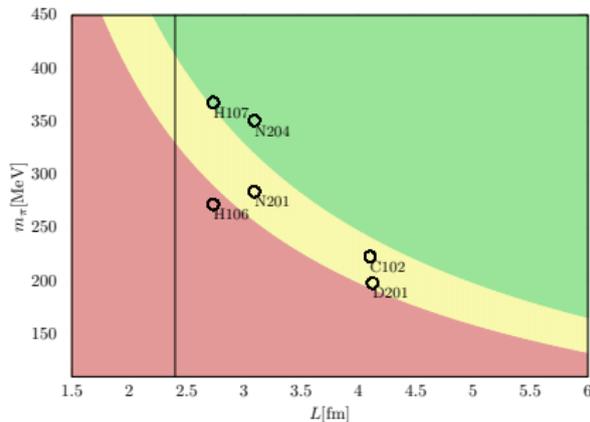- target statistics chosen considering largest τ_{int} (often YM action density)

CLS 2+1 flavor ensembles: Volumes used

$Tr(M) = $ const.

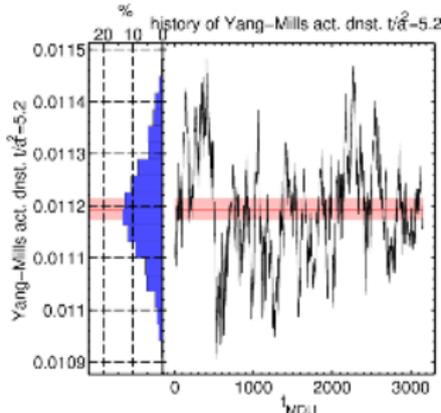$m_s = $ const.

plots by Jakob Simeth, RQCD

- red: $m_\pi L \leq 4$; yellow: $4 \leq m_\pi L \leq 5$; green $5 \leq m_\pi L$
- Most ensembles with $m_\pi L \geq 4$
- Some smaller volumes to check finite size effects

Autocorrelation towards the continuum limit

Action density at t_0 as defined by $t^2 \langle E \rangle = 0.3$
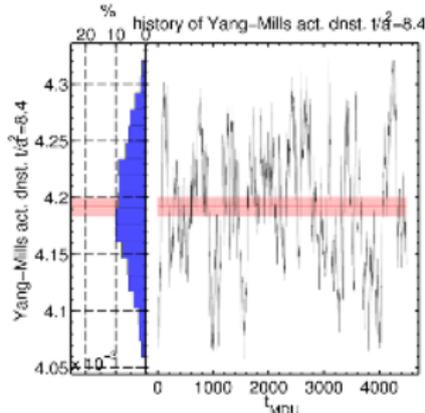
N203	**N302**	**J501**
$a \approx 0.064$fm	$a \approx 0.050$fm	$a \approx 0.039$fm
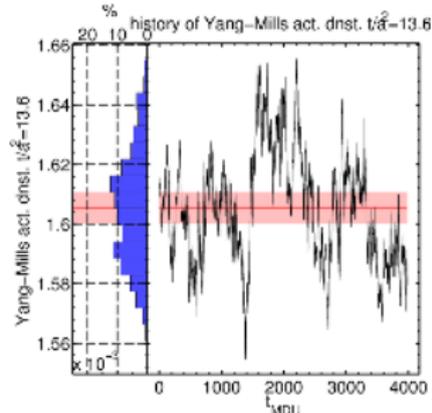
$\tau_{\text{int}} = 60(32)$ MDU $\qquad$ $\tau_{\text{int}} = 49(22)$ MDU $\qquad$ $\tau_{\text{int}} = 150(98)$ MDU

- Autocorrelation time is expected to increase significantly
- Uncertainty is still sizable

Autocorrelation towards physical quark masses

Action density at t_0 as defined by $t^2 \langle E \rangle = 0.3$
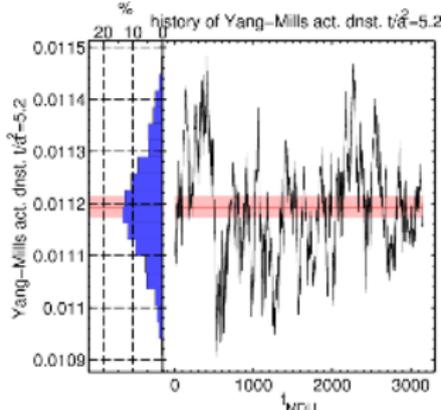
N203
$m_\pi \approx 340$ MeV

N200
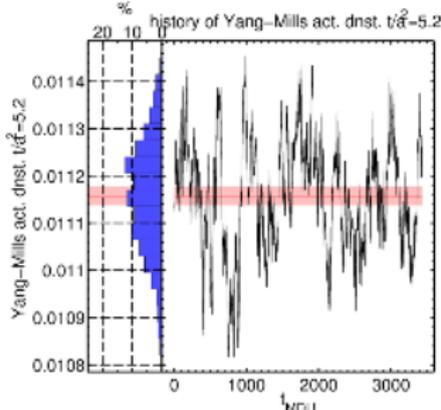$m_\pi \approx 280$ MeV

D200
$m_\pi \approx 200$ MeV

$\tau_{int} = 60(32)$ MDU

$\tau_{int} = 45(21)$ MDU
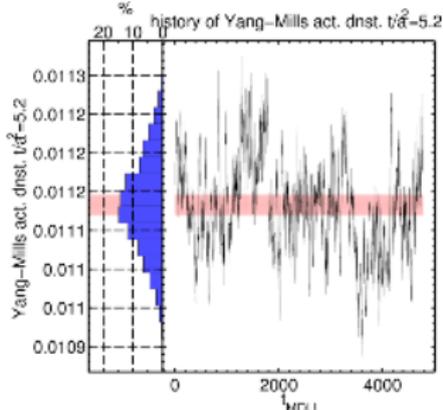
$\tau_{int} = 101(55)$ MDU

- Close to previously estimated $\tau_{exp} = 14(3) \frac{t_0}{a^2}$

Bruno *et al.* JHEP 1502 043 (2015)

"E250" –Description and thermalization strategy

- At this lattice spacing periodic boundary conditions are chosen ($\tau_{\exp}$ not yet completely dominated by topology)
- Physical ud/s run at $\beta = 3.55$ ($a \approx 0.064$ fm)
- To keep $m_\pi L \geq 4$: $L^3 \times T = 96^3 \times 192a^4$
- Thermalization strategy:
  1. Start from an $SU(3)$ run with 3 light quarks and periodic boundary conditions
  2. Perform a number of runs to thermalize this small volume ($L^3 \times T = 48^3 \times 64$)
  3. Triple the time extent $48^3 \times 64 \rightarrow 48^3 \times 192$
  4. Double the spatial extent $48^3 \times 192 \rightarrow 96^3 \times 192$
- "Small volume" runs performed on JUQUEEN; large volume runs on MogonII (Mainz University)
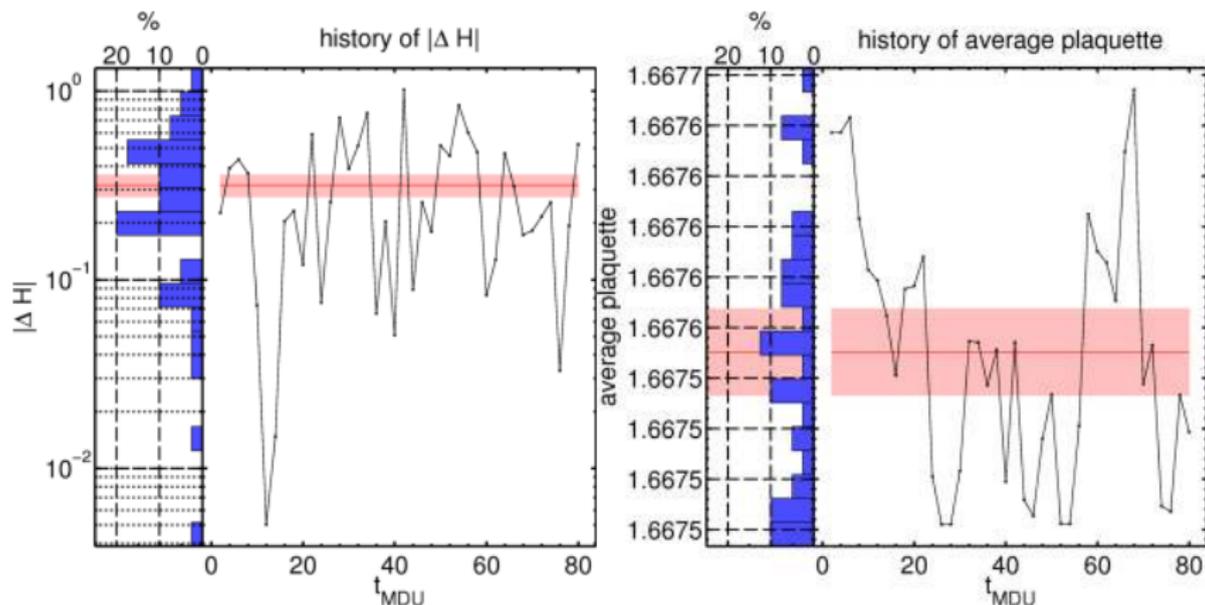
- First stable run – not yet fully thermalized
- Run uses local partition of size 24×8^3 and 692 nodes/ 13824 cores
- Made possible by early usage time on Mogon II

Some tuning: A look at the force norms
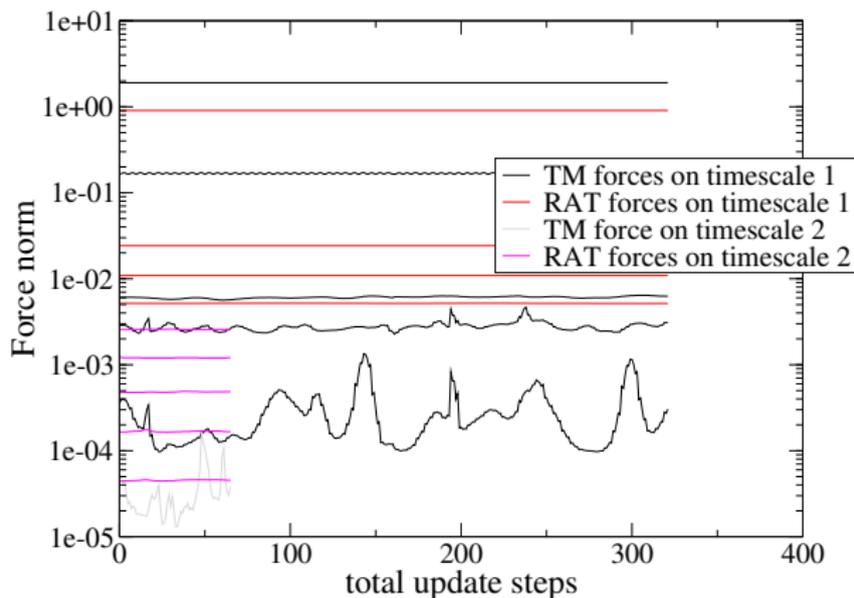
- Force terms for light quarks (black, grey) and strange (red, magenta)
- lvl 0 and lvl 1: 4th order Omelyan integrator;
  lvl 2: 2nd order Omelyan integrator
- lvl 2 forces are updated least often

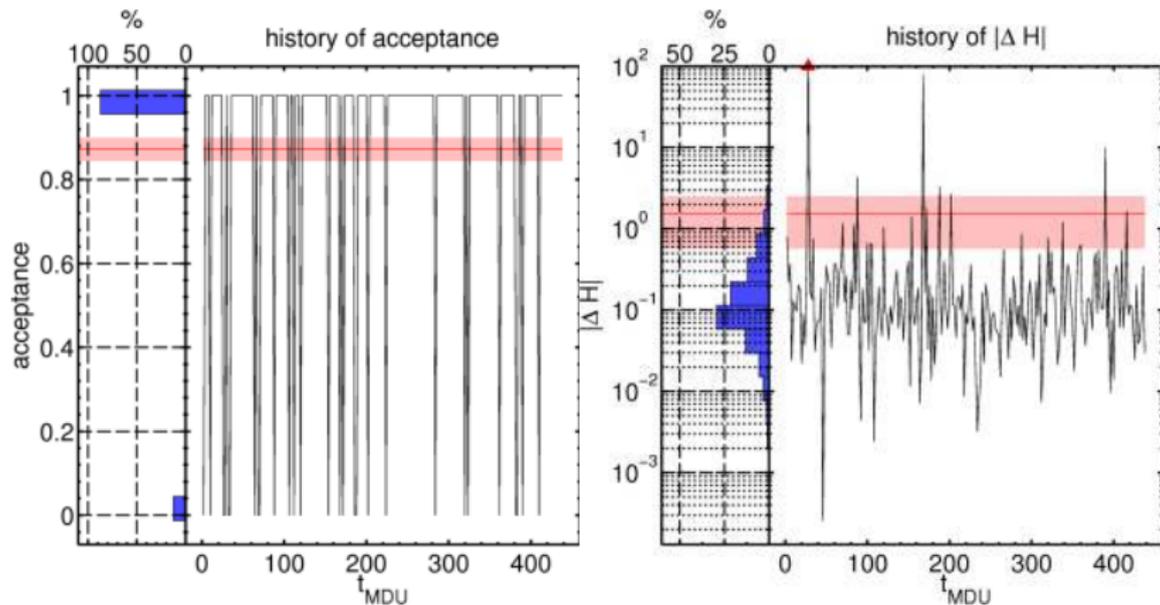# After some initial changes: A look at the norm fluctuations
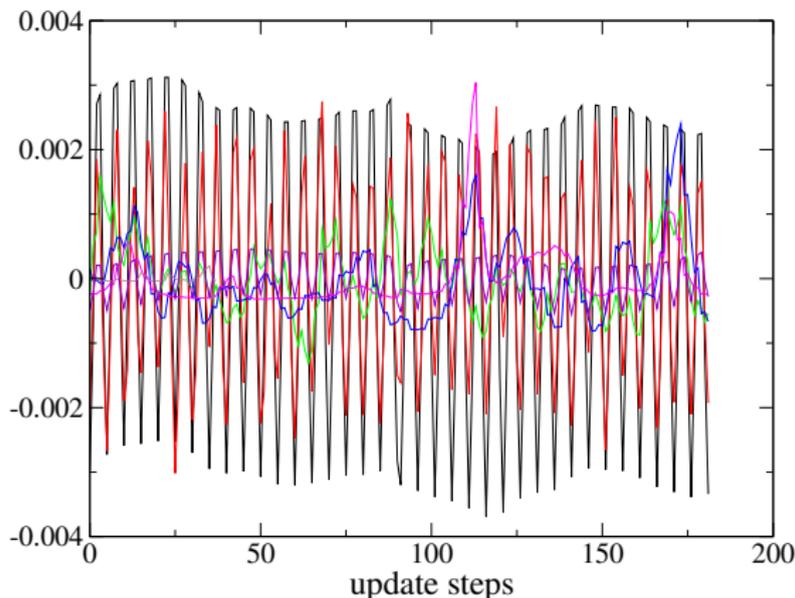
- after various tests
  (rearrangements of forces, further Hasenbusch masses, etc.)
- Observed dH seems largely driven by the force fluctuations

Plots from the current run: dH

Acceptance: 0.872(27)
Shown: 436 MDU, 109 configurations

Plots: average Plaquette & topological charge
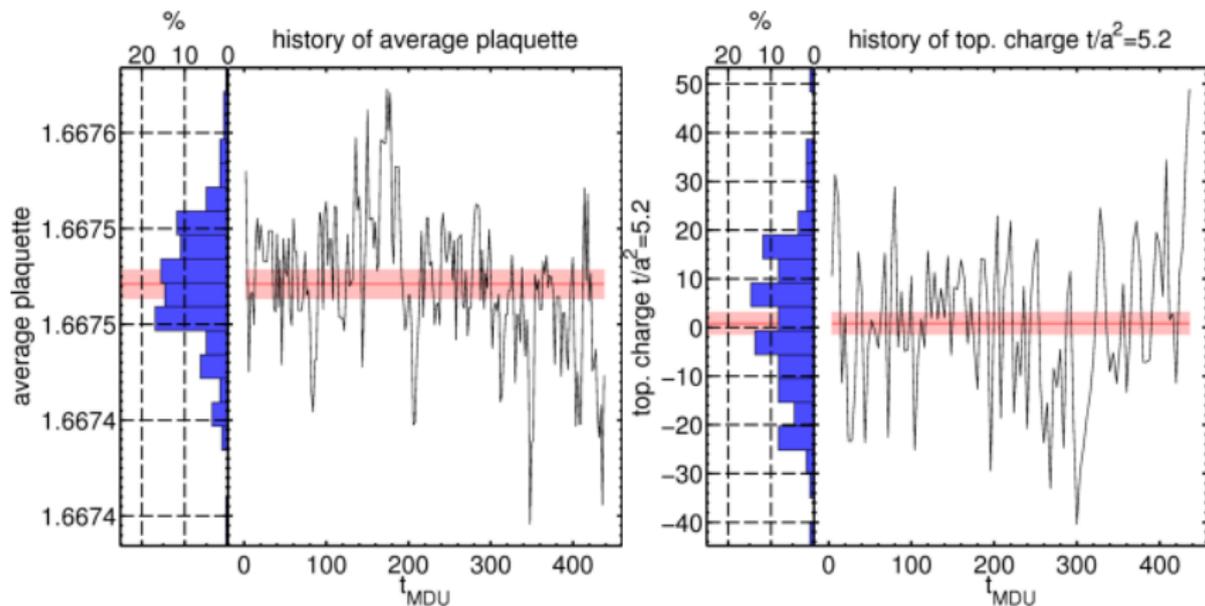
- Proper analysis will need a much longer chain
- Looks very promising

A look at the reweighting factors

RW0: Rational approximation

RW1: Twisted mass reweighting
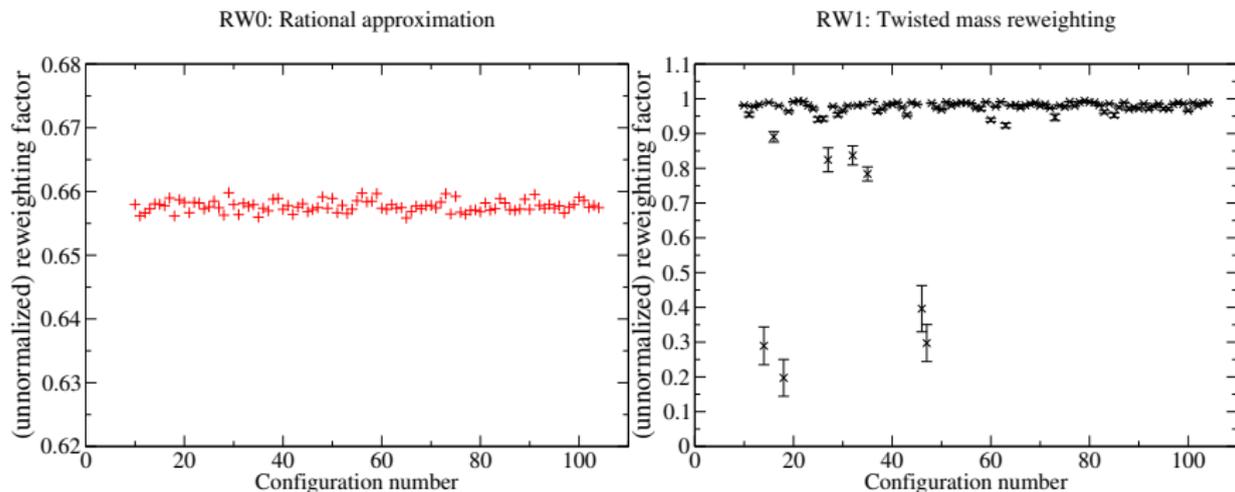
- Twisted mass reweighting estimated with 24 random sources and no intermediate twisted mass parameter μ
- Might have to improve estimate (see also pion)

Pion correlator
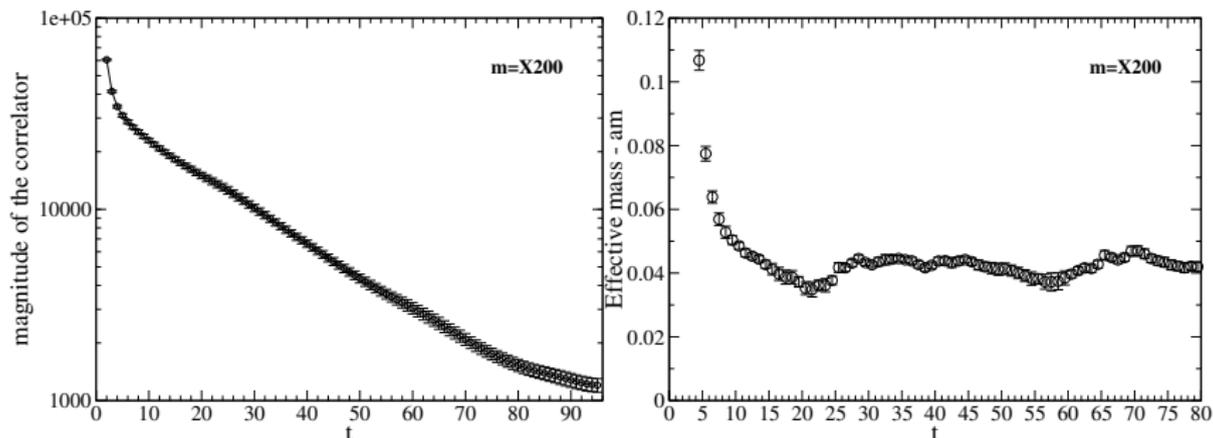
- Results from 70 configs without averaging over (random) source locations
- Larger autocorrelation visible
- Currently results in $m_\pi \approx 130(3)$MeV

Challenges

- Runs with $L^3 \times T = 48^3 \times 64$ proceeded smoothly
- Runs at intermediate volume needed various minor parameter adjustments (more frequent updates of the deflation subspace)
- Runs with $L^3 \times T = 96^3 \times 192$
  - Large deflation blocksize was needed in order to maintain a manageable size of the little Dirac operator
    $\rightarrow$ Iteration counts higher than desirable/ deflation not as efficient
  - Run only stable with large deflation blocksize
    $6^4 \rightarrow 6 \times 4 \times 8^2 \rightarrow 8 \times 4 \times 8^2$
  - Indicates that a multigrid setup with 3 levels might be preferable for this lattice volume (but not obvious that it would pay off)
  - Even larger lattices would likely need further algorithmic improvements
- Fluctuation of twisted mass reweigthing factor larger than desirable?

Conclusions and Outlook

- Large library of CLS 2+1 flavor ensembles

  Bruno *et al.* JHEP 1502 043 (2015)
  Bali *et al.* PRD 94 074501 (2016)

- Many physics studies started (and a number close to publication)

- Stable run at (very close to) physical m_l, m_s with $a \approx 0.064$ fm

- Not enough statistics for a detailed study of autocorrelation, pion masses, nucleon masses, decay constants, . . .

- might profit from a 3 level multigrid setup at the current lattice volume

- Physical light-quark mass run will be crucial to reduce systematic uncertainties (examples focus on Mainz projects)

  - Hadronic vacuum polarization contribution to a_μ
  - Baryon structure calculations
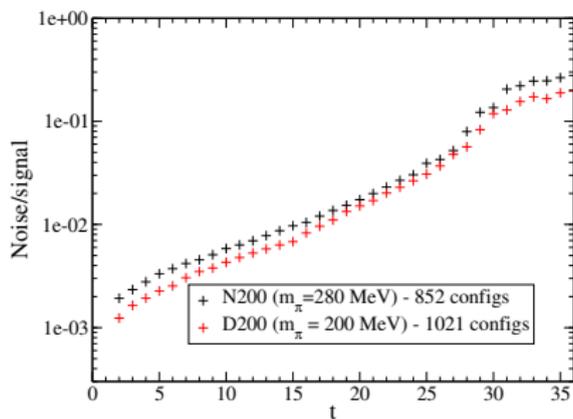 - Scale setting

...

Thank you!

Nucleon effective masses
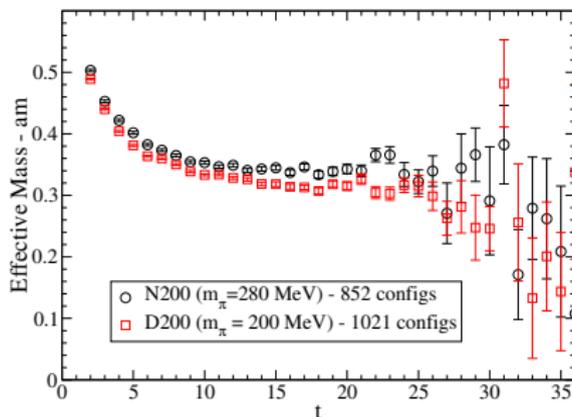
Data from Tim Harris, Konstantin Ottnad, Mainz

Setup

- All-mode-averaging (AMA)
  12 ($n_c \times n_D$) exact inversions and 16×12 sloppy inversions
- Results from sources in a single timeslice
- Effective mass from the local-smeared correlator

Nucleon noise/signal

Data from Tim Harris, Konstantin Ottnad, Mainz

- Slope in (most of) plateau region does not reach asymptotic value (given by $m_N - \frac{3}{2}m_\pi$)
- Suggests that in practice noise/signal scaling is not as severe
- Exponential growth qualitatively observed