(Towards) CLS simulations at physical pion mass

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Representing the CLS effort
With plots from Hubert Simma, Jakob Simeth

Outline

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1. Introduction - The CLS 2+1 flavor ensembles
    - The CLS 2+1 flavor ensembles – Key features
    - Landscape of CLS ensembles
2. Towards the physical point
    - Autocorrelation times towards the physical point
    - Statistical uncertainty towards physical light-quark masses
3. Simulations and challenges: “X200”
    - Thermalization strategy
    - Current status
4. Conclusions and Outlook

Coordinated Lattice Simulations – Members

- Berlin (NIC/DESY-Zeuthen/HU Berlin)
- CERN
- Mainz
- Madrid
- Münster
- Odense/ CP3-Origins
- Regensburg
- Rome (Roma I, Roma II)
- Wuppertal

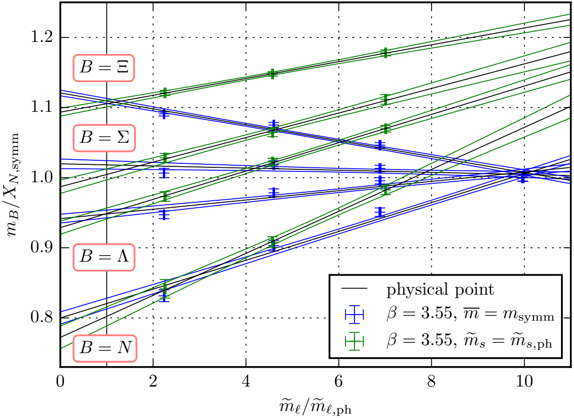
The CLS 2+1 flavor ensembles – Key features

- 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

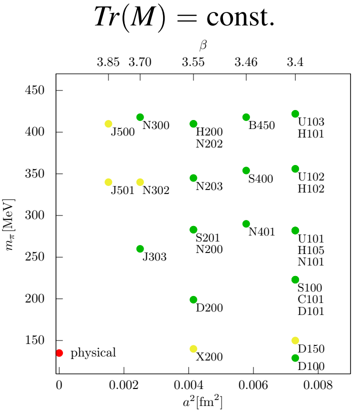
Baryon masses: trajectory with fixed $Tr(M)$ vs. $m_s = \text{const.}$

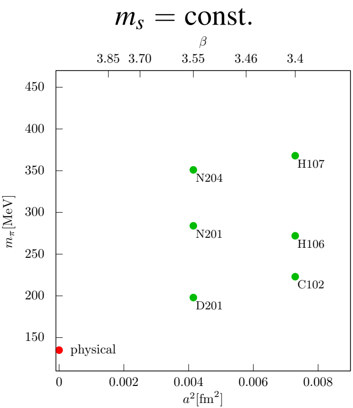


`plot from Bali et al. RQCD, arXiv:1702.01035`

- Example of octet baryon masses at $a \approx 0.064$ fm (from RQCD)
- Illustrates typical behavior

CLS 2+1 flavor ensembles: Overview

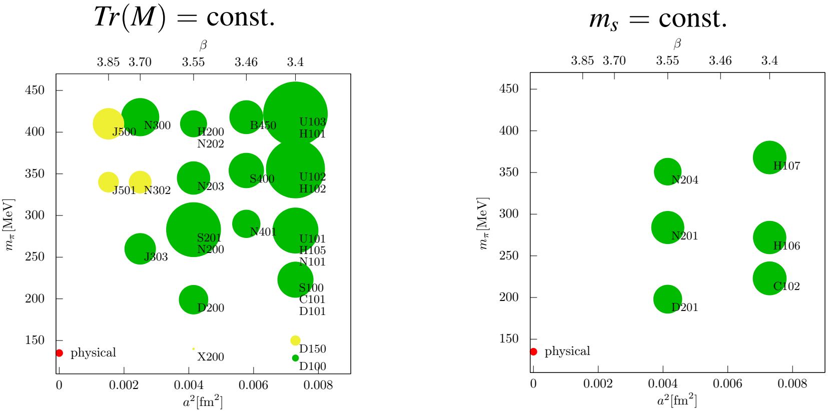




`plots by Jakob Simeth, RQCD`

- 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



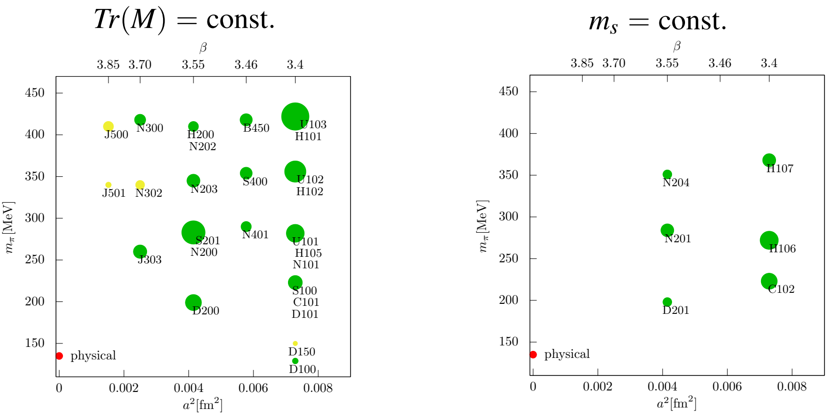
$Tr(M) = \text{const.}$

$m_s = \text{const.}$

plots by Jakob Simeth, RQCD

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

CLS 2+1 flavor ensembles: Statistics



$Tr(M) = \text{const.}$

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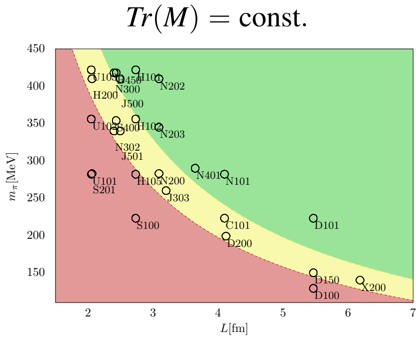
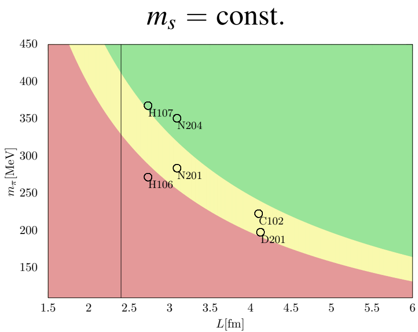
plots by Jakob Simeth, RQCD

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

CLS 2+1 flavor ensembles: Volumes used



$Tr(M) = \text{const.}$



$m_s = \text{const.}$

`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

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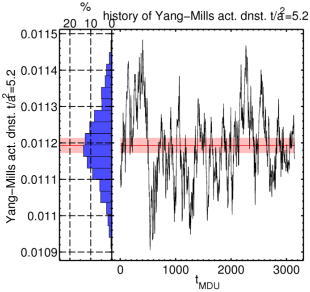
Autocorrelation towards the continuum limit

Action density at t_0 as defined by $t^2\langle E\rangle = 0.3$

N203

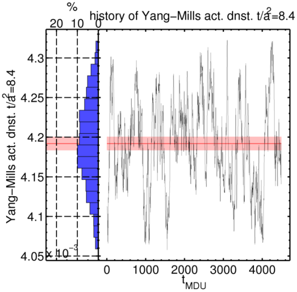
$a \approx 0.064\text{fm}$



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

N302

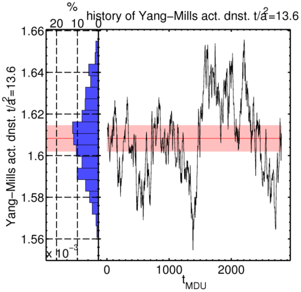
$a \approx 0.050\text{fm}$



$\tau_{\text{int}} = 49(22)$ MDU

J501

$a \approx 0.039\text{fm}$



$\tau_{\text{int}} = 138(95)$ MDU

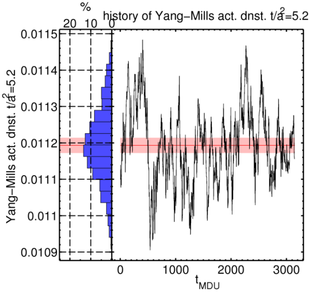
- Autocorrelation time is expected to increase significantly
- Uncertainty is still sizable

Autocorrelation towards physical quark masses

Action density at t_0 as defined by $t^2\langle E\rangle = 0.3$

N203

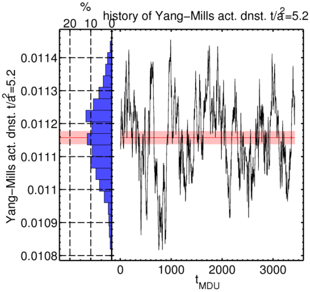
$m_\pi \approx 340$ MeV



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

N200

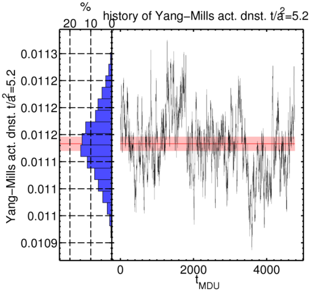
$m_\pi \approx 280$ MeV



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

D200

$m_\pi \approx 200$ MeV



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

Noise/Signal at light quark masses – Introduction

- For the nucleon we have (argument by Parisi, Lepage)

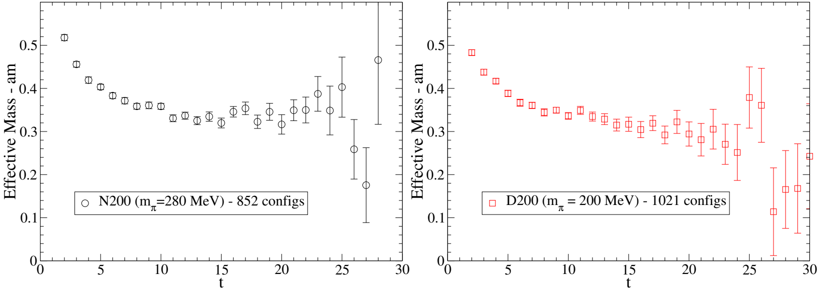
$$\begin{aligned} N\sigma^2_{N,\mathbf{p}=0} &= \left\langle C_N(\mathbf{p}=0,t;m)^2 \right\rangle - \left\langle C_N(\mathbf{p}=0,t;m)\right\rangle^2 \\ &\propto Z_{3\pi}\mathrm{e}^{-3m_\pi t} + Z_N^2\mathrm{e}^{-2m_N t} \end{aligned}$$

- The noise to signal ratio therefore degrades exponentially

$$\frac{\sigma_N(t)}{\langle C_N(t)\rangle} \simeq \frac{1}{\sqrt{N}}\mathrm{e}^{\left(m_N-\frac{3}{2}m_\pi\right)t}$$

- Similar argument for Nuclei, heavy mesons, *etc.*

Nucleon effective masses

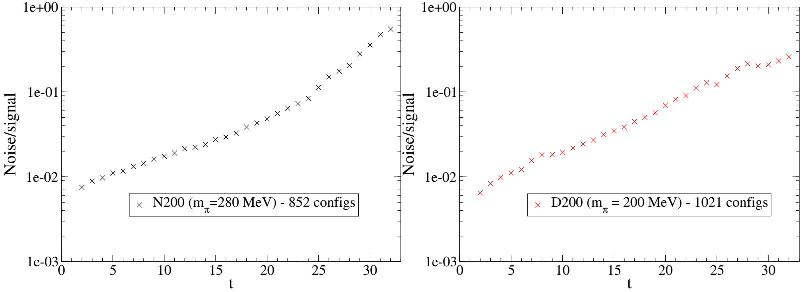


`Data from Tim Harris, Konstantin Ottnad, Mainz`

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

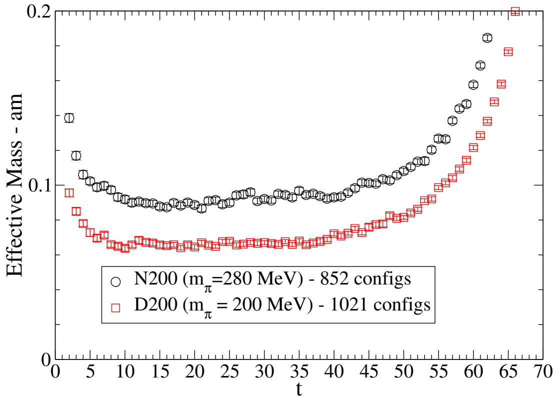
Nucleon noise/signal



`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

Pion effective masses



- Strong effects from open boundary visible
- These are well understood
- There are plenty of usable timeslices
- Note: Thermal effects (with periodic bc) can also be a nuisance

Pion decay constant

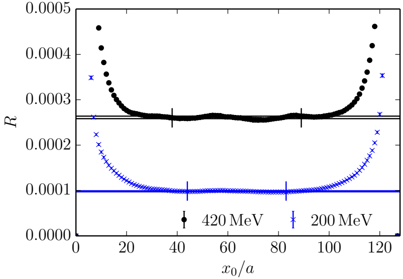
`Results from Bruno, Korzec, Schaefer, arXiv:1608.08900`

$\beta = 3.40; a \approx 0.087$

Ensemble	#configs	m_π [MeV]	af_π
H101	2016	420	0.06351(34)
H102	2005	350	0.06057(34)
H105	2708	280	0.05723(57)
C101	1234	220	0.05561(40)

$\beta = 3.55; a \approx 0.064$

Ensemble	#configs	m_π [MeV]	af_π
N202	579	420	0.04829(20)
N203	1543	340	0.04632(17)
N200	1712	280	0.04422(18)
D200	1191	200	0.04233(16)

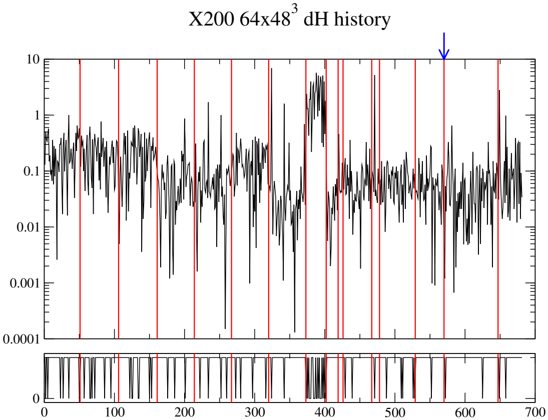


Outline

“X200” –Description and thermalization strategy

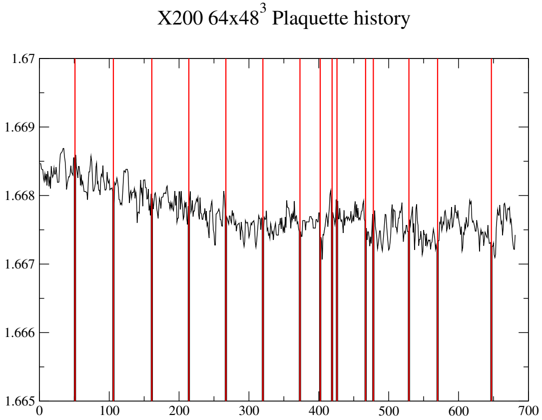
- Physical ud/s run at $\beta = 3.55$ ($a \approx 0.064$ fm)
- To keep $m_\pi L \geq 4$: $L^3 \times T = 96^3 \times 192$
- Thermalization strategy:
  1. Start from an $SU(3)$ run with 3 light quarks and periodic boundary conditions
  2. Perform a number of runs to thermalize this small volume ($L^3 \times T = 48^3 \times 64$)
  3. Triple the time extent $48^3 \times 64 \to 48^3 \times 192$
  4. Double the spatial extent $48^3 \times 192 \to 96^3 \times 192$
- At this fairly coarse lattice spacing periodic boundary conditions are chosen

Small volume run - dH history



Acceptance history for the thermalization of a small volume physical quark mass run. The vertical red lines indicate changes of run parameters. The arrow indicates where the target quark masses have been reached.

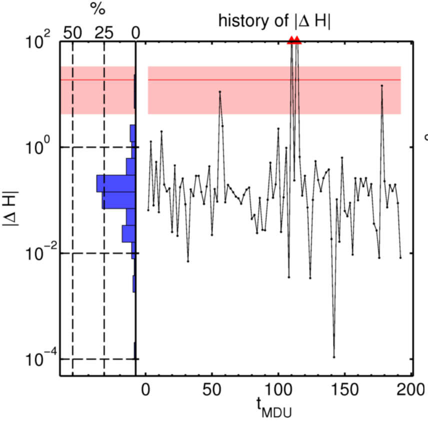
Small volume run - Plaquette history

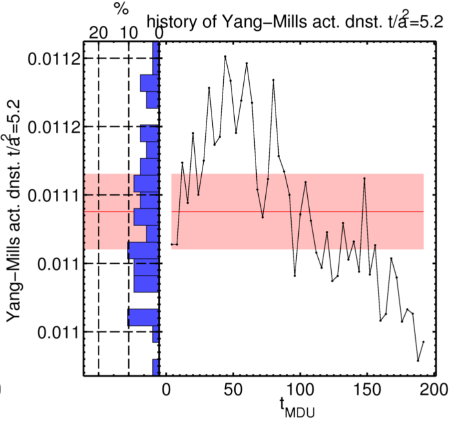


Plaquette history for the thermalization of a small volume physical quark mass run.

- Overall no significant difficulty in (partially) thermalizing the small volume

Intermediate run of size $L^3 \times T = 48^3 \times 192$

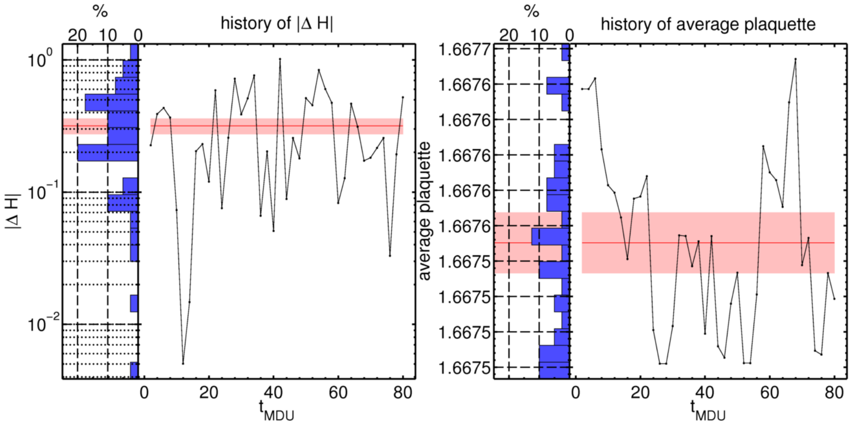




Challenges

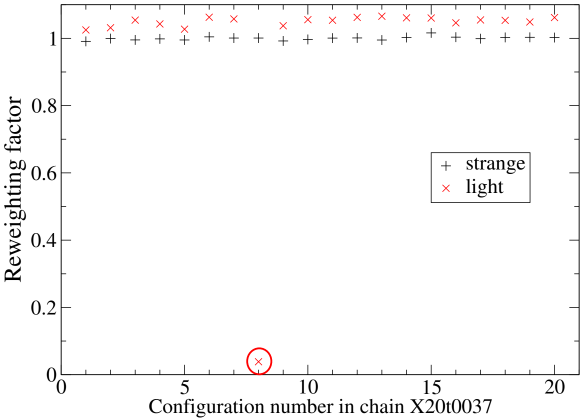
- Runs with $L^3 \times T = 48^3 \times 64$ proceeded smoothly
- Runs at intermediate volume needed various minor parameter adjustments (more frequent updates of the deflation subspace)
- Runs with $L^3 \times T = 96^3 \times 192$
  - Run only stable with large deflation blocksize $6^4 \rightarrow 6 \times 4 \times 8^2 \rightarrow 8 \times 4 \times 8^2$
  - Large deflation blocksize was needed in order to maintain a manageable size of the little Dirac operator → Iteration counts higher than desirable/ deflation not as efficient
  - 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

JUQUEEN → Cluster MOGON II (JGU Mainz)



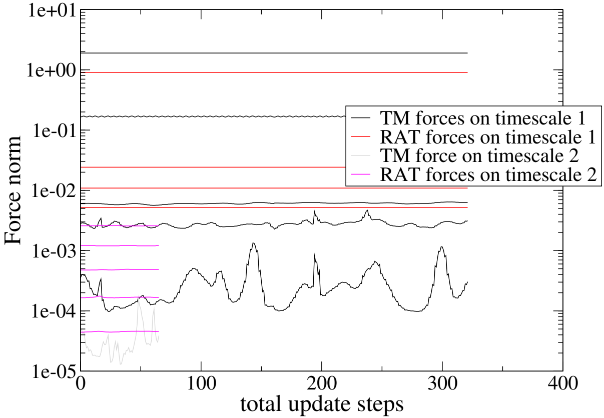
- First stable run – not yet fully thermalized
- Run uses local partition of size 24×8^3 and 692 nodes/ 13824 cores
- Made possible by early usage time on Mogon II

JUQUEEN → Cluster MOGON II (JGU Mainz)



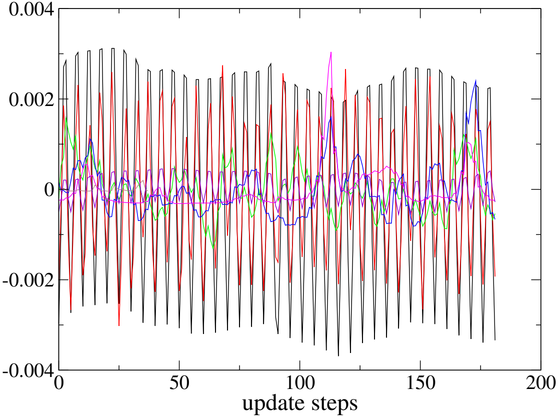
- Reweighting factors for first stable run; mostly small fluctuations

Further improvements: A look at the force norms



- integrators: lvl0 and lvl1: 4th order Omelyan integrator; lvl2: 2nd order Omelyan integrator
- lvl 2 forces are updated less often
- Lead to a slight adjustment in Hasenbusch masses

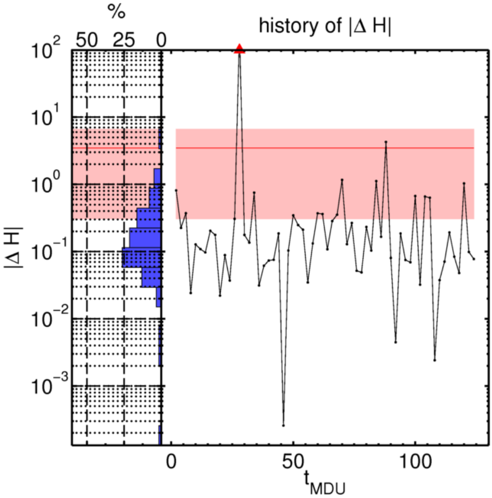
After some initial changes: A look at the norm fluctuations



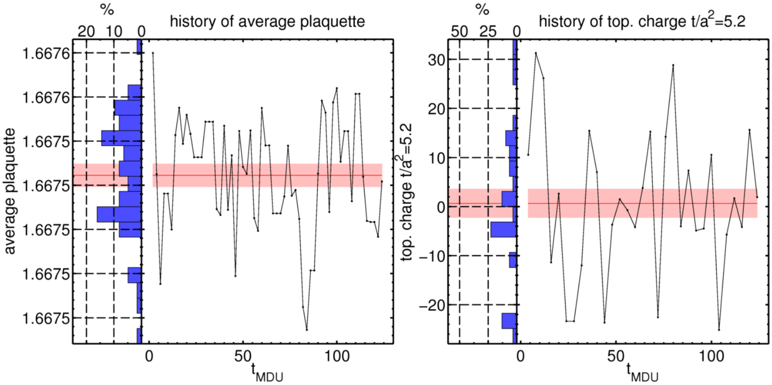
- after various tests
  (rearrangements of forces, further Hasenbusch masses, etc.)
- It seems that observed dH is largely driven by the force fluctuations

Plots from the current run: dH

Acceptance: 0.790(53)
Shown:
124 MDU, 31 configurations
Completed (as of today):
188 MDU, 47 configurations



Plots: average Plaquette & topological charge



- Proper analysis will need a much longer chain
- Looks very promising

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Conclusions and Outlook

- Large library of CLS 2+1 flavor ensembles
- 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 already profit from a lvl3 multigrid setup at the current lattice volume

. . .

Thank you!