Scale setting on the (2+1+1)-flavor HISQ ensembles: current status

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Hadron physics and heavy quarks on the lattice,
Trinity College, Dublin, June 4 — 7, 2024

Outline

- FLAG: gradient flow scales
- HISQ: action, ensembles
- Taste-breaking effects
- The gradient flow: definitions, corrections, integration
- Relative scale and the integrated autocorrelation time
- Absolute scale: a few examples — w_0/r_1, $w_0 f_\pi$, $w_0 M_\Omega$
- Conclusion

FLAG 2023 update: gradient flow scales

Collaboration	Ref.	N_f	publication status	chiral extrapolation	continuum extrapolation	finite volume	physical scale	$\sqrt{t_0}$ [fm]	w_0 [fm]
ETM 21	[43]	2+1+1	A	★	★	★	f_π	0.14436(61)	0.17383(63)
CalLat 20A	[115]	2+1+1	A	★	★	★	m_Ω	0.1422(14)	0.1709(11)
BMW 20	[119]	1+1+1+1	A	★	★	★	m_Ω		0.17236(29)(63)[70]
ETM 20	[1057]	2+1+1	C	★	★	★	f_π		0.1706(18)
MILC 15	[116]	2+1+1	A	★	★	★	$F_{p4s}(f_\pi)^\#$	0.1416(+8/-5)	0.1714(+15/-12)
HPQCD 13A	[40]	2+1+1	A	★	○	★	f_π	0.1420(8)	0.1715(9)
RQCD 22	[1058]	2+1	P	★	★	★	m_Ξ	0.1449(+7/-9)	
CLS 21	[1059]	2+1	C	★	★	★	f_π, f_K	0.1443(7)(13)	
CLS 16	[117]	2+1	A	○	★	★	f_π, f_K	0.1467(14)(7)	
QCDSF/UKQCD 15B	[718]	2+1	P	○	○	○	$m_P^{SU(3)}$	0.1511(22)(6)(5)(3)	0.1808(23)(5)(6)(4)
RBC/UKQCD 14B	[10]	2+1	A	★	★	★	m_Ω	0.14389(81)	0.17250(91)
HotQCD 14	[120]	2+1	A	★	★	★	$r_1(f_\pi)^\#$		0.1749(14)
BMW 12A	[118]	2+1	A	★	★	★	m_Ω	0.1465(21)(13)	0.1755(18)(4)

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Lattice action

- One-loop Symanzik tadpole-improved gauge action.

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- RHMC updating, on the finest ensembles — RHMD

  Kennedy, Horvath, Sint, heplat/9809092

  Clark, Kennedy, hep-lat/0608015

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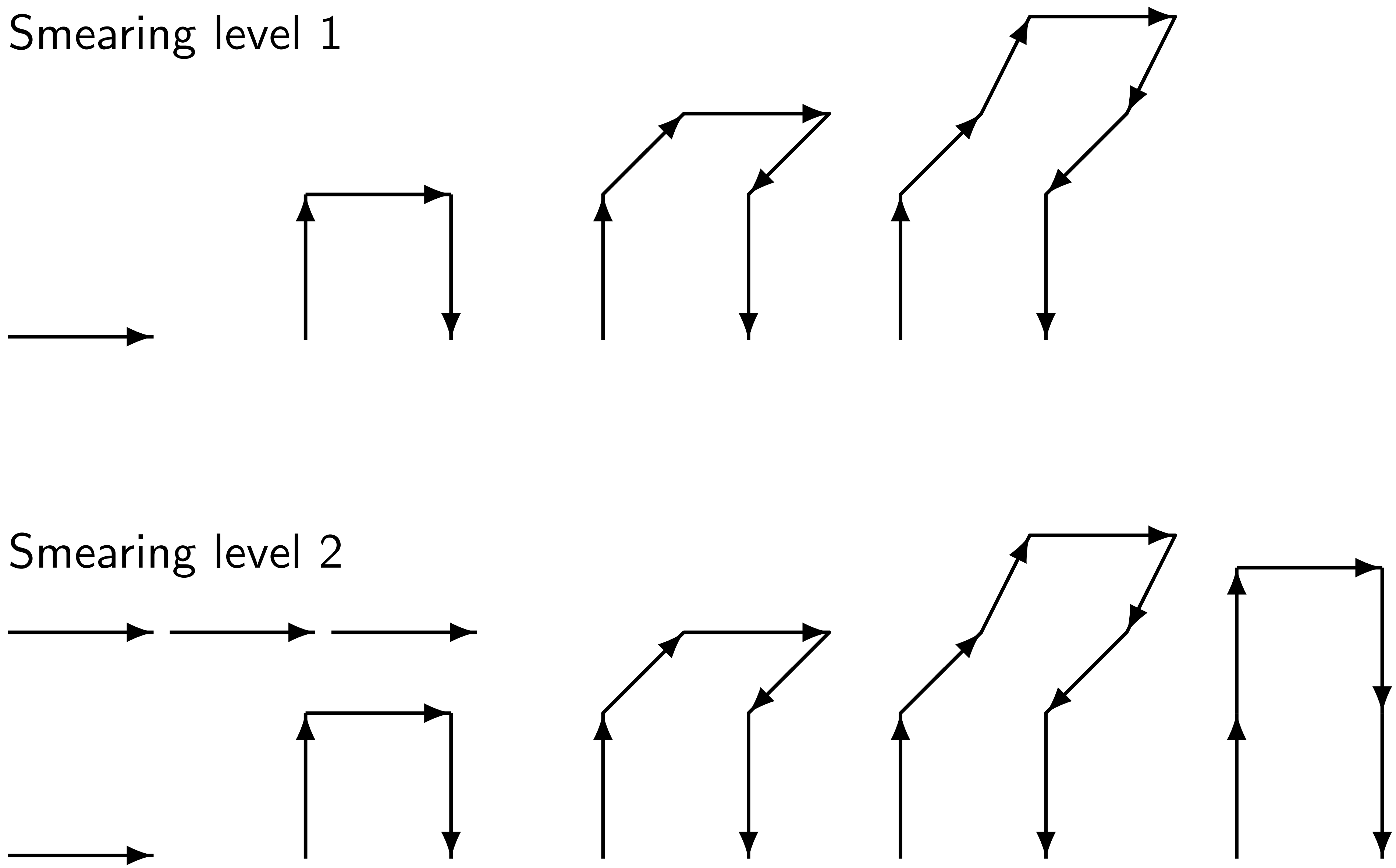
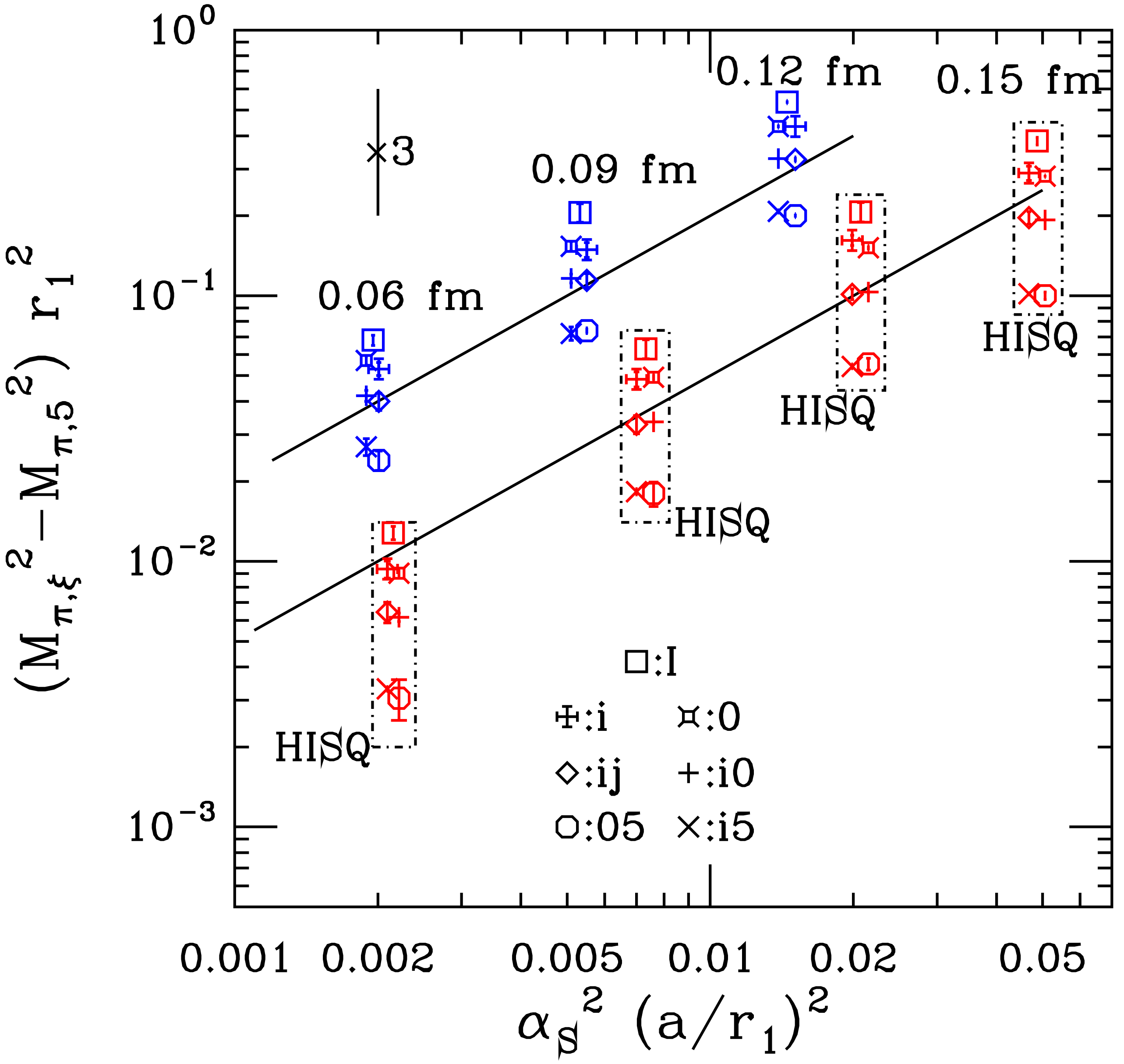


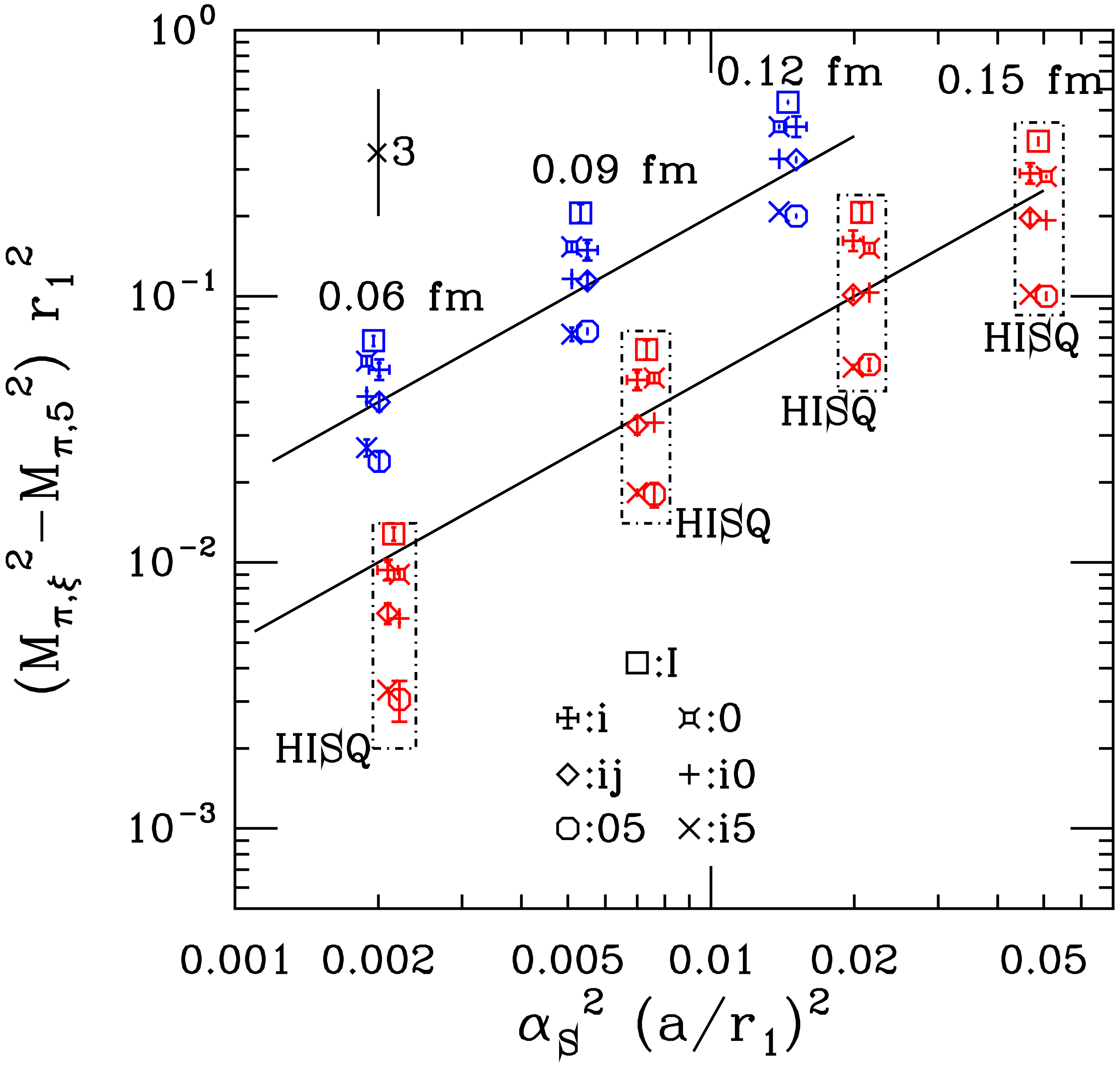
Pion mass taste splittings

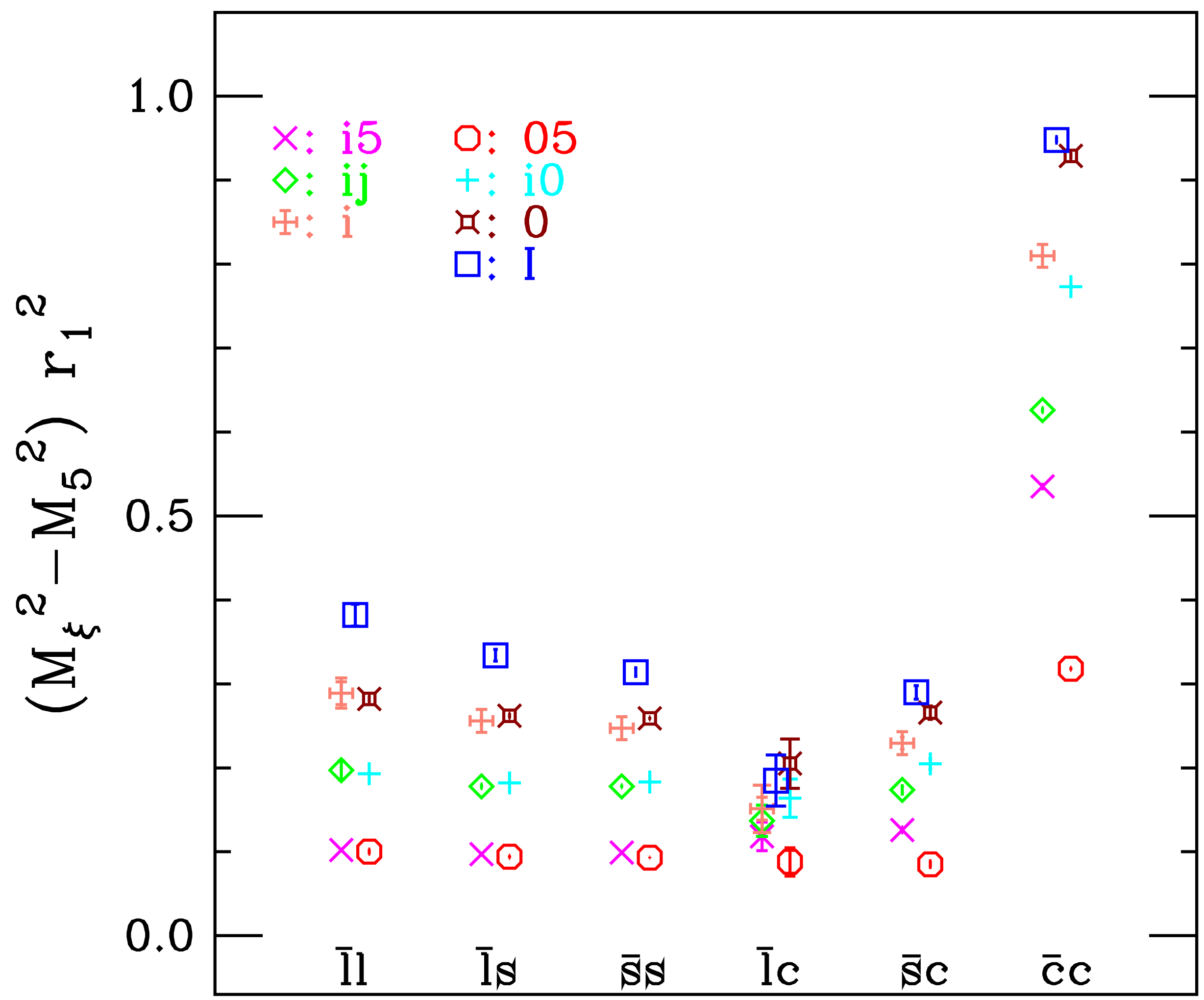


MILC, 1212.4768

- HISQ vs asqtad pion taste splittings (left).

Pion mass taste splittings





MILC, 1212.4768

- HISQ vs asqtad pion taste splittings (left).
- Splitting pattern for different quark masses (right).

MILC HISQ ensembles

$\approx a$ (fm)	Key	β	am'_l	am'_s	am'_c	$(L/a)^3\times(T/a)$	L (fm)	M_π (MeV)	$M_\pi L$	$N_{\rm conf}$
0.15	$m_s/5$	5.80	0.013	0.065	0.838	$16^3\times48$	2.45	305	3.8	1020
0.15	$m_s/10$	5.80	0.0064	0.064	0.828	$24^3\times48$	3.67	214	4.0	1000
0.15	physical	5.80	0.00235	0.0647	0.831	$32^3\times48$	4.89	131	3.3	1000
0.12	$m_s/5$	6.00	0.0102	0.0509	0.635	$24^3\times64$	2.93	305	4.5	1040
0.12	unphysA	6.00	0.0102	$0.03054^\dagger$	0.635	$24^3\times64$	2.93	304	4.5	1020
0.12	small	6.00	0.00507	0.0507	0.628	$24^3\times64$	2.93	218	3.2	1020
0.12	$m_s/10$	6.00	0.00507	0.0507	0.628	$32^3\times64$	3.91	217	4.3	1000
0.12	large	6.00	0.00507	0.0507	0.628	$40^3\times64$	4.89	216	5.4	1028
0.12	unphysB	6.00	0.01275	$0.01275^\dagger$	0.640	$24^3\times64$	2.93	337	5.0	1020
0.12	unphysC	6.00	0.00507	$0.0304^\dagger$	0.628	$32^3\times64$	3.91	215	4.3	1020
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0.12	unphysE	6.00	0.00507	$0.012675^\dagger$	0.628	$32^3\times64$	3.91	214	4.2	1020
0.12	unphysF	6.00	0.00507	$0.00507^\dagger$	0.628	$32^3\times64$	3.91	213	4.2	1020
0.12	unphysG	6.00	0.0088725	$0.022815^\dagger$	0.628	$32^3\times64$	3.91	282	5.6	1020
0.12	physical	6.00	0.00184	0.0507	0.628	$48^3\times64$	5.87	132	3.9	999
0.09	$m_s/5$	6.30	0.0074	0.037	0.440	$32^3\times96$	2.81	316	4.5	1005
0.09	$m_s/10$	6.30	0.00363	0.0363	0.430	$48^3\times96$	4.22	221	4.7	999
0.09	physical	6.30	0.0012	0.0363	0.432	$64^3\times96$	5.62	129	3.7	484

Table from FNAL-MILC-TUMQCD, 1712.09262

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MILC HISQ ensembles

'2015
'2020

0.06	$m_s/5$	6.72	0.0048	0.024	0.286	$48^3 \times 144$	2.72	329	4.5	1016
0.06	$m_s/10$	6.72	0.0024	0.024	0.286	$64^3 \times 144$	3.62	234	4.3	572
0.06	physical	6.72	0.0008	0.022	0.260	$96^3 \times 192$	5.44	135	3.7	842
0.042	$m_s/5$	7.00	0.00316	0.0158	0.188	$64^3 \times 192$	2.73	315	4.3	1167
0.042	physical	7.00	0.000569	0.01555	0.1827	$144^3 \times 288$	6.13	134	4.2	420
0.03	$m_s/5$	7.28	0.00223	0.01115	0.1316	$96^3 \times 288$	3.09	309	4.8	724

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  - Retuned physical m_l/m_s at $a = 0.15$, 0.12 and 0.09 (CalLat) fm with larger statistics.
    CalLat, 2011.12166
  - Larger volume $128^3 \times 96$ at physical m_l/m_s $a = 0.09$ fm.
  - 6 ensembles at $a = 0.06$ and 0.09 fm with lighter-than-physical strange quark mass.

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The gradient flow

- Smoothing of the original gauge field $U_{x,\mu}$ towards stationary points of the action S^f:

Lüscher, 1006.4518

$$\frac{dV_{x,\mu}}{dt} = -\left\{\partial_{x,\mu} S^f(t)\right\} V_{x,\mu}, \quad V_{x,\mu}(t=0) = U_{x,\mu},$$

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- Scale setting:

Lüscher, 1006.4518 Borsanyi et al., 1203.4469

$$t^2 \langle S^o(t) \rangle \Big|_{t=t_0} = Const \quad \text{or} \quad \left[t \frac{d}{dt} t^2 \langle S^o(t) \rangle \right]_{t=w_0^2} = Const,$$

where the observable $S^o = S_{clover}$ or S_{Wilson} or $S_{Symanzik}$.

- In practice $Const = 0.3$.

Integration of the flow

- The flow equation evolves $V_{x,\mu}$ on a manifold

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- Two approaches for constructing Runge-Kutta manifold integrators:
  - with commutators, Munthe-Kaas, Appl. Num. Math. (1999)
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- Luscher's (3,3) (i.e. 3-stage 3-order) method is a member of a new class based on classical (!), so called, 2N-storage Runge-Kutta integrators. Bazavov, 2007.04225 Bazavov, Chuna, 2101.05320

Integration of the flow

- We use (6,4) 2N-storage method. Berland, Bogey, Bailly, Computers and Fluids (2006)
- For all ensembles we integrate the flow at two step sizes $\Delta t = 1/20$, $1/40$ to fully control the global integration error.

The gradient flow

- For a given combination of the dynamical action, flow action and the observable the leading discretization effects can be canceled at tree level:

$$t^2 S(t) \quad \rightarrow \quad t^2 S_{corr}(t) = \frac{t^2 S(t)}{1 + \sum_{m=1}^{4} C_m (a^{2m}/t^m)}$$

Fodor et al, 1406.0827

- Expansion in a^2/t

$$\langle t^2 S(t) \rangle_a = \frac{3(N^2-1)g_0^2}{128\pi^2}(C(a^2/t) + O(g_0^2))$$

The gradient flow

	SWS	WWC	SSS	SWW	WSW	WSC
C_2	1/72	-1/24	-1/24	-1/24	5/72	-7/72
C_4	7/320	-1/512	1/32	1/32	23/1280	19/2560
C_6	-8539/1935360	-1/5120	-283/27648	-283/27648	2077/483840	-2237/1935360
C_8	76819/18579456	-1/65536	3229/442368	3229/442368	16049/9289728	14419/74317824
	SSW	WWW	WSS	WWS	SWC	SSC
C_2	-7/72	1/8	1/8	13/72	-5/24	-19/72
C_4	35/768	3/128	3/128	13/384	167/2560	145/1536
C_6	-5131/276480	13/2048	13/2048	277/30720	-58033/1935360	-12871/276480
C_8	10957/884736	77/32768	77/32768	323/98304	457033/24772608	52967/1769472

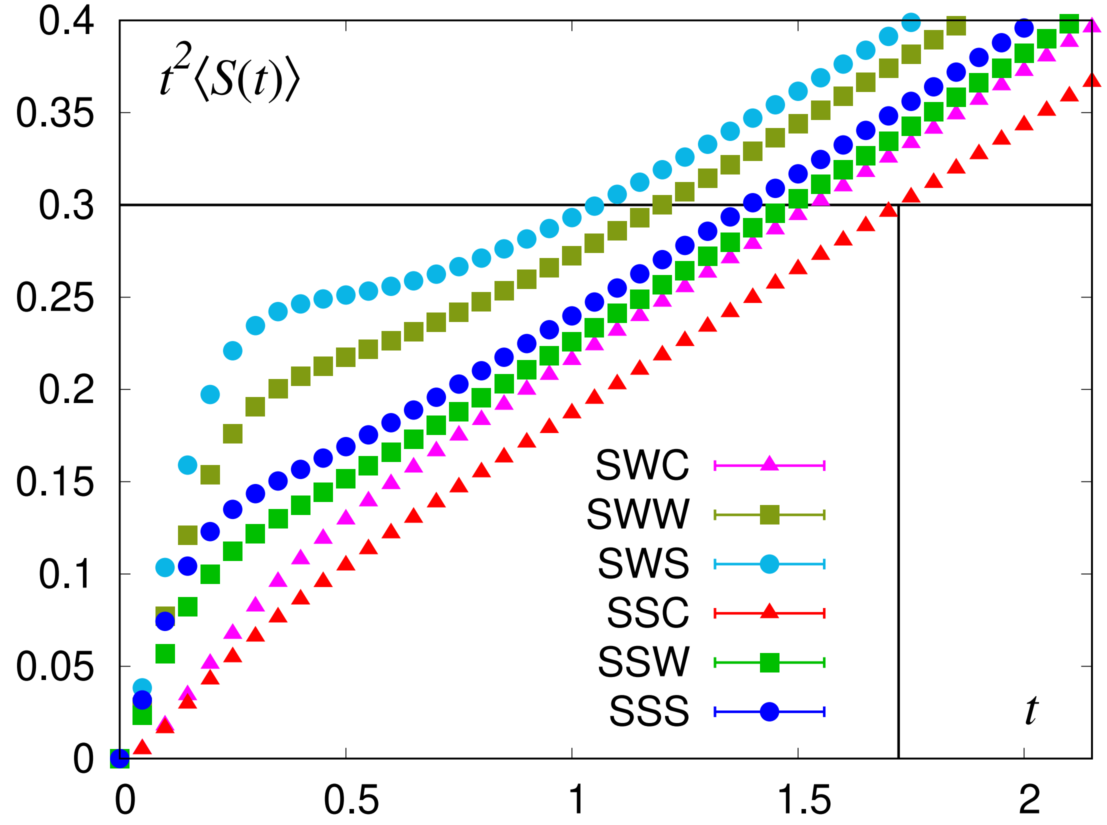
The gradient flow

	SWS	WWC	SSS	SWW	WSW	WSC
C_2	1/72	-1/24	-1/24	-1/24	5/72	-7/72
C_4	7/320	-1/512	1/32	1/32	23/1280	19/2560
C_6	-8539/1935360	-1/5120	-283/27648	-283/27648	2077/483840	-2237/1935360
C_8	76819/18579456	-1/65536	3229/442368	3229/442368	16049/9289728	14419/74317824

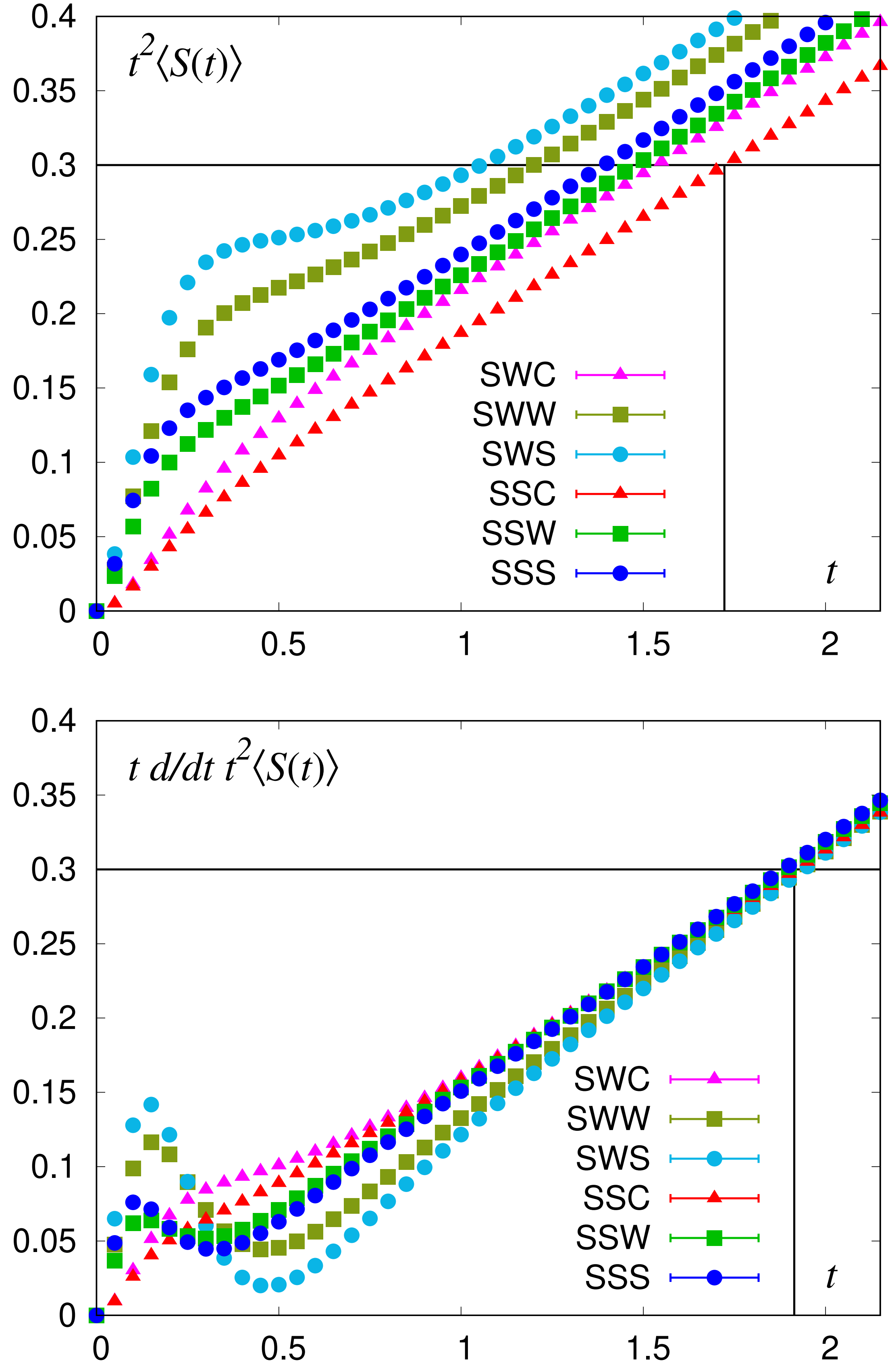
	SSW	WWW	WSS	WWS	SWC	SSC
C_2	-7/72	1/8	1/8	13/72	-5/24	-19/72
C_4	35/768	3/128	3/128	13/384	167/2560	145/1536
C_6	-5131/276480	13/2048	13/2048	277/30720	-58033/1935360	-12871/276480
C_8	10957/884736	77/32768	77/32768	323/98304	457033/24772608	52967/1769472

- Corrections for the relevant gauge-flow-observable combinations that we measure.

Action density vs flow time, $a = 0.12$ fm



Action density vs flow time, $a = 0.12$ fm



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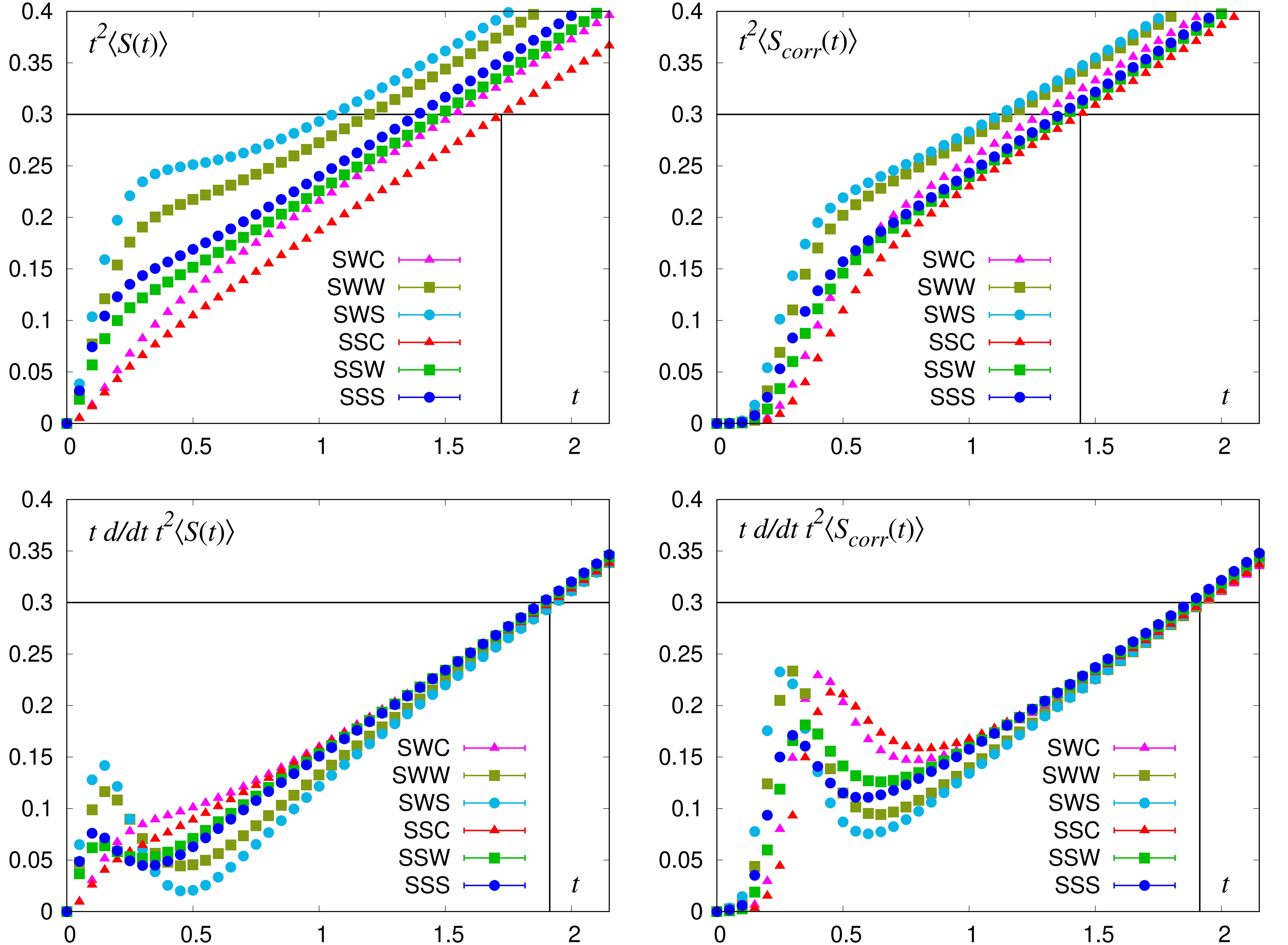
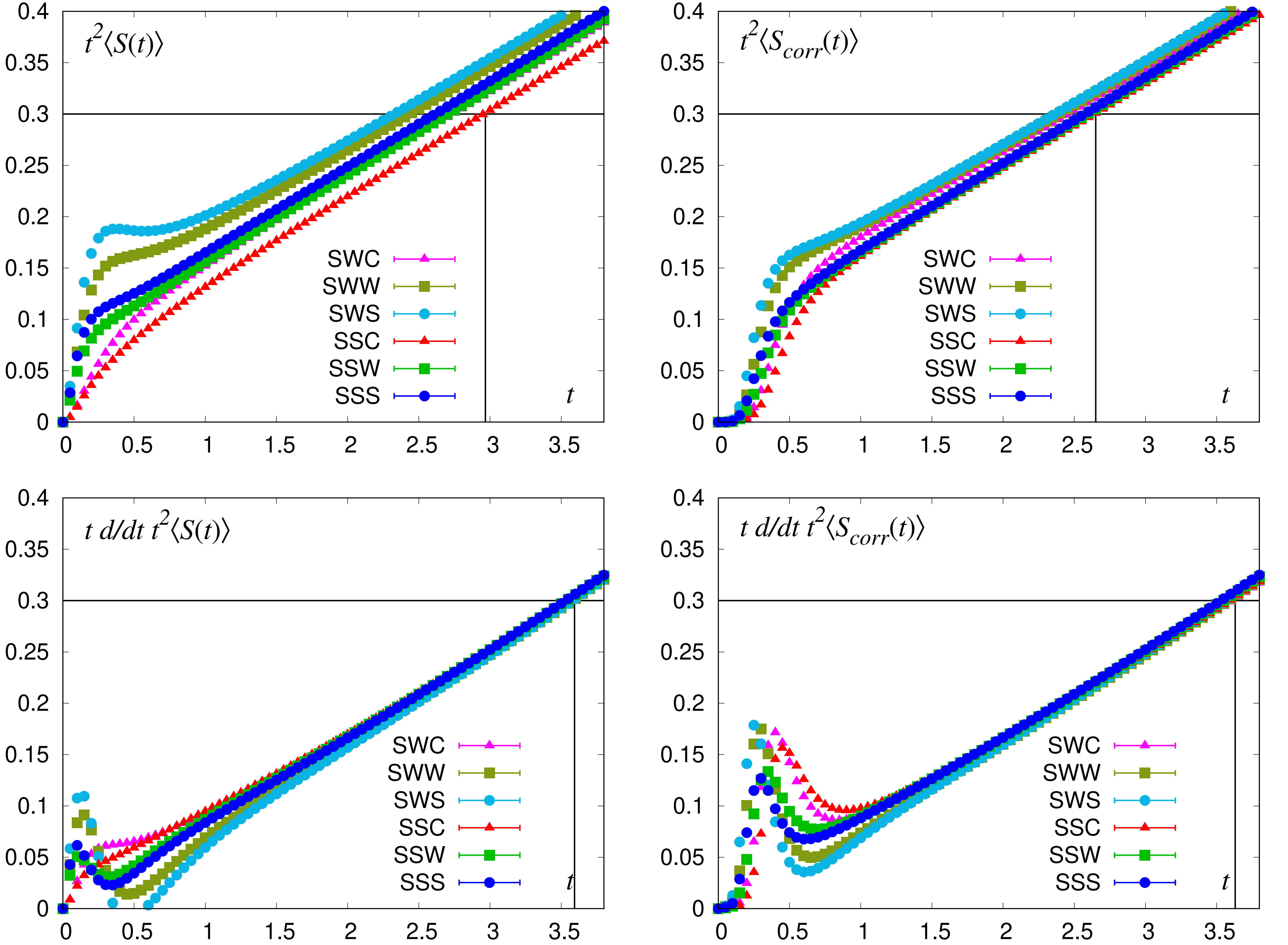


Action density vs flow time, $a = 0.09$ fm



Integration error

- Define the integration error as

$$\Delta S \equiv \langle S^o(t, \Delta t = 1/40)\rangle \Big|_{t=w_0^2} - \langle S^o(t, \Delta t = 1/20)\rangle \Big|_{t=w_0^2}$$

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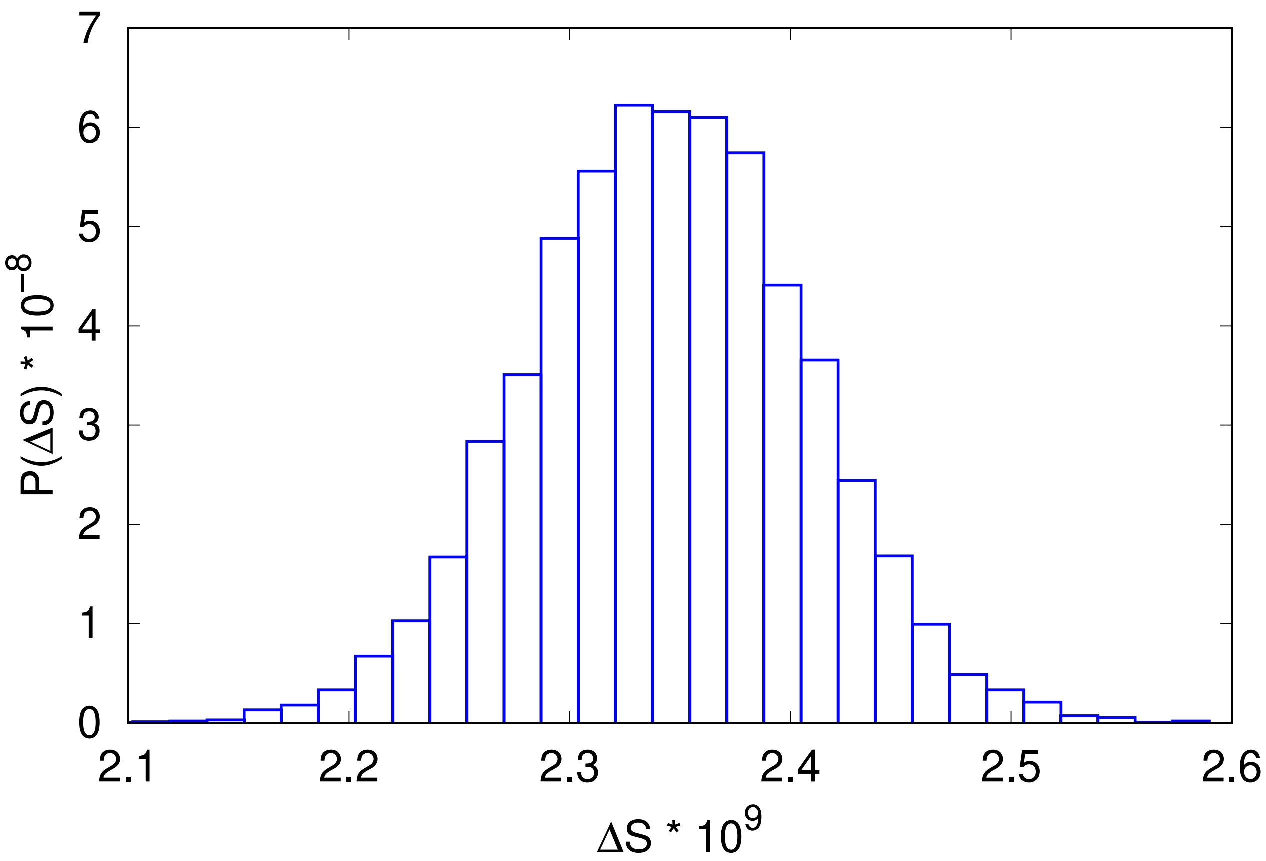

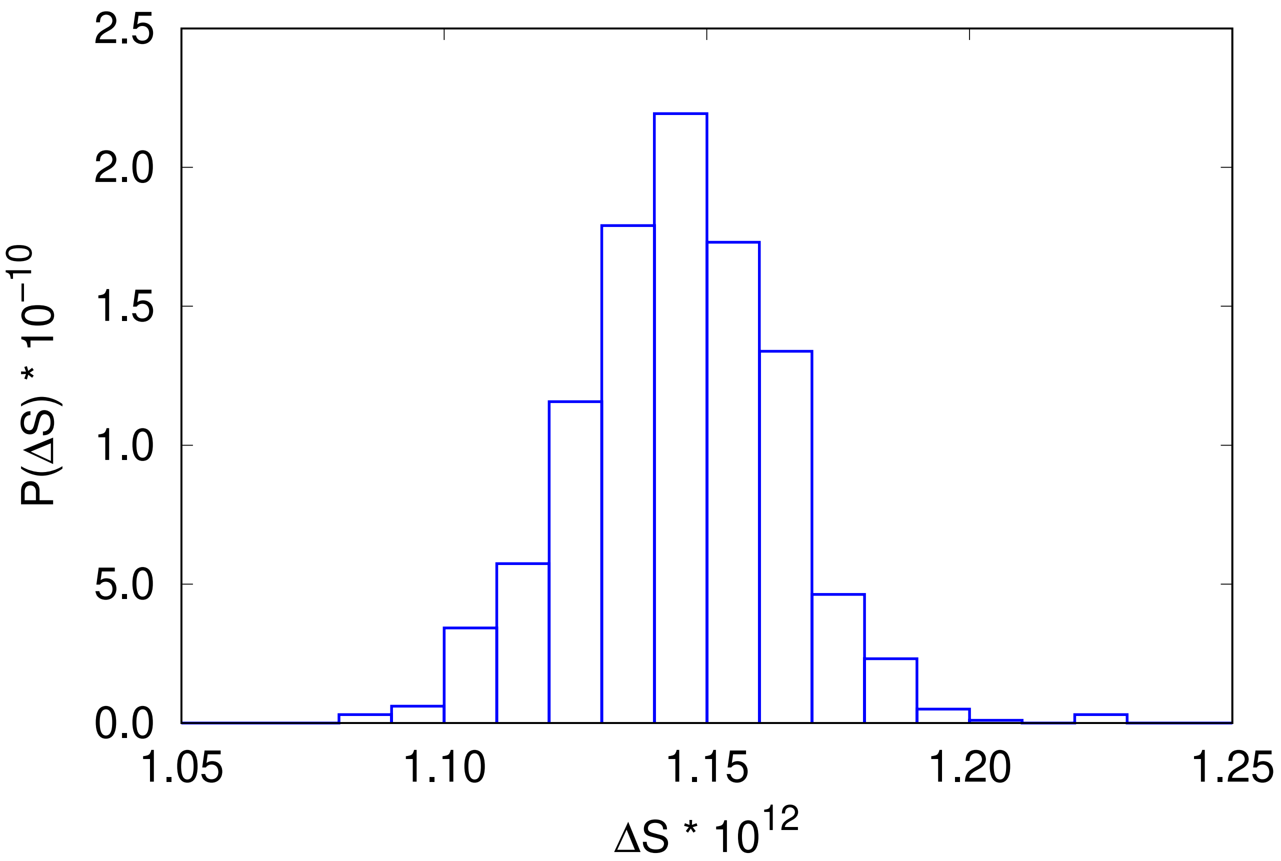

- The integration error on the physical mass ensembles at $a = 0.12$ fm (left) and $a = 0.042$ fm (right).

Autocorrelations

- Define the autocorrelation function for an observable $\mathcal{O}$:

$$C(n) \equiv \langle \mathcal{O}_0 \mathcal{O}_n \rangle - \langle \mathcal{O} \rangle^2$$

- The integrated autocorrelation time

$$\tau_{int} = 1 + 2 \sum_{n=1}^{N-1} \left(1 - \frac{n}{N} \right) \frac{C(n)}{C(0)}, \qquad \sigma^2(\bar{\mathcal{O}}) = \frac{\sigma^2(\mathcal{O})}{N} \tau_{int}$$

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- Window method to estimate the integrated autocorrelation time

$$\tau_{int}(n) = 1 + 2 \sum_{n'=1}^{n} \frac{C(n')}{C(0)}$$

- If the autocorrelation function is a single exponential

$$C(n) = C(0) \exp(-an) \quad \text{then} \quad \tau_{int}^1 = \frac{e^a + 1}{e^a - 1}$$

Example: τ_{int} with the window method

- Mock data, single variable, Metropolis updating with progressively worse acceptance rate.
- Time series of 10,000,000 events.

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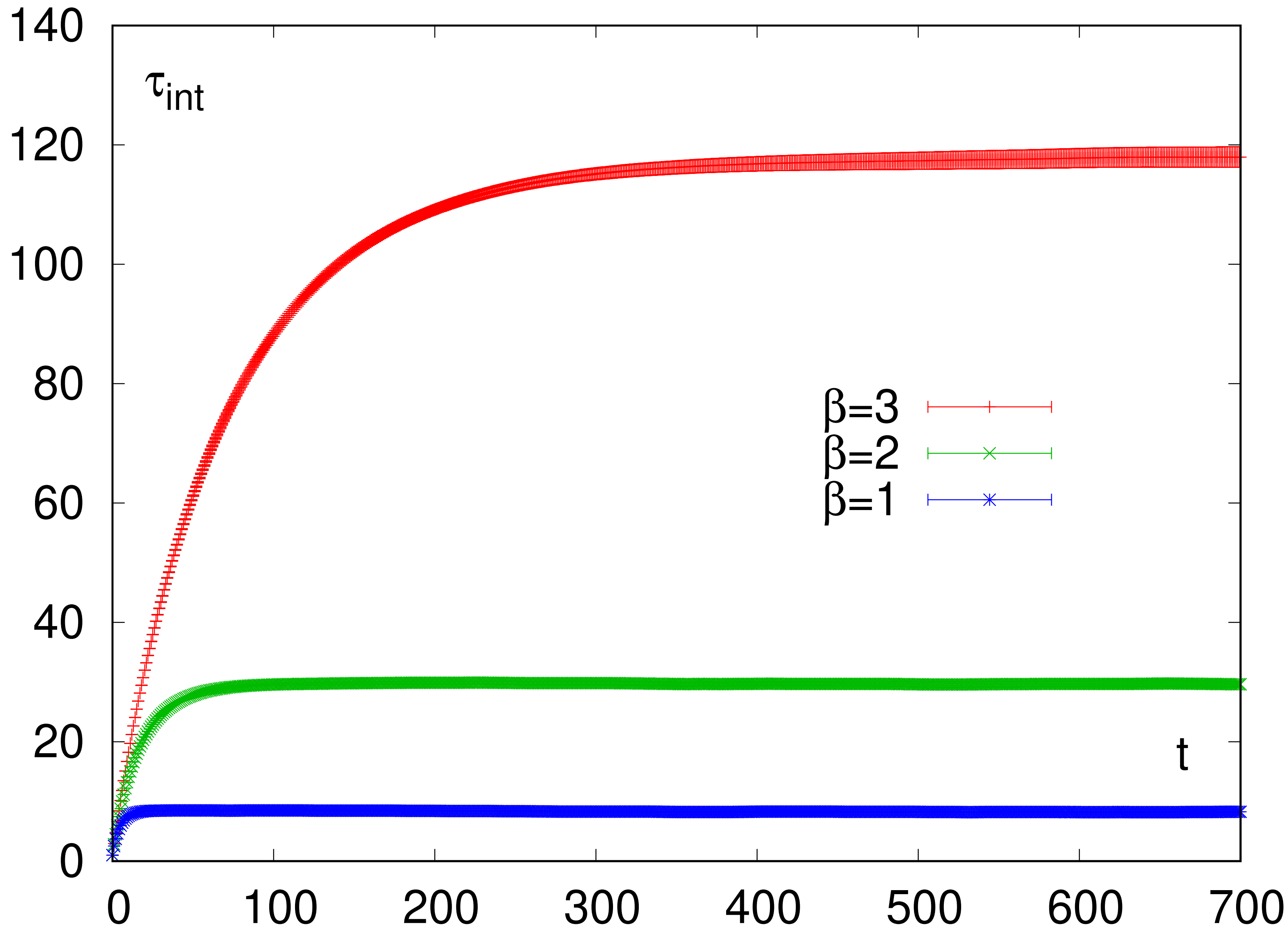
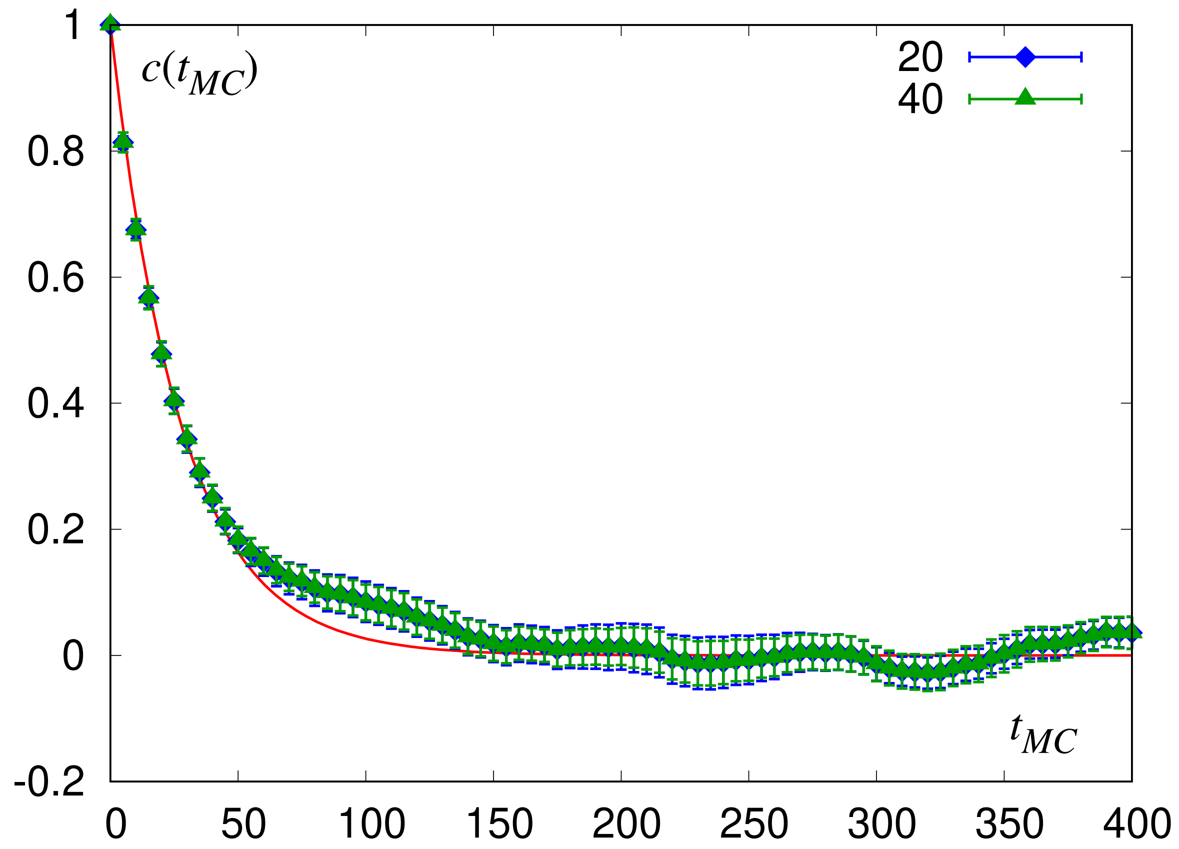
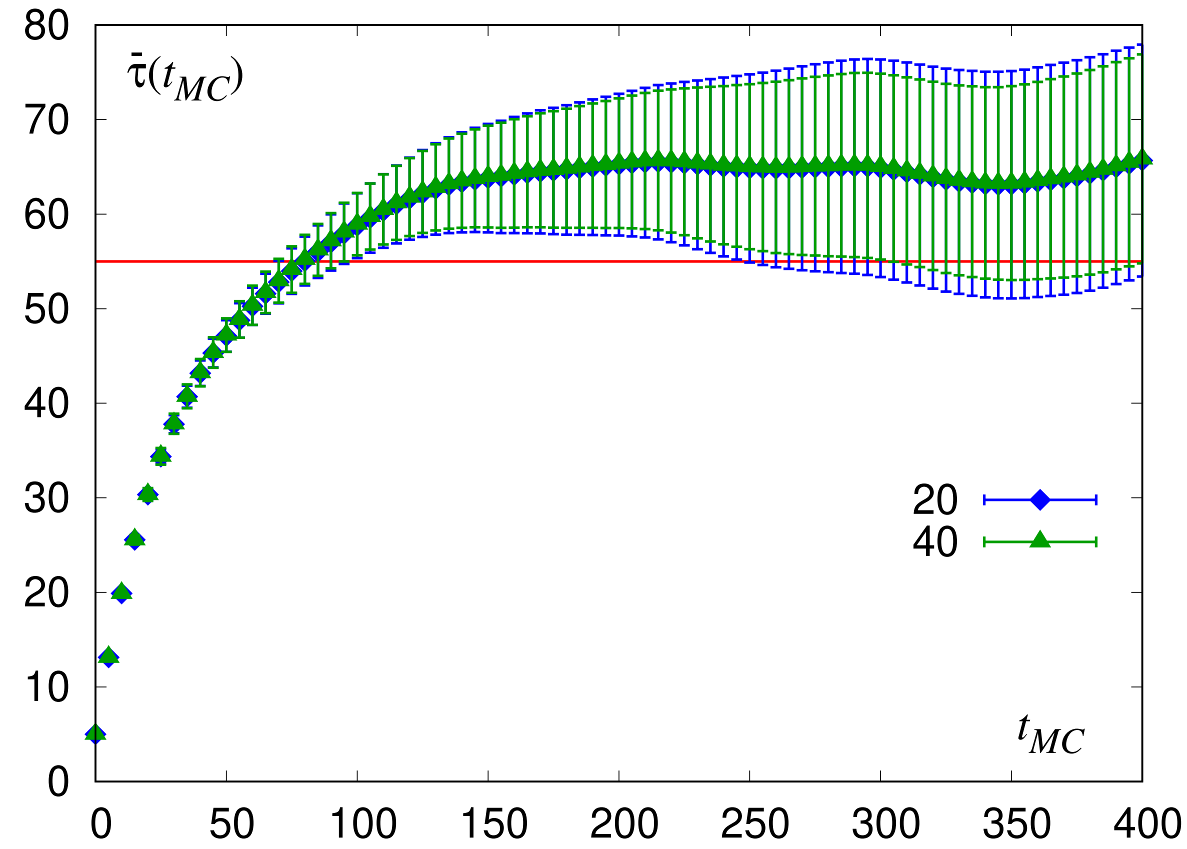


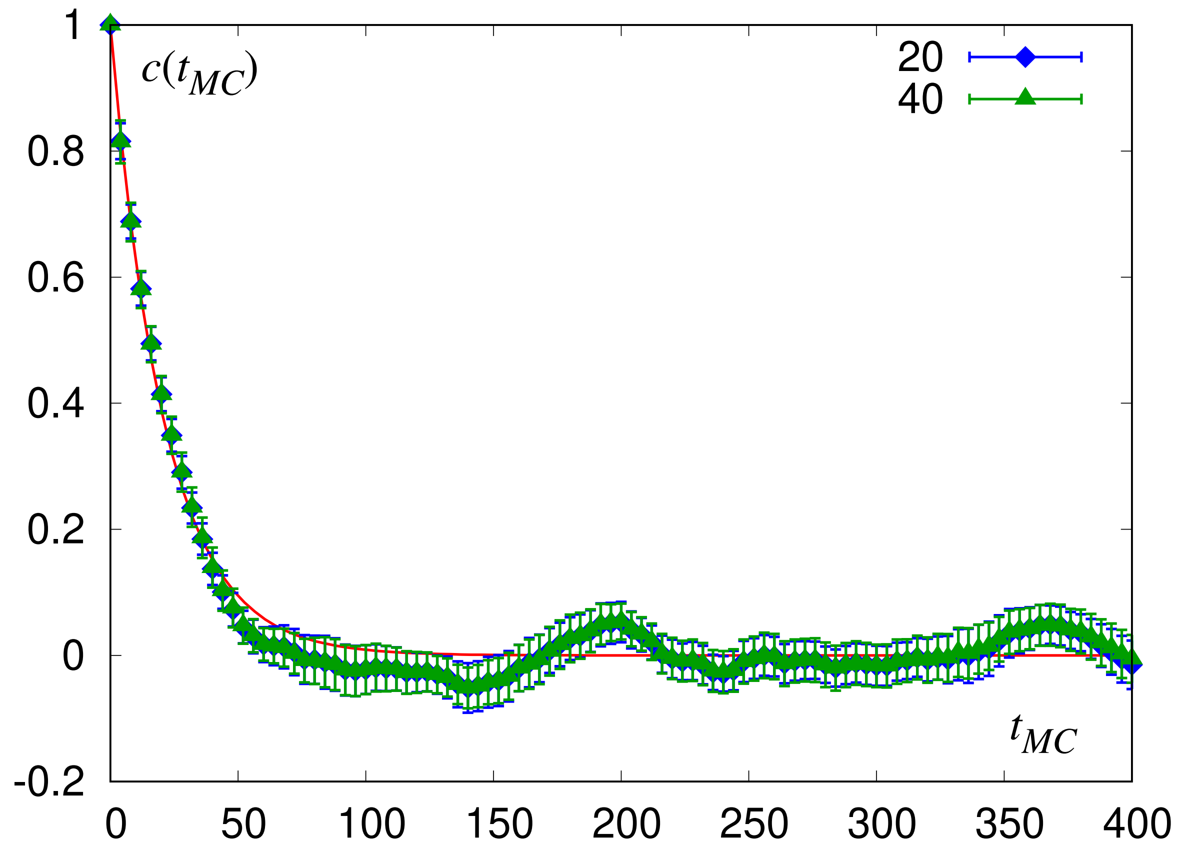
Autocorrelations: $a = 0.12$ fm, physical pion

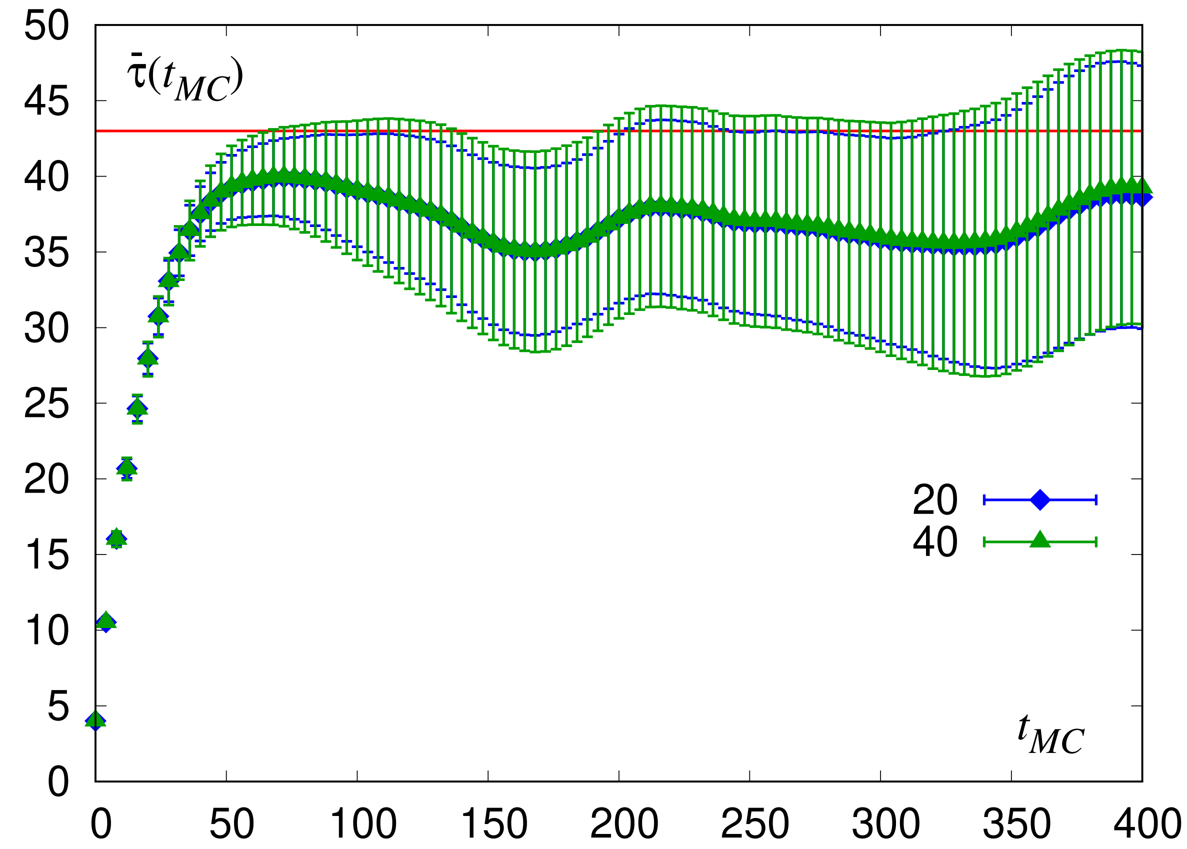




- MC time series: ~45,000 time units
- Observable: Clover action density at $t \sim w_0^2$
- Normalized autocorrelation function (left) and integrated autocorrelation time $\tau_{int}(t_{MC})$ (right)
- Single-exponential fit: $\tau_{int}^1 = 55 \pm 3$

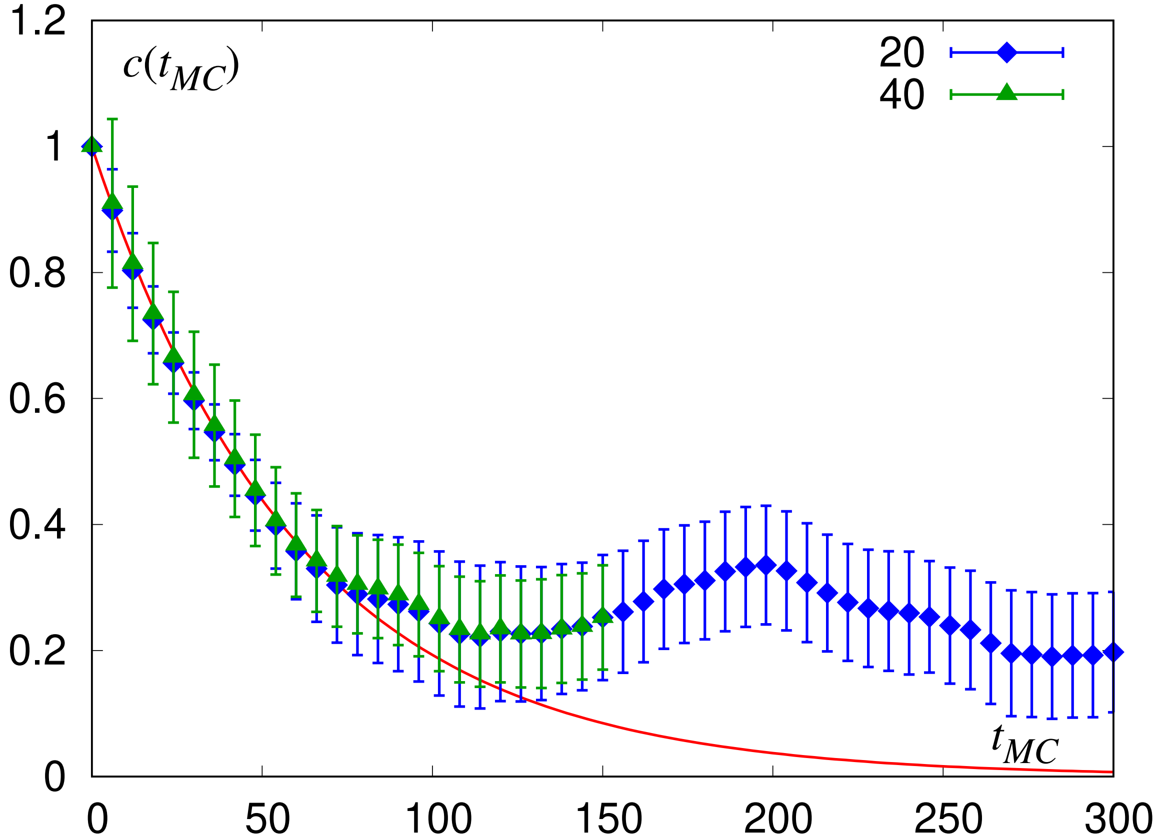
Autocorrelations: $a = 0.09$ fm, physical pion

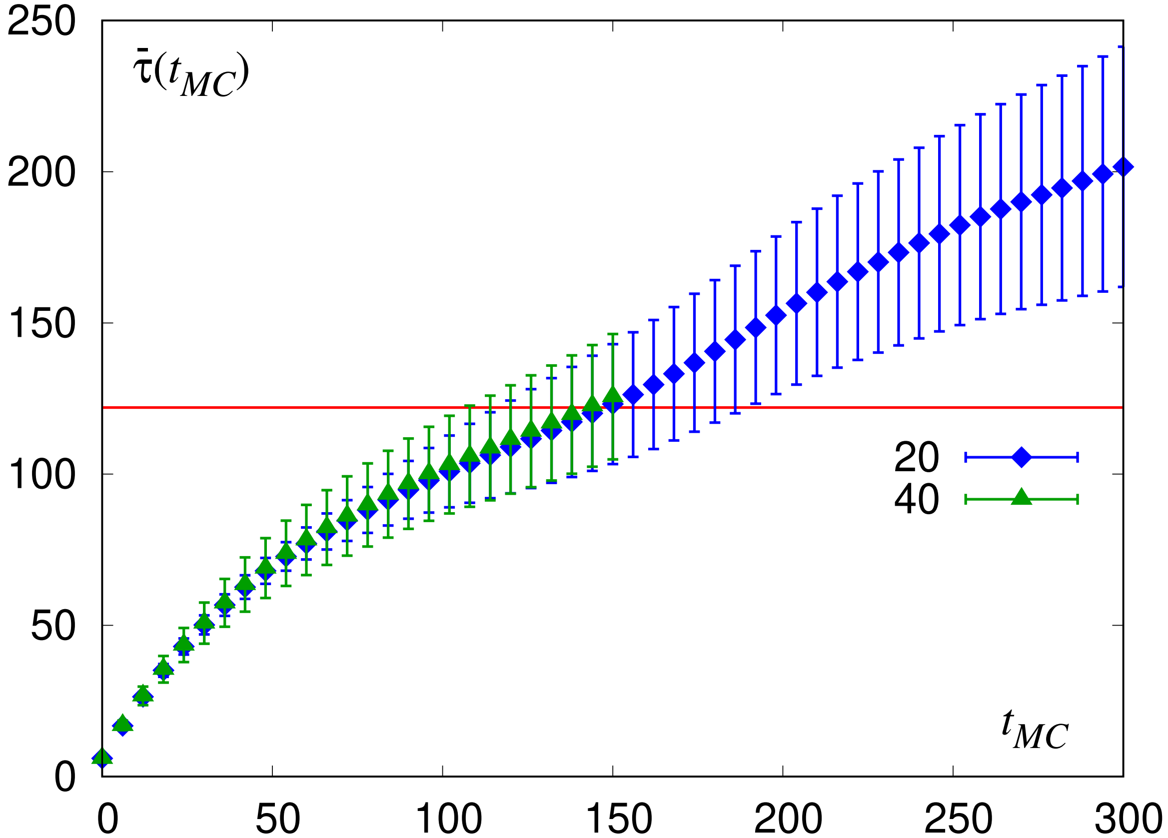




- MC time series: ~20,000 time units
- Observable: Clover action density at $t \sim w_0^2$
- Normalized autocorrelation function (left) and integrated autocorrelation time $\tau_{int}(t_{MC})$ (right)
- Single-exponential fit: $\tau_{int}^1 = 43 \pm 3$

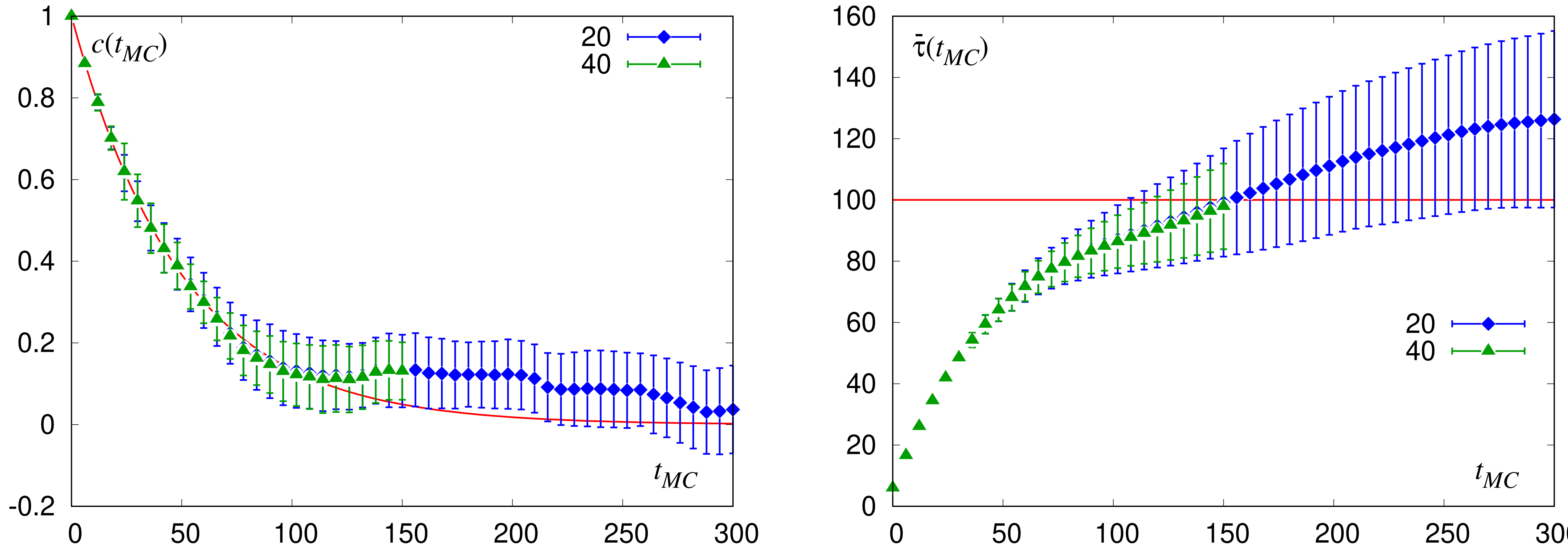
Autocorrelations: $a = 0.06$ fm, 300 MeV pion





- MC time series: ∼6,000 time units
- Observable: Clover action density at $t \sim w_0^2$
- Normalized autocorrelation function (left) and integrated autocorrelation time $\tau_{int}(t_{MC})$ (right)
- Single-exponential fit: $\tau_{int}^1 = 122 \pm 31$

Autocorrelations: $a = 0.042$ fm, physical pion

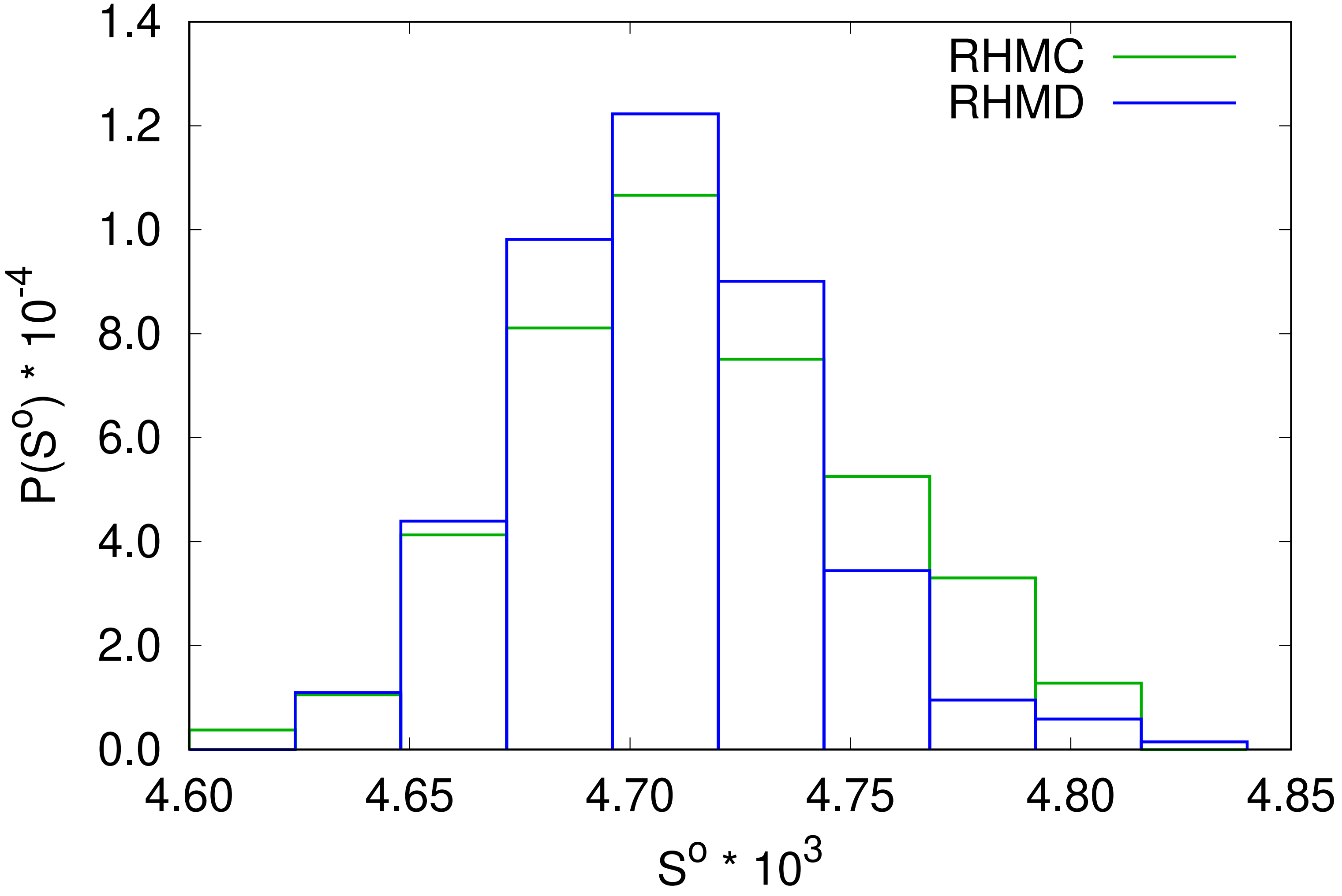


- MC time series: ∼6,000 time units
- Observable: Clover action density at $t \sim w_0^2$
- Normalized autocorrelation function (left) and integrated autocorrelation time $\tau_{int}(t_{MC})$ (right)
- Single-exponential fit: $\tau_{int}^1 = 100 \pm 12$

Relative scale

- Statistical uncertainty:
  - Propagated with jackknife on binned data.
  - Bin size is extrapolated to infinity.

RHMC vs RHMD

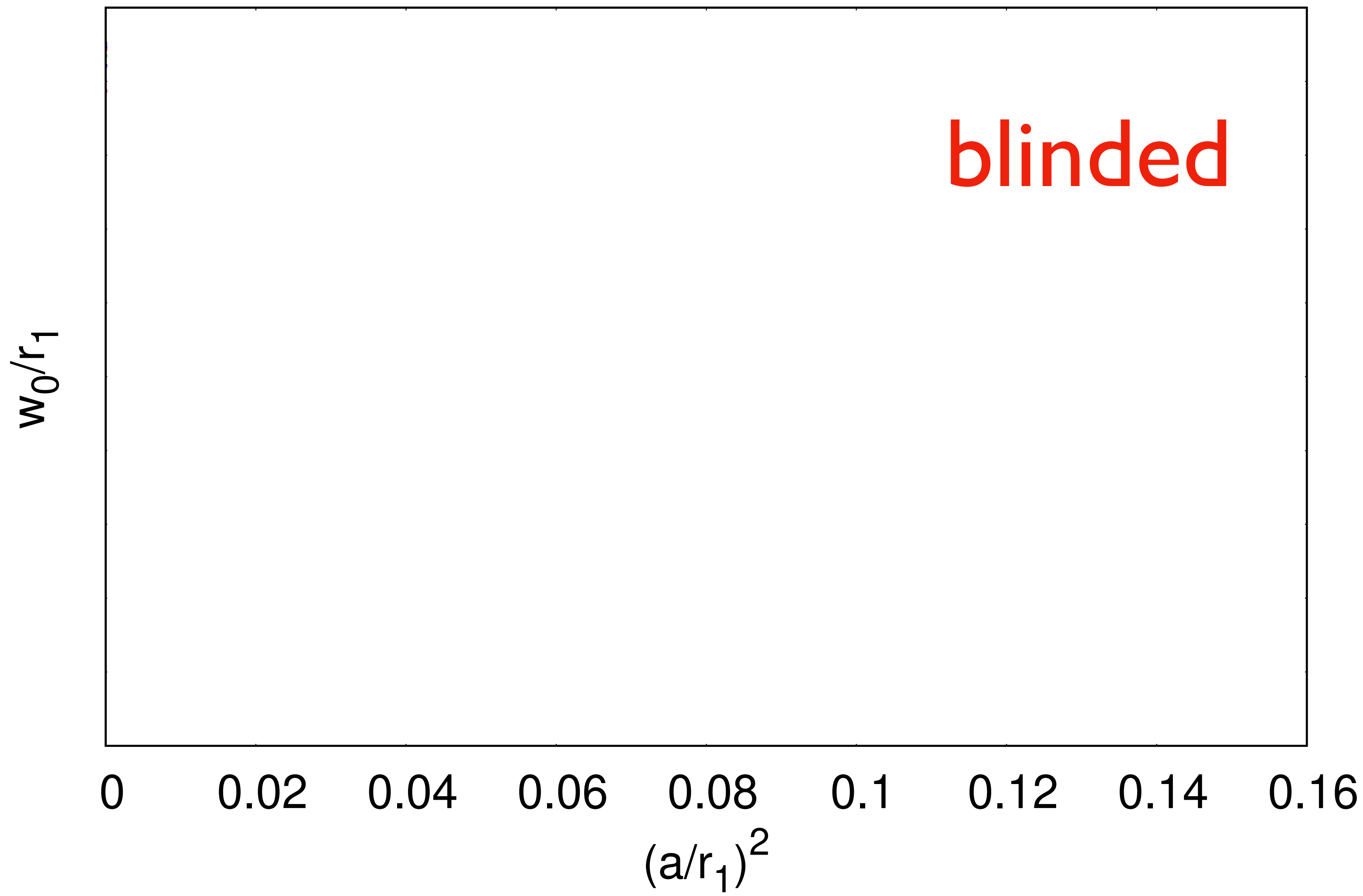


- Histogram of the clover observable at $t = w_0^2$ on the $m_\pi = 200$ MeV$a = 0.06$ fm ensemble
- w_0/a in SSCc: 2.9557(34) RHMC vs 2.9520(47) RHMD

Absolute scale

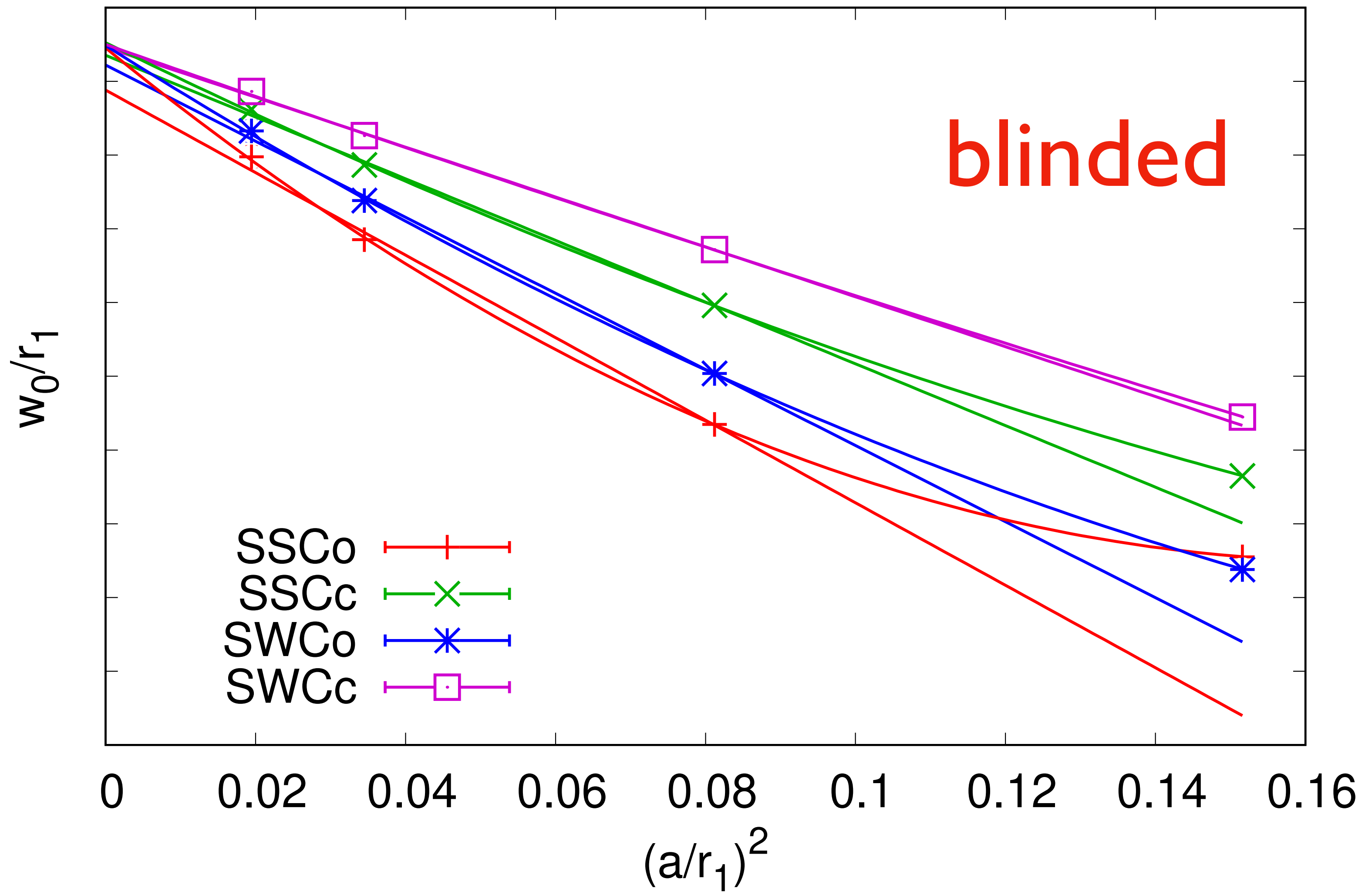
- Our plan:
  - $w_0 f_{p4s}$ on all ensembles (also as a crosscheck of 1503.02769).
  - $w_0 M_\Omega$ on physical mass ensembles.

w_0/r_1



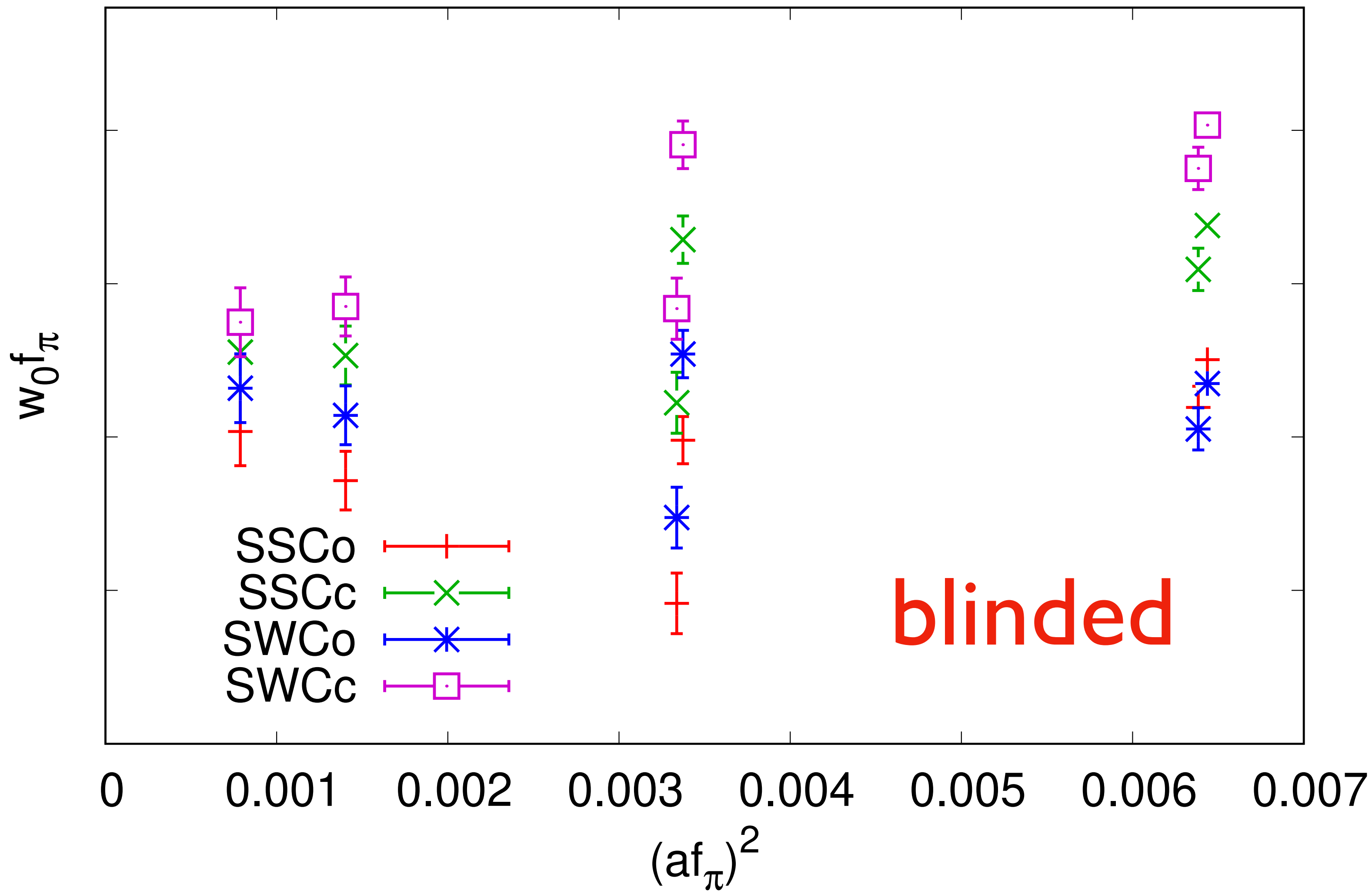
- Crosscheck against the r_1 scale that has been recently determined on most of the HISQ ensembles. TUMQCD, 2206.03156

w_0/r_1



- Crosscheck against the r_1 scale that has been recently determined on most of the HISQ ensembles. TUMQCD, 2206.03156
- Simple fits: linear and quadratic in a^2.

$w_0 f_\pi$



- The $w_0 f_\pi$ quantity on the physical mass $a = 0.042, 0.06, 0.09$ (original and retuned) and 0.12 (original and retuned) fm ensembles.
- No corrections of the mass mistuning yet. The magnitude of the effect seems comparable to the spread of the flow-observable schemes.

Omega baryon

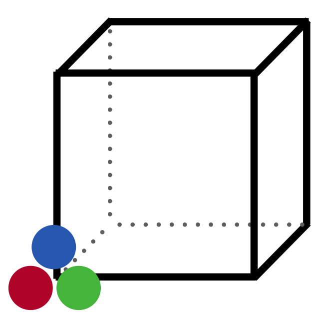
- We use HISQ in the valence sector for computing M_Ω.
- General challenges:
  - Signal-to-noise for baryons deteriorates as, e.g. for the nucleon $\sim \exp\{-(M_N - 3M_\pi/2)t\}$.
  - Excited states at early Euclidean times.
  - Staggered baryon spectroscopy.

Golterman, Smit, NPB 255 (1985)
Kilcup, Sharpe, NPB 283 (1987)
Bailey, hep-lat/0611023
Hughes, Lin, Meyer, 1912.00028

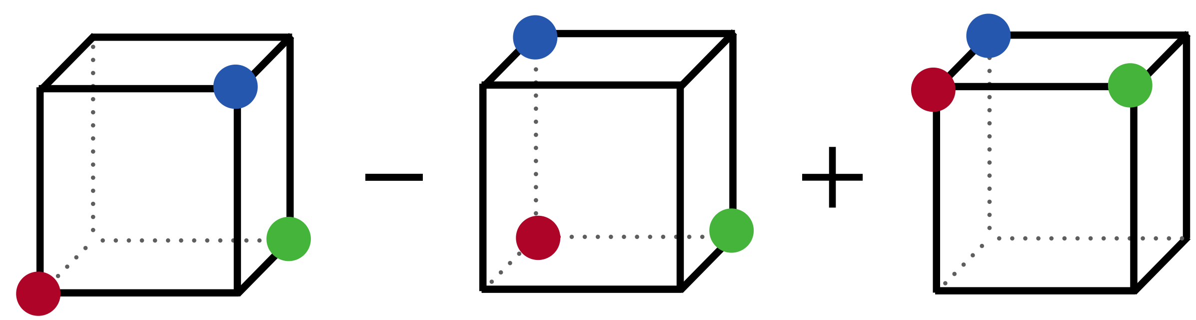
Staggered baryons

- Three interpolating operators for three Omega baryon tastes.
- Coulomb gauge fixing.
- Wall and Gaussian smeared sources, point and smeared sinks.
- May need GEVP for the final analysis.
- Perform Bayesian model averaging for all fits (different number of states and t_{min}). Jay, Neil, 2008.01069

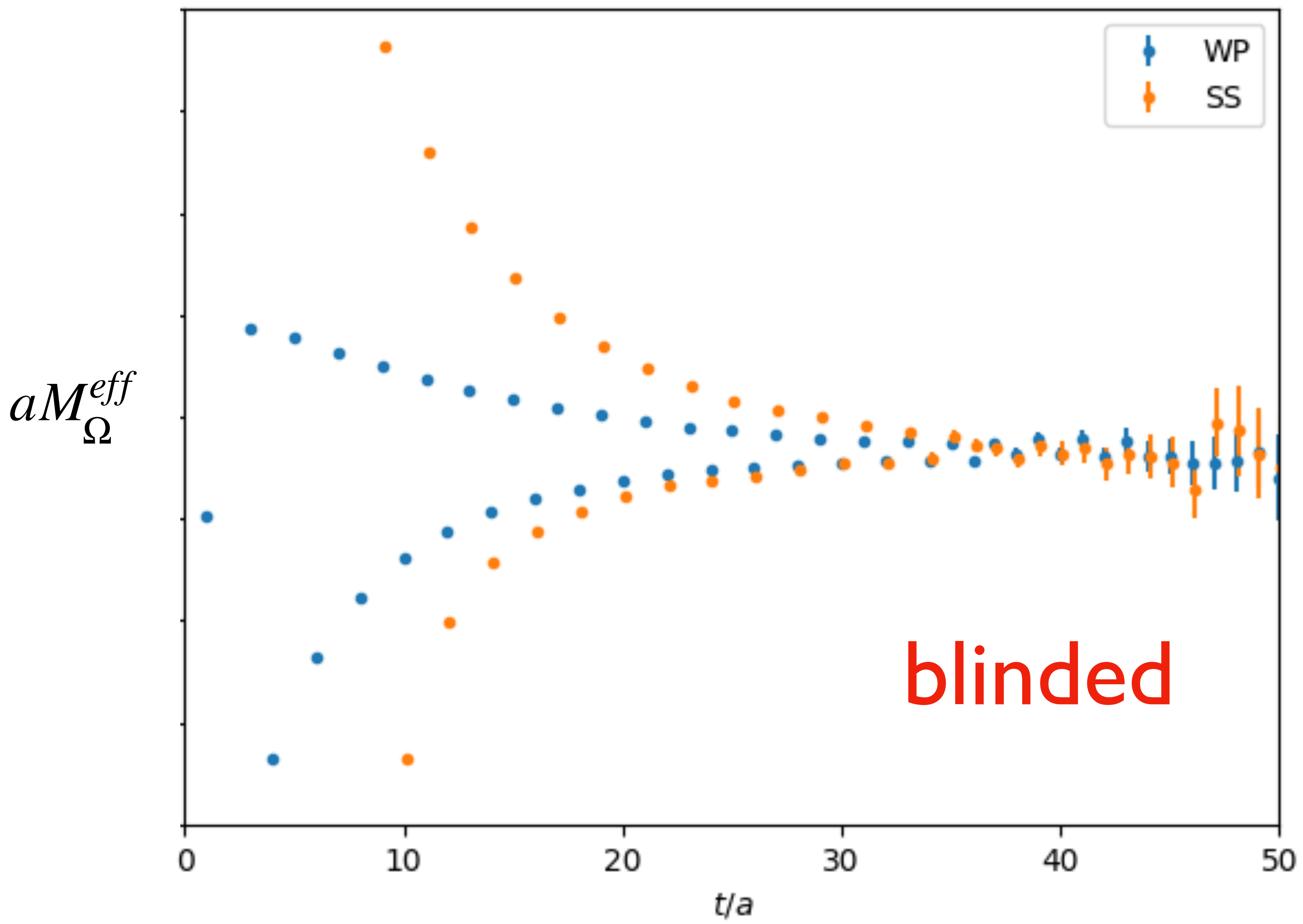
$O_{\Omega,1} =$



$O_{\Omega,2} =$



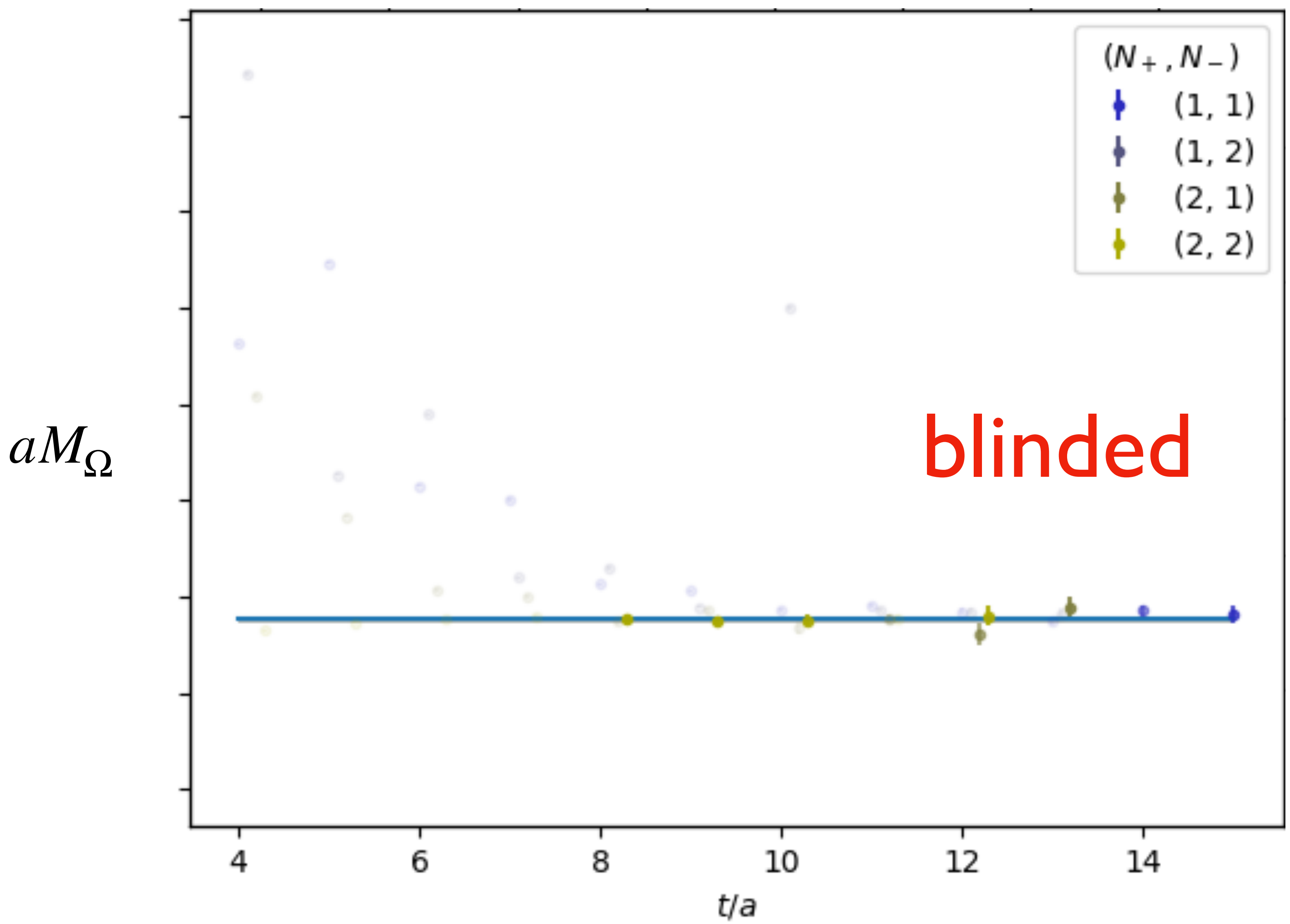
M_Ω: effective mass at $a = 0.06$ fm, physical mass



Note:

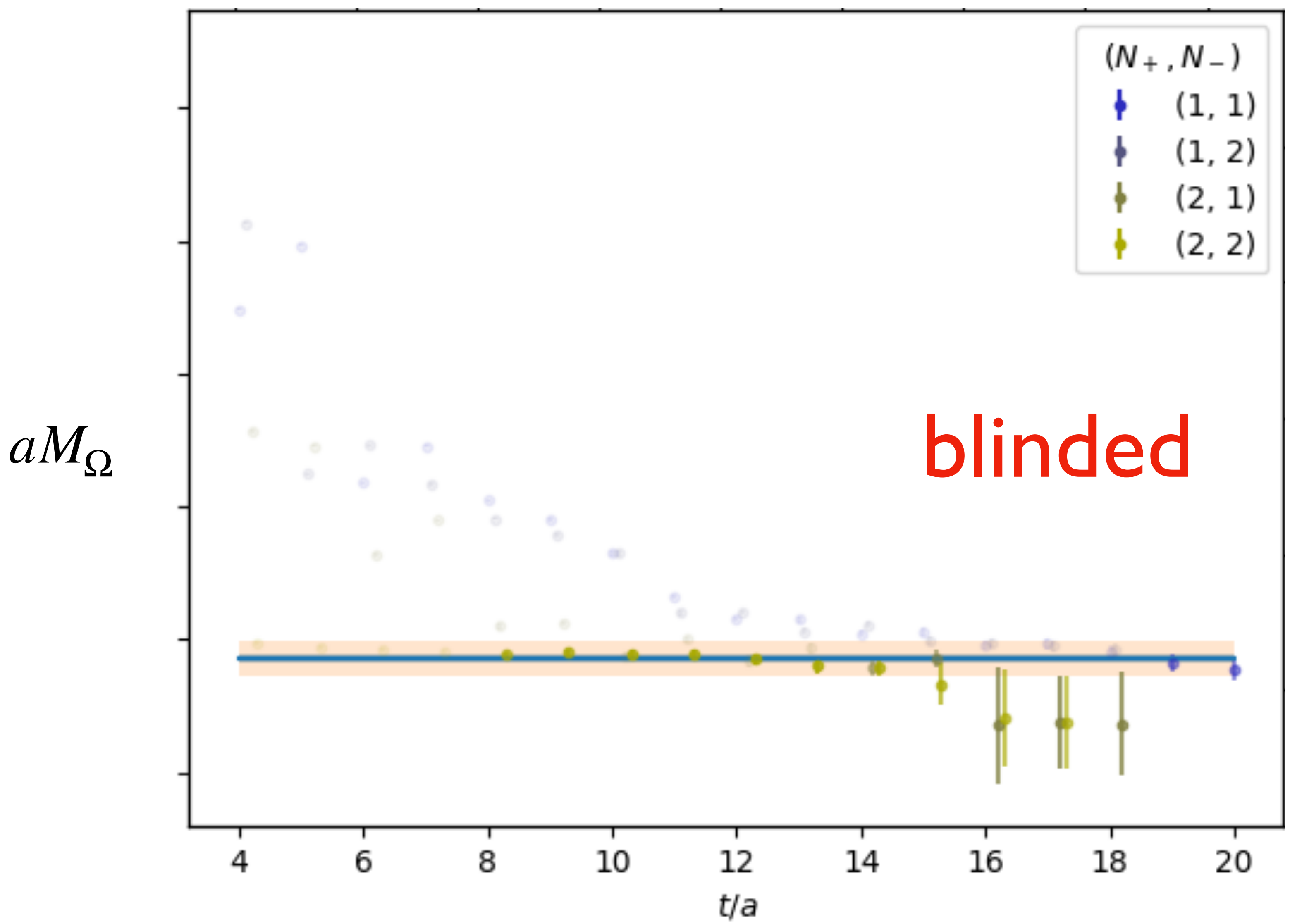
- Oscillating opposite parity state.
- Wall sources significantly help.

M_Ω: Fits at $a = 0.12$ fm



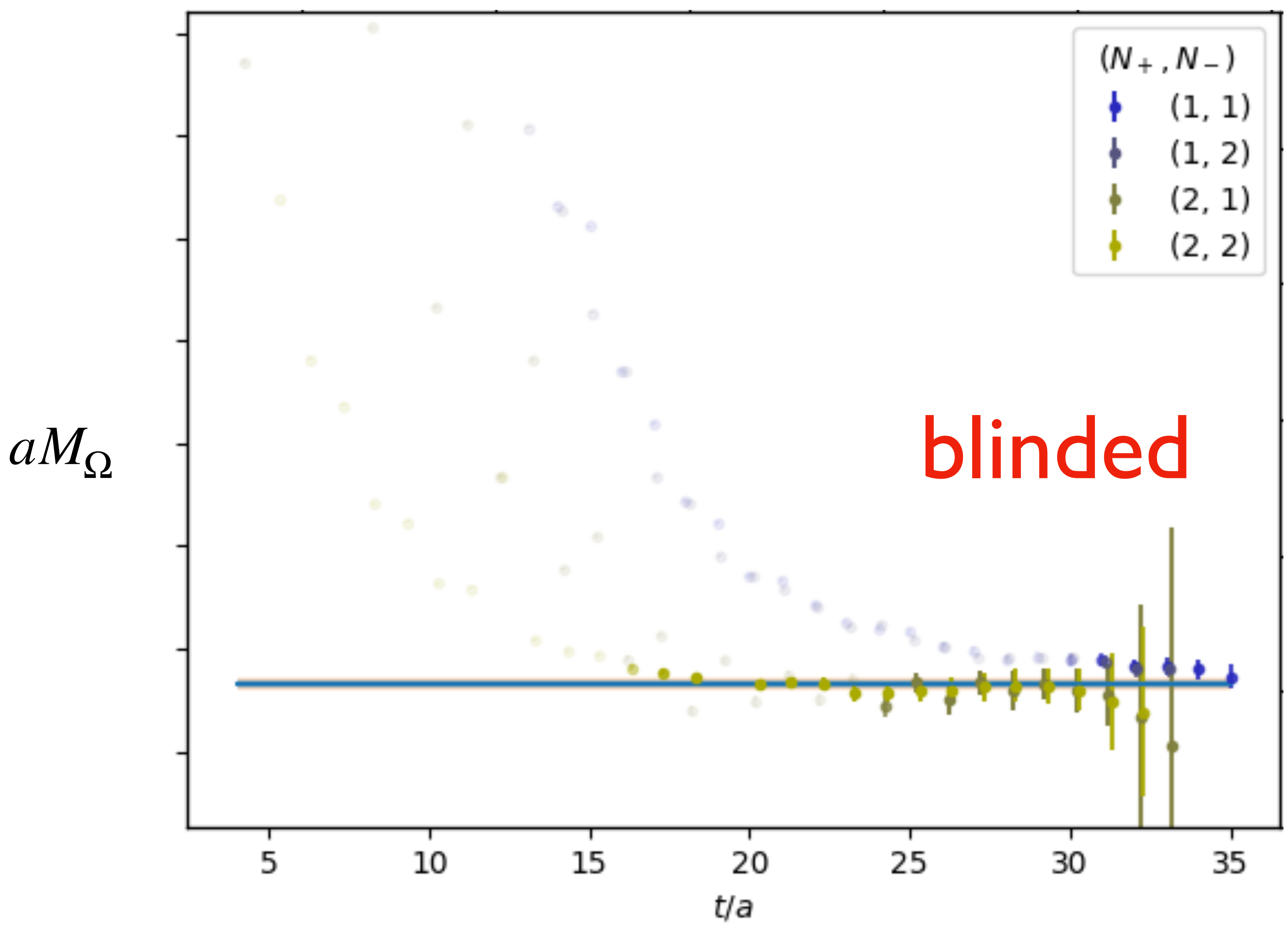
- Fitted Omega baryon mass as function of t_{min}.
- The horizontal line is the result of Bayesian model averaging.
- Dimmed points represent least favored fits.

M_Ω: Fits at $a = 0.09$ fm



- Fitted Omega baryon mass as function of t_{min}.
- The horizontal line is the result of Bayesian model averaging.
- Dimmed points represent least favored fits.

M_Ω: Fits at $a = 0.06$ fm



- Fitted Omega baryon mass as function of t_{min}.
- The horizontal line is the result of Bayesian model averaging.
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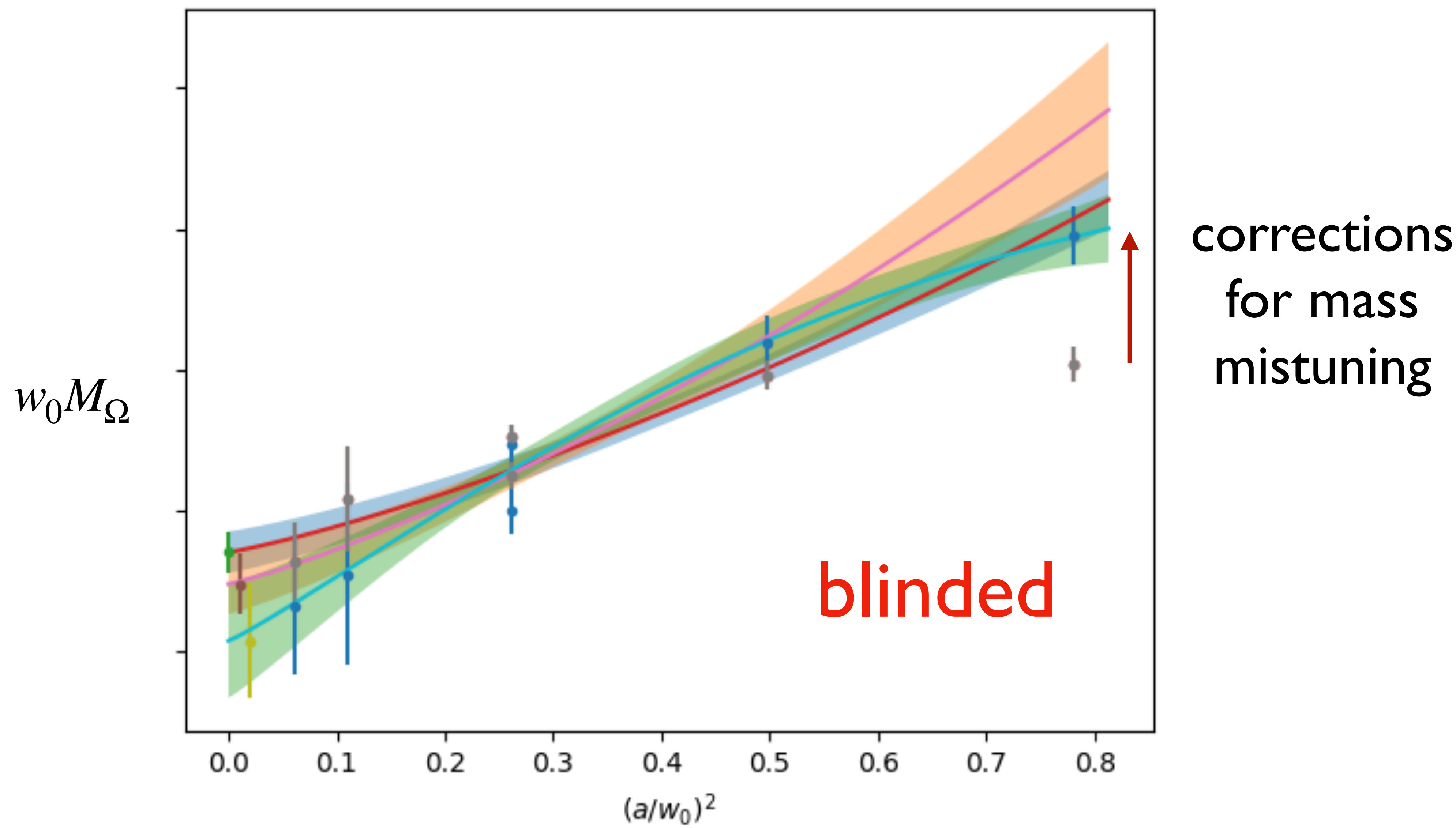
M_Ω: continuum extrapolation



- Continuum extrapolations:
  - $\alpha_s a^2$ (with and without $a = 0.15$ fm)
  - $\alpha_s a^2 + a^4$

Conclusion

- Ongoing program of the gradient flow scales $\sqrt{t_0}/a$ and w_0/a computations for all MILC HISQ ensembles with two flow and three observable combinations.
- Ongoing computation of aM_Ω with HISQ on the physical-mass ensembles.
- Next steps:
  - Adding electromagnetic effects for M_Ω.
  - Full chiral-continuum analysis of $w_0 f_{p4s}$.