Simulations with N_f=2+1 Flavors of Anisotropic Clover Fermions

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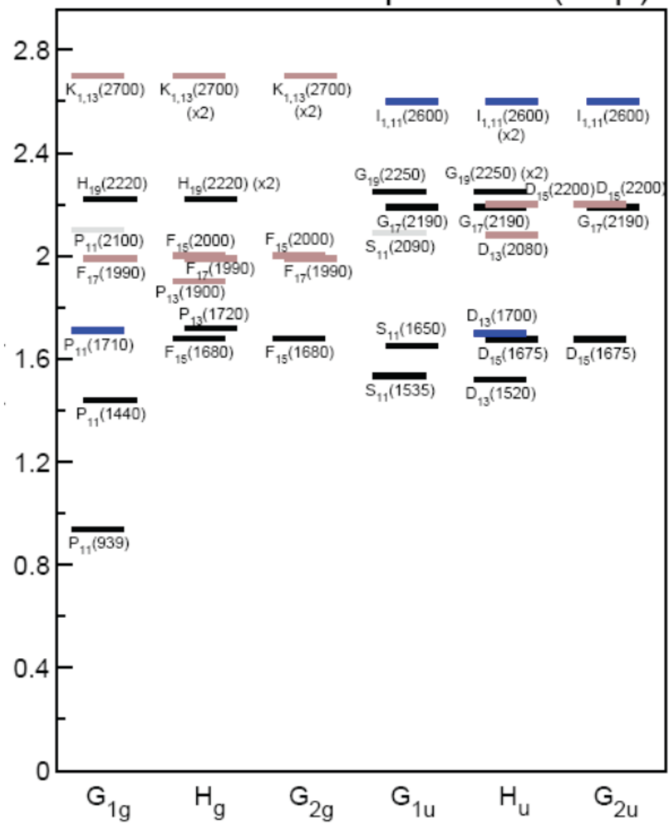
Perspectives and Challenges for Full-QCD Lattice Calculations
ECT, Trento, Italy
May 07, 2008

Physics Research Directions

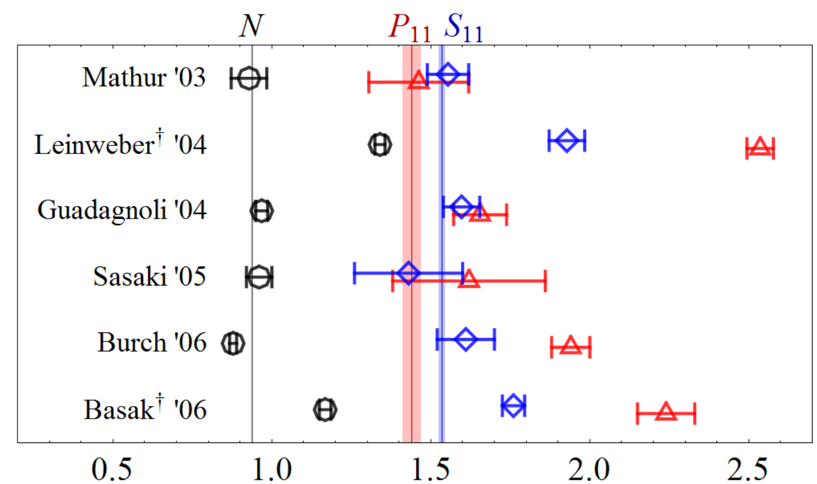
Wanted:

- Spectrum:
  - Excited-state baryon resonances (Hall B)
  - Conventional and exotic (hybrid) mesons (Hall D)

Nucleon Mass Spectrum (Exp)



Example: N, P_{11}, S_{11} spectrum

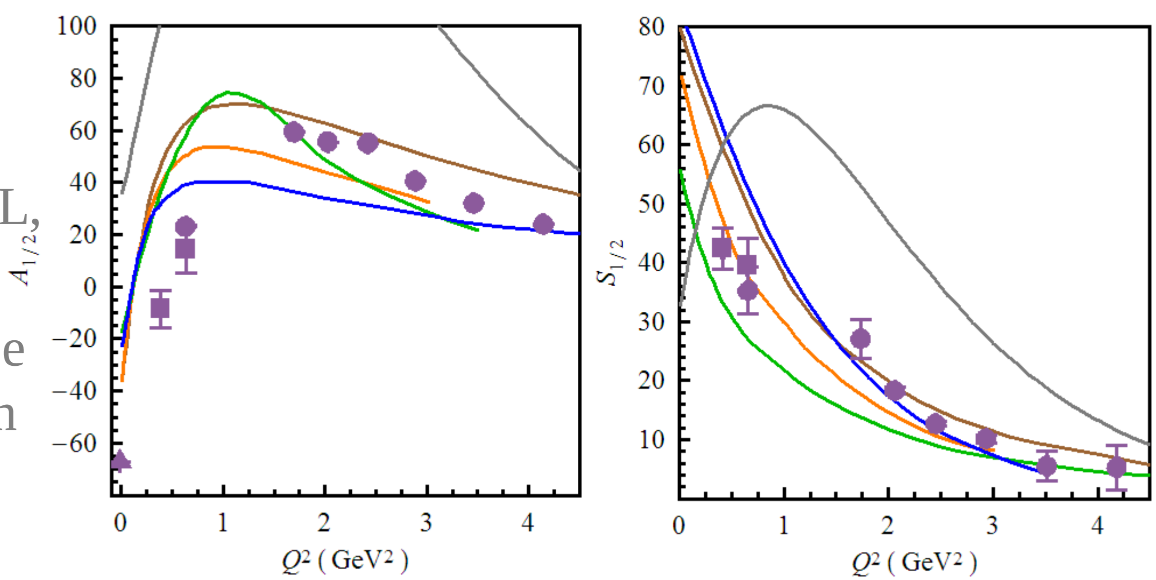


Physics Research Directions

Wanted:

- Spectrum:
  - Excited-state baryon resonances (Hall B)
  - Conventional and exotic (hybrid) mesons (Hall D)
- Form factors: ground-state and excited-state form factors and transition form factors
  - Experiments at Jefferson Laboratory (**CLAS**), MIT-Bates, LEGS, Mainz, Bonn, GRAAL, and Spring-8
  - Many models disagree (a selection are shown here)

Example: *N-P_{11} transition FF*



Physics Research Directions

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- Spectrum:
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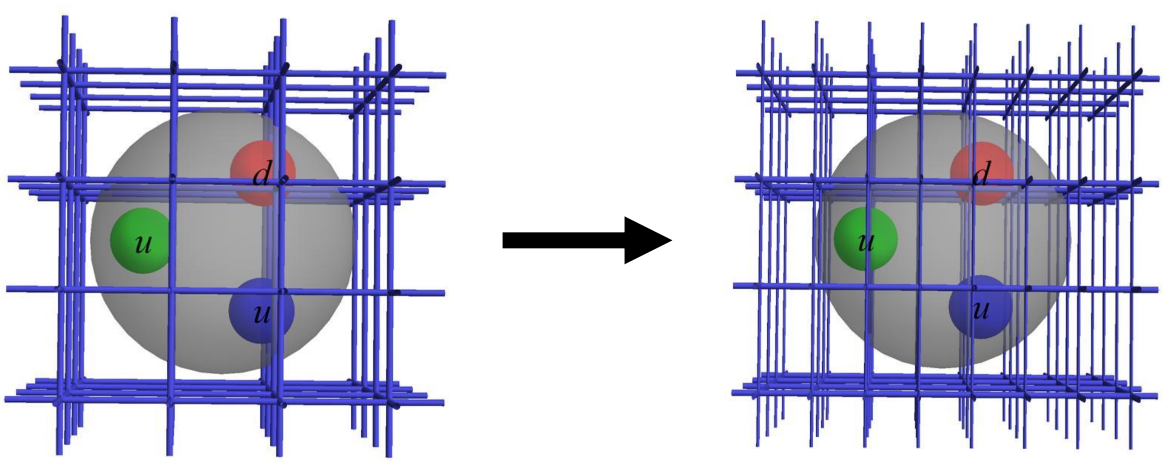
Solution: increase resolution

Anisotropic lattices ($a_t < a_{x,y,z}$)



Only Interested in Ground State?

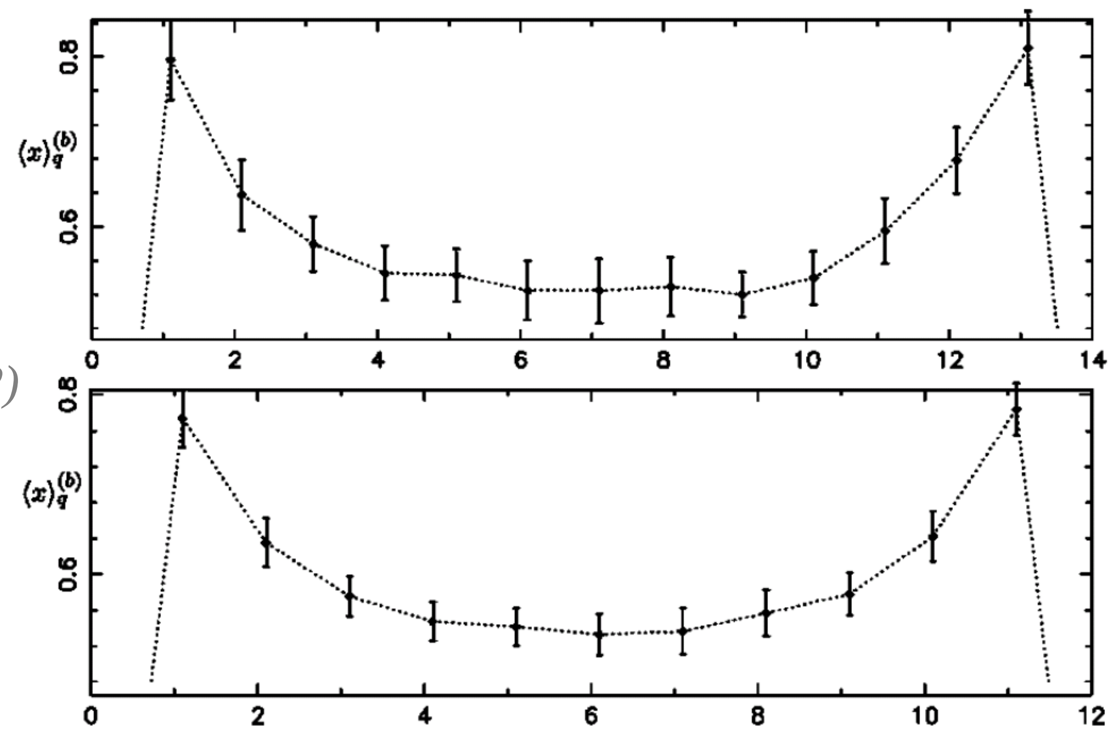
- Going to larger t does not always work well with three-point correlators
- Example:

  Quark helicity distribution

  LHPC & SESAM

  Phys. Rev. D ***66****, 034506 (2002)*

  50% increase in error budget at $t_{sep} = 14$



- Confronting the excited states might be a better solution than avoiding them.

Actions

- Anisotropic Symanzik gauge action with bare anisotropy γ_g

$$S_G = \frac{\beta}{N_c\gamma_g}\left\{\sum_{x,s>s'}\left[\frac{5}{3}\mathcal{P}_{ss'} - \frac{1}{12}\mathcal{R}_{ss'}\right] + \sum_{x,s}\left[\frac{4}{3}\mathcal{P}_{st} - \frac{1}{12}\mathcal{R}_{st}\right]\right\}$$

(Morningstar, Peardon '99)

- Anisotropic clover fermion action with **3d stout-link smeared** U's (spatially smeared only)

$$S_F^{SW} = \overline{\psi}\left[m_0 + D_t(U') + \frac{1}{\gamma_f}D_s(U')\right]\psi - \overline{\psi}\left[c_t\sum_s \sigma_{ts}F_{ts}(U') + \frac{c_s}{\gamma_g}\sum_{rs}\sigma_{rs}F_{rs}(U')\right]\psi$$

  - Tree-level values for c_t and c_s $\quad c_s = \frac{\gamma_g}{\gamma_f}, \quad c_t = \frac{1}{2}\left(\frac{\gamma_g}{\gamma_f} + 1/\xi\right)$

    (P. Chen 2001)

- Tadpole improvement factors u_s (gauge) and u_s' (fermion)
- Coefficients to tune: γ_g, γ_f, m_0, β

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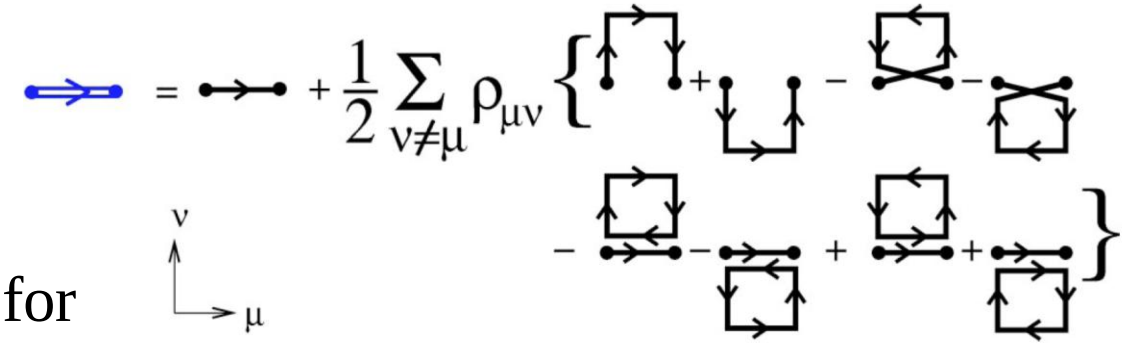
- Tadpole improvement factors u_s (gauge) and u_s' (fermion)
- Coefficients to tune: γ_g, γ_f, m_0, β
- "SLAC" = *S*tout *L*ink *A*nisotropic *C*lover

3D Stout-Link Smearing

Morningstar, Peardon '04

- Smoothes out dislocations; impressive glueball results
- Updating **spatial** links only
- Differentiable!
  Direct implementation for dynamical simulation



Why 3d Stout-link smearing?

i. Still have positive-definite transfer matrix in time (good for spectroscopy with multiple excited states)

ii. Light quark action (more) stable

iii. Tadpole $c_{s,t}$ is closer to nonperturbative one

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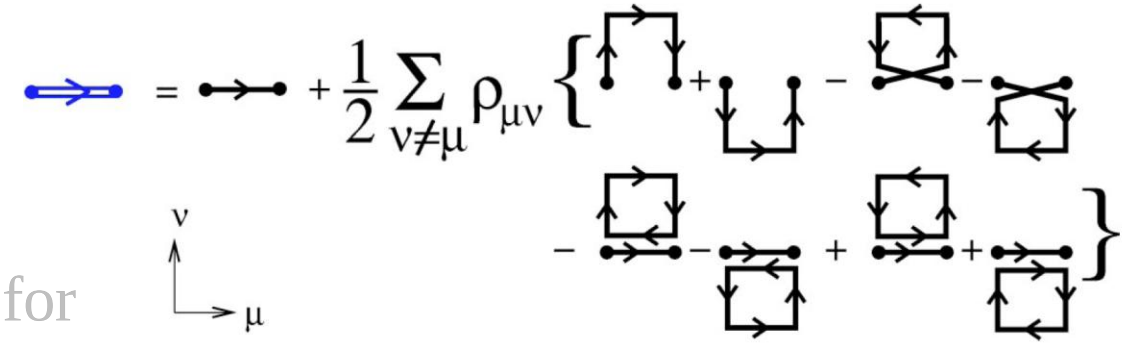
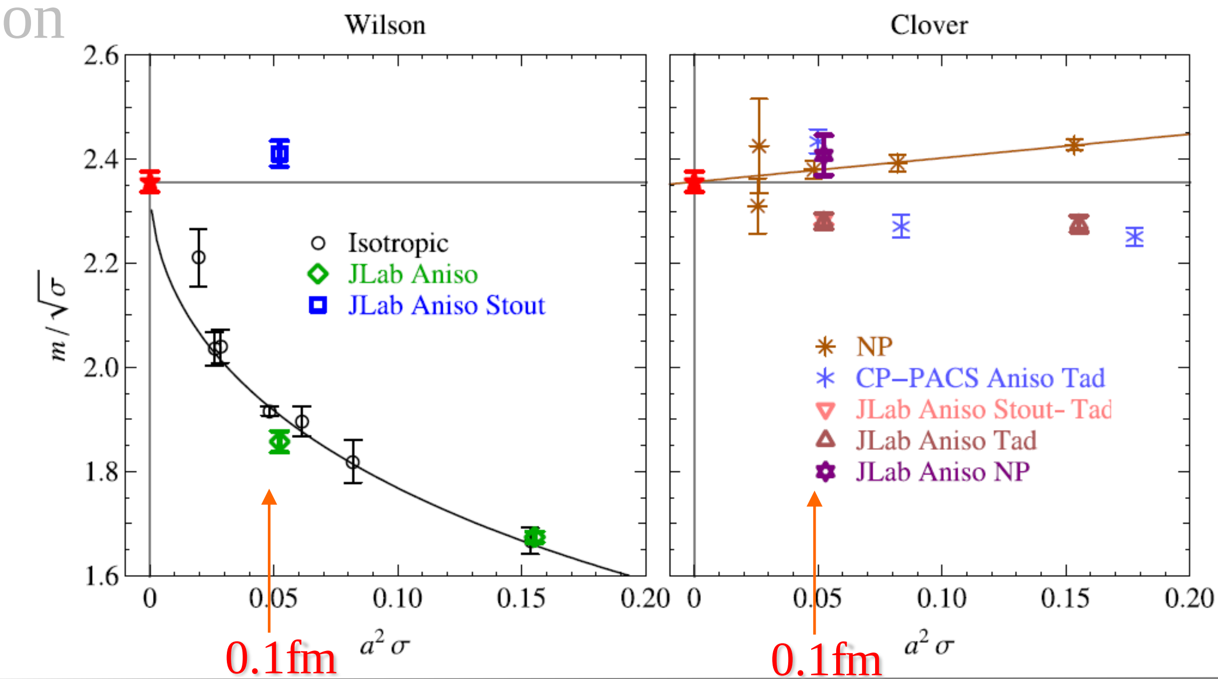


Scaling Study:

with $n_\rho = 2$ and $\rho = 0.22$

Quenched Wilson gauge comparison

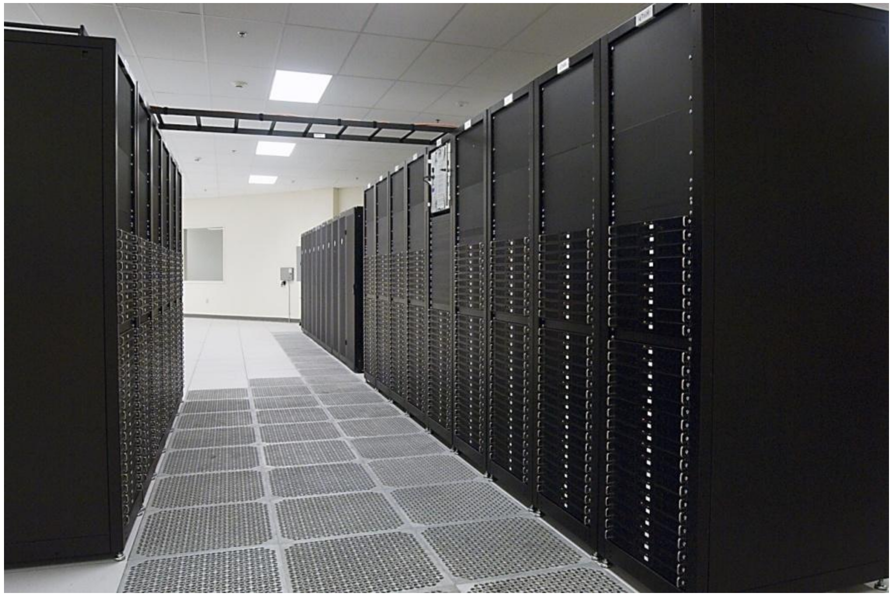
Clover: small scaling violations



Computational Facilities

- Two major resources:

USQCD



7n cluster (13 TF) @ JLab

INCITE

Jaguar cluster (119 TF) @ ORNL

Algorithm

- Rational Hybrid Monte Carlo (RHMC)
- Multi-scale anisotropic molecular dynamics update
- Even-odd preconditioning for the clover term
- Stout-link smearing in fermion actions

$$\frac{d\tilde{Q}}{dU_{\mathrm{thin}}} = \frac{d\tilde{Q}}{dU_{\mathrm{stout}}} \frac{dU_{\mathrm{stout}}}{dU_{\mathrm{thin}}}$$

- Split gauge term
- Three time scales
  - δt_1: Omelyan integrator for $\mathrm{tr}\ \log A_{ee}$ and $\phi_i^\dagger r^{-\frac{1}{2}}(\tilde{Q})\phi$
  - δt_2: Leapfrog integrator $S_{G,(\mathrm{S})}$
  - δt_3: Leapfrog integrator $S_{G,(\mathrm{T})}$
  - Choice: $(\delta t_1, \delta t_2, \delta t_3) = (1/4, 1/4, 1/3)$ for $12^3 \times 96$
    $(1/5, 1/3, 1/2)$ for $12^3 \times 32$
- Acceptance rate: 60–70%

Dynamical Generation Costs

- Cost in terms of cost of producing one MD trajectory

$$\text{Cost}_{\text{traj}} = \xi^{1.25}\left(\frac{\text{fm}}{a_s}\right)^6 \cdot \left[\left(\frac{L_s}{\text{fm}}\right)^3\left(\frac{L_t}{\text{fm}}\right)\right]^{5/4} \cdot [C_1 + C_2/m_l]\,.$$

Anisotropy

Ops + HMC

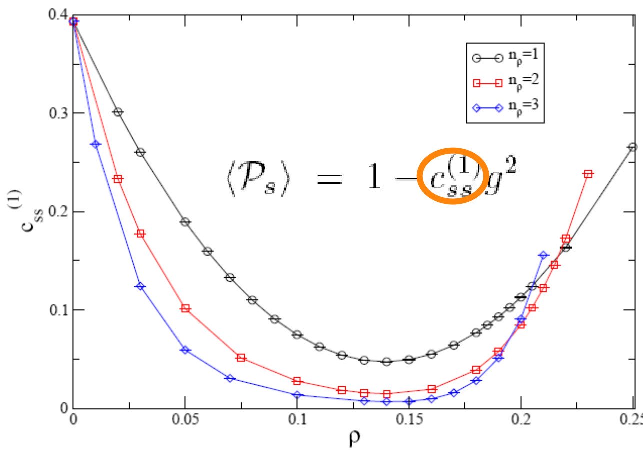
Solver iteration

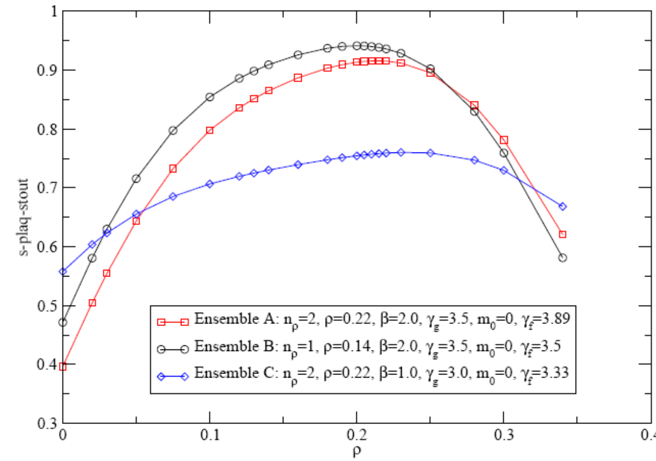
- Extra cost – a dimension taken to (near) continuum limit!
- Improvement: Temporal preconditions of clover Dirac operator *(Edwards, Joo, Peardon, work in progress)*
  - Gain factor of 2.5 in quenched study
  - Ready to implement on next anisotropic runs

Tadpole Factors and Stout Smearing

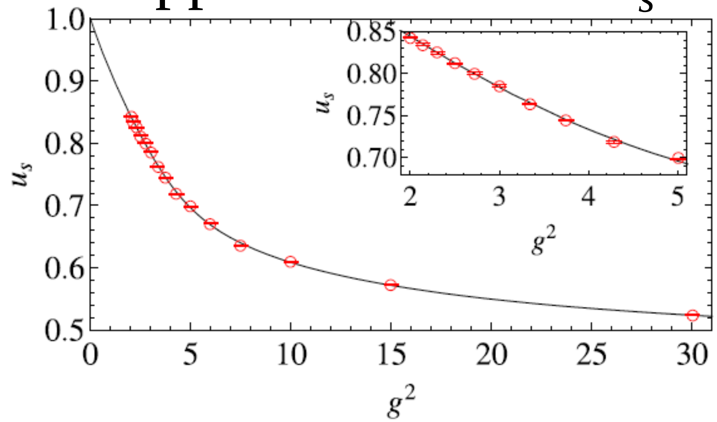
- Stout parameter study:

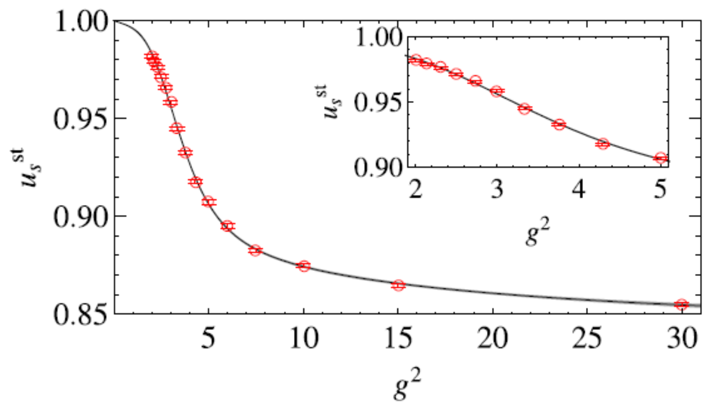
one-loop (Foley et al.) numerical





- Conservative choices: $n_\rho = 2$ and $\rho = 0.14$ ($< 1/2d$)
- Padé approximation for u_s over a wide range of $g^2 = 6/\beta$





N_f=3 Nonperturbative Tuning

- Nonperturbatively determine γ_g, γ_f, m_0 on anisotropic lattice

$$S_F^{SW} = \overline{\psi}\left[m_0 + D_t(U') + \frac{1}{\gamma_f}D_s(U')\right]\psi - \overline{\psi}\left[c_t\sum_s \sigma_{ts}F_{ts}(U') + \frac{c_s}{\gamma_g}\sum_{rs}\sigma_{rs}F_{rs}(U')\right]\psi$$

- Three calculations:
  - Background field in time: PCAC gives M_t

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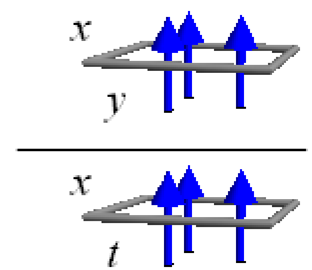
  - Background field in space: sideways potential gives $\gamma_{g,\mathrm{R}}$

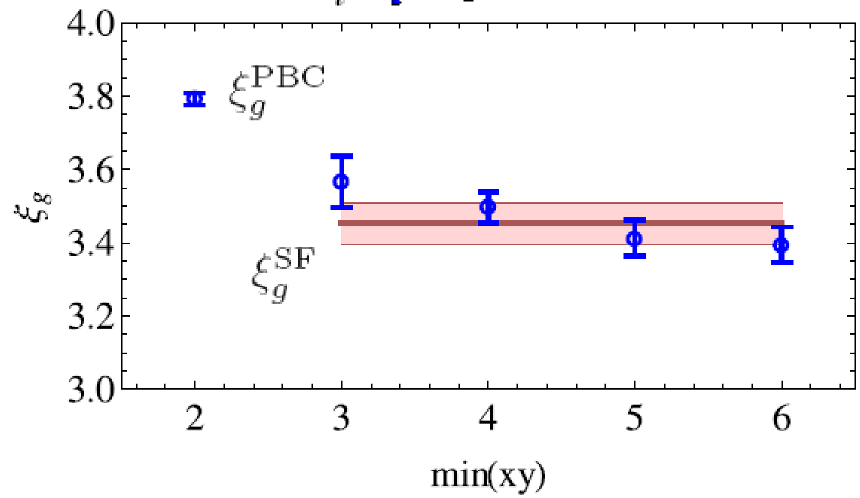
Klassen Method: ratio of Wilson loops

Wanted: $V_s(ya_s) = V_s(ta_s/\xi_\mathrm{R})$

⇨ Condition: $R_{ss}(x,y) = R_{st}(x,t)$



$$L(\xi_g) = \sum_{x,y}\frac{(R_{ss}(x,y) - R_{st}(x,\xi_g y))^2}{(\Delta R_s)^2 + (\Delta R_t)^2}$$



Comparison with PBC result

Example:

($\gamma_g = 4.4$, $\gamma_f = 3.4$, $m_0 = -0.0570$, $\beta = 1.5$)

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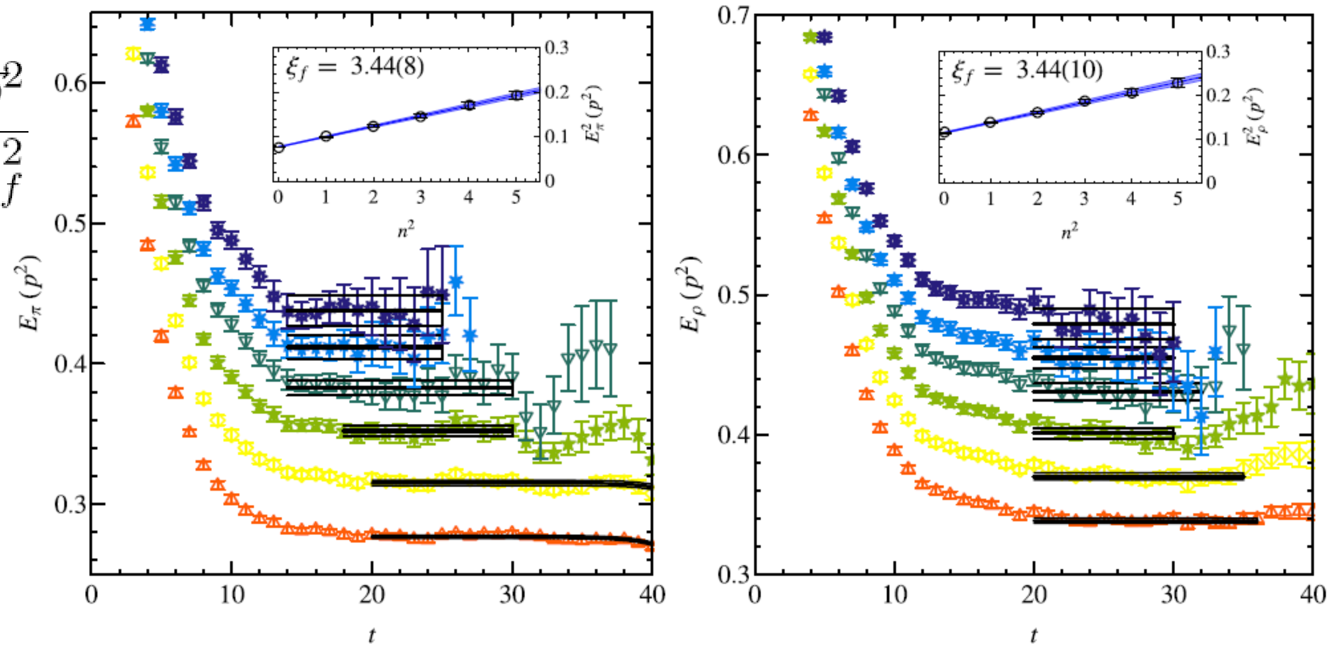
- Three calculations:
  - Background field in time: PCAC gives M_t
  - Background field in space: sideways potential gives $\gamma_{g,\mathrm{R}}$
  - Antiperiodic in time: dispersion relation gives $\gamma_{f,\mathrm{R}}$, (m_0, r_0, etc.)

$$E(\vec{p})^2 = m^2 + \frac{\vec{p}^2}{\xi_f^2}$$



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m_0	γ_g	γ_f	M_t	ΔM_t	$\Delta M_t^{(0)}$
−0.0950	4.3	3.5	−0.0122(9)	0.0003(10)	−0.001547
−0.0950	4.3	3.4	−0.0121(9)	0.0003(9)	−0.00167
−0.0950	4.3	3.3	−0.0141(8)	0.0002(9)	−0.001798
−0.0734	4.3	3.5	0.0160(9)	−0.0007(9)	−0.001547
−0.0734	4.3	3.4	0.0149(7)	−0.0007(6)	−0.00167
−0.0734	4.3	3.3	0.0139(7)	0.0006(11)	−0.001798
−0.0618	4.2	3.5	0.0431(11)	0.0002(4)	−0.001427
−0.0618	4.2	3.4	0.036(2)	−0.0004(8)	−0.001545
−0.0618	4.2	3.3	0.0339(11)	0.0004(8)	−0.001672
−0.0618	4.3	3.5	0.0321(9)	0.0003(5)	−0.001547
−0.0618	4.3	3.4	0.0303(6)	−0.0001(5)	−0.00167
−0.0618	4.3	3.3	0.0297(6)	−0.0003(4)	−0.001798
−0.0618	4.4	3.4	0.0218(5)	−0.0004(5)	−0.001791
−0.0618	4.4	3.3	0.0213(7)	0.0001(6)	−0.001923
−0.0570	4.3	3.4	0.0349(7)	0.0002(5)	−0.00167
−0.0570	4.3	3.3	0.0342(10)	0.0004(7)	−0.001798
−0.0570	4.3	3.2	0.0311(12)	0.0005(8)	−0.001935
−0.0570	4.3	3.1	0.0300(9)	0.0025(8)	−0.002078
−0.0570	4.4	3.3	0.0248(12)	0.0002(8)	−0.001923
−0.0570	4.4	3.2	0.0239(6)	0.0005(7)	−0.002065
−0.0570	4.4	3.1	0.0220(7)	0.0012(11)	−0.002212

m_0	γ_g	γ_f	ξ_g
−0.0950	4.3	3.5	3.48(5)
−0.0950	4.3	3.4	3.42(3)
−0.0950	4.3	3.3	3.40(3)
−0.0743	4.3	3.4	3.47(10)
−0.0734	4.3	3.4	3.46(4)
−0.0618	4.2	3.5	3.48(4)
−0.0618	4.2	3.4	3.41(3)
−0.0618	4.2	3.3	3.42(2)
−0.0618	4.3	3.5	3.50(4)
−0.0618	4.3	3.4	3.47(4)
−0.0618	4.3	3.3	3.43(4)
−0.0618	4.3	3.2	3.38(7)
−0.0618	4.4	3.3	3.47(5)
−0.0570	4.3	3.4	3.48(7)
−0.0570	4.3	3.3	3.43(9)
−0.0570	4.3	3.2	3.39(3)
−0.0570	4.3	3.1	3.36(4)
−0.0570	4.4	3.3	3.50(4)
−0.0570	4.4	3.2	3.54(5)
−0.0570	4.4	3.1	3.399(16)

m_0	γ_g	γ_f	ξ_f	m_π	m_ρ	m_π/m_ρ
−0.0743	4.3	3.4	3.43(4)	0.1501(9)	0.222(3)	0.677(9)
−0.0618	4.2	3.5	3.62(5)	0.2830(9)	0.348(2)	0.814(5)
−0.0618	4.2	3.4	3.38(4)	0.2753(10)	0.337(2)	0.816(5)
−0.0618	4.2	3.3	3.18(3)	0.2604(10)	0.319(5)	0.817(11)
−0.0618	4.3	3.4	3.47(6)	0.2232(15)	0.290(4)	0.769(9)
−0.0618	4.4	3.3	3.25(6)	0.1639(17)	0.217(5)	0.754(16)
−0.0570	4.3	3.3	3.23(4)	0.2401(13)	0.299(4)	0.804(8)
−0.0570	4.3	3.2	3.19(5)	0.2290(16)	0.292(4)	0.784(10)
−0.0570	4.3	3.1	2.99(4)	0.2164(18)	0.261(7)	0.828(20)
−0.0570	4.4	3.3	3.43(6)	0.193(3)	0.255(6)	0.758(17)
−0.0570	4.4	3.2	3.22(8)	0.182(3)	0.233(5)	0.780(17)
−0.0570	4.4	3.1	2.91(11)	0.151(3)	0.194(6)	0.78(2)

N_f=3 Nonperturbative Tuning

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- Three calculations:
  - Background field in time: PCAC gives M_t
  - Background field in space: sideways potential gives $\gamma_{g,\mathrm{R}}$
  - Antiperiodic in time: dispersion relation gives $\gamma_{f,\mathrm{R}}$, (m_0, r_0, etc.)
- Parametrize anisotropies and PCAC mass linearly:

$$\begin{aligned}
\xi_g(\gamma_g,\gamma_f,m_0) &= a_0 + a_1\gamma_g + a_2\gamma_f + a_3 m_0 \\
\xi_f(\gamma_g,\gamma_f,m_0) &= b_0 + b_1\gamma_g + b_2\gamma_f + b_3 m_0 \\
M_t(\gamma_g,\gamma_f,m_0) &= c_0 + c_1\gamma_g + c_2\gamma_f + c_3 m_0.
\end{aligned}$$

- Use space & time BC simulations to fit a's, b's, c's separately
- Improvement condition: solve 3×3 linear system for each m_q, with $\xi = a_s/a_t = 3.5$

$$\begin{aligned}
\xi_g(\gamma_g^*,\gamma_f^*,m_0^*) &\stackrel{!}{=} \xi \\
\xi_f(\gamma_g^*,\gamma_f^*,m_0^*) &\stackrel{!}{=} \xi \\
M_t(\gamma_g^*,\gamma_f^*,m_0^*) &\stackrel{!}{=} m_q
\end{aligned}$$

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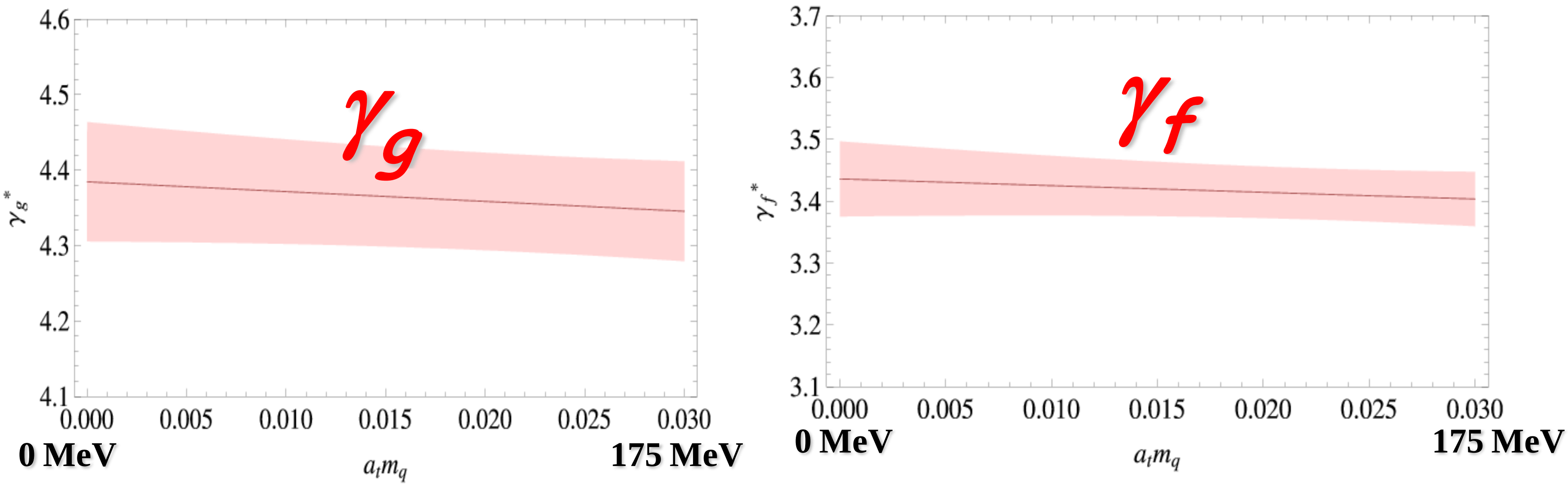
- $N_f = 3$, $\xi = 3.5$, $\beta = 1.5$ arxiv:0803.3960
  - Plot of γ_g and γ_f versus input current quark mass
  - Mild dependence on quark mass; fix γ_g and γ_f



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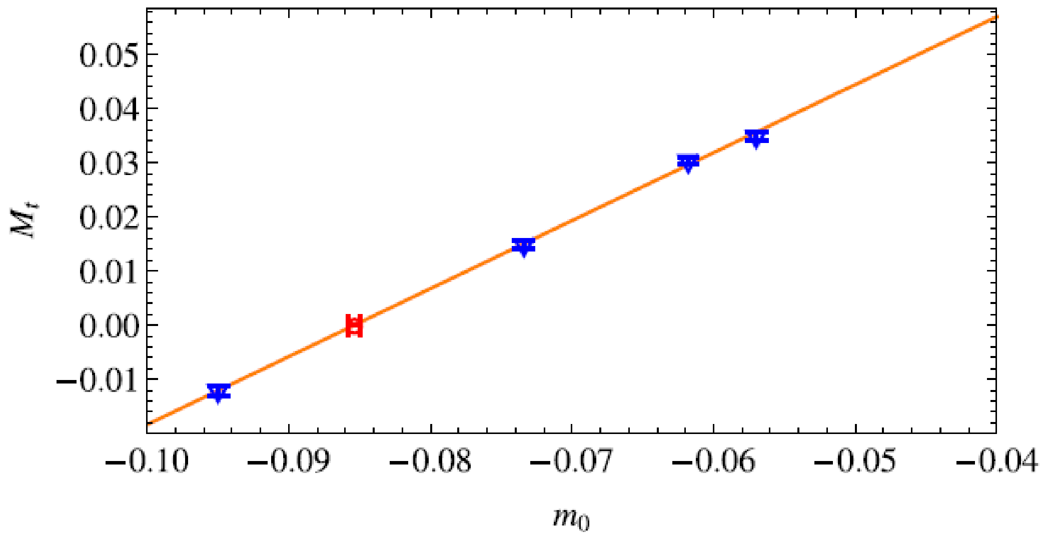
  - Mild dependence on quark mass; fixed γ_g and γ_f
- PCAC mass measured in SF scheme: $m_{\rm cr} = -0.0854(5)$



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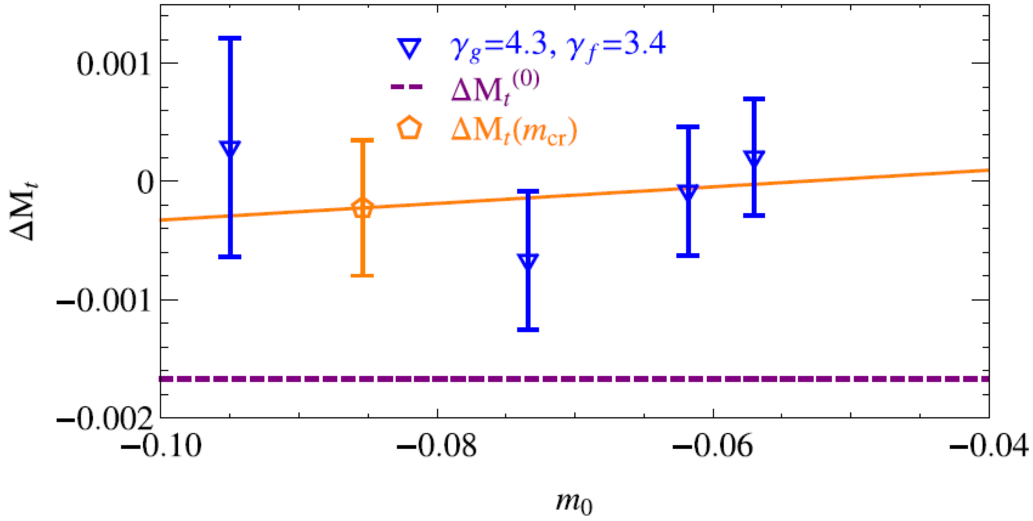
  - Plot of γ_g and γ_f versus input current quark mass
  - Mild dependence on quark mass; fixed γ_g and γ_f
- PCAC mass measured in SF scheme: $m_{\rm cr} = -0.0854(5)$
- Check NP $c_{s,t}$ condition in SF scheme



2+1-Flavor Runs

- Mass-independent scheme (fixed $\beta = 1.5$ approach)
- Scale and masses are defined in chiral limit

(Edwards, Joo, Lin, Peardon, work in progress)

L_x	L_t	m_l	m_s	L (fm)	m_π L	m_π (MeV)
12	96	−0.0540	−0.0540	1.44	11.6	~ 1600
12	96	−0.0699	−0.0540	1.44	8.3	
12	96	−0.0794	−0.0540	1.44	5.9	
12	96	−0.0826	−0.0540	1.44	9.6	
16	96	−0.0826	−0.0540	1.92	6.3	~ 660
12	96	−0.0618	−0.0618	1.44	9.7	~ 1340
16	128	−0.0743	−0.0743	1.92	8.1	~ 850
16	128	−0.0808	−0.0743	1.92	5.6	
16	128	−0.0830	−0.0743	1.92	4.5	
16	128	−0.0840	−0.0743	1.92	3.8	
24	128	−0.0840	−0.0743	2.88	5.7	~ 390

Algorithm

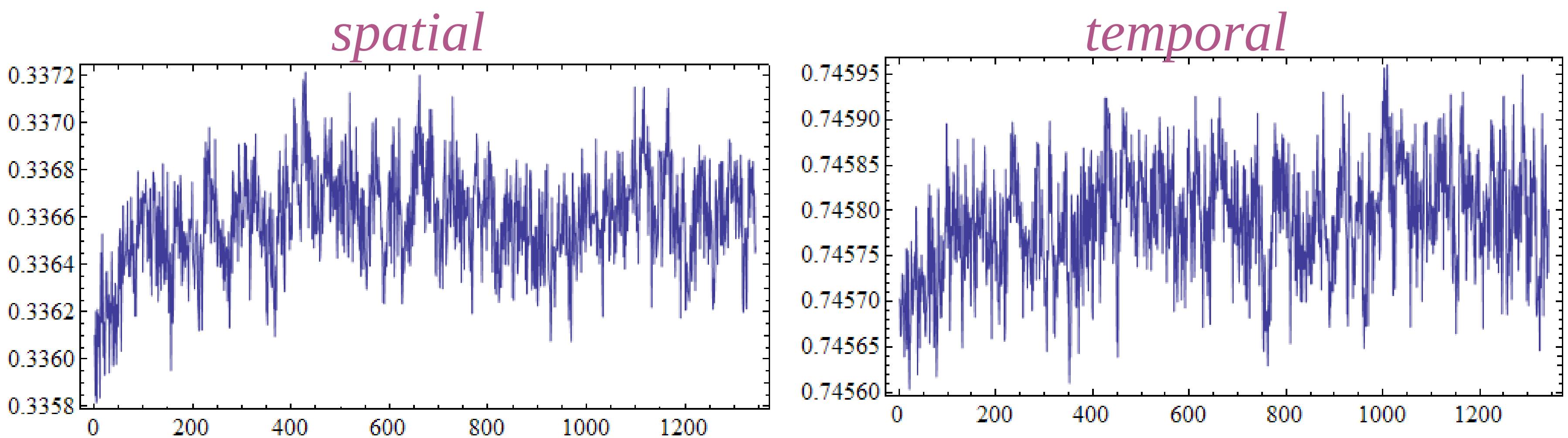
- Rational Hybrid Monte Carlo (RHMC)
- Multi-scale anisotropic molecular dynamics update
- Even-odd preconditioning for the clover term
- Stout-link smearing in fermion actions

$$\frac{d\tilde{Q}}{dU_{\mathrm{thin}}} = \frac{d\tilde{Q}}{dU_{\mathrm{stout}}} \frac{dU_{\mathrm{stout}}}{dU_{\mathrm{thin}}}$$

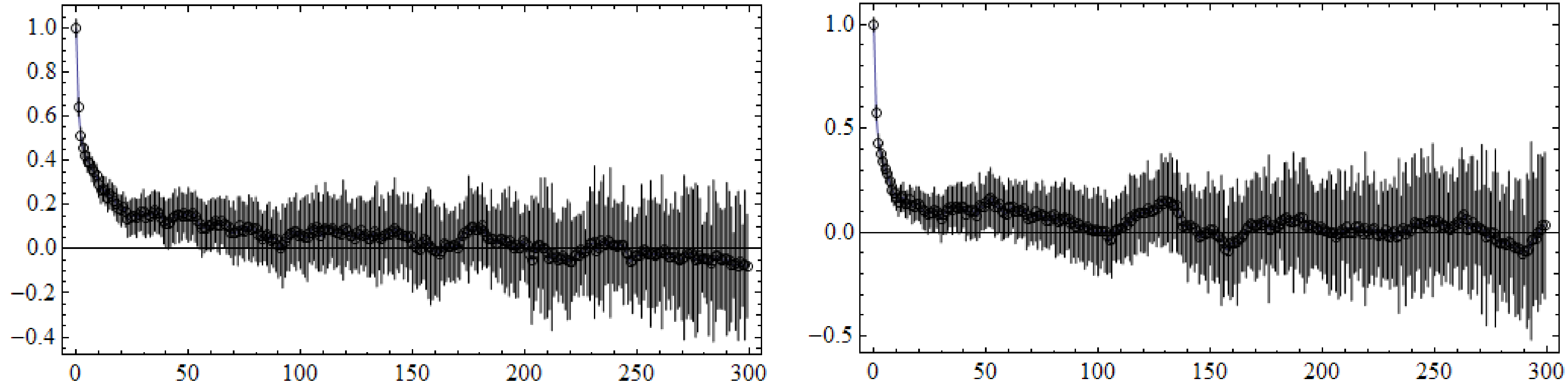
- Split gauge term
- Three time scales
  - δt_1: Omelyan integrator for $\mathrm{tr}\,\log A_{ee}$ and $\phi_i^{\dagger} r^{-\frac{1}{2}}(\tilde{Q})\phi$
  - δt_2: Omelyan integrator $S_{G,(\mathrm{S})}$
  - δt_3: Omelyan integrator $S_{G,(\mathrm{T})}$
  - Choice: $\delta t_1 = \delta t_2$
- Acceptance rate: 75%

Autocorrelation

- Example: $24^3 \times 128$ volume, with pion mass 315 MeV
- Plaquette history

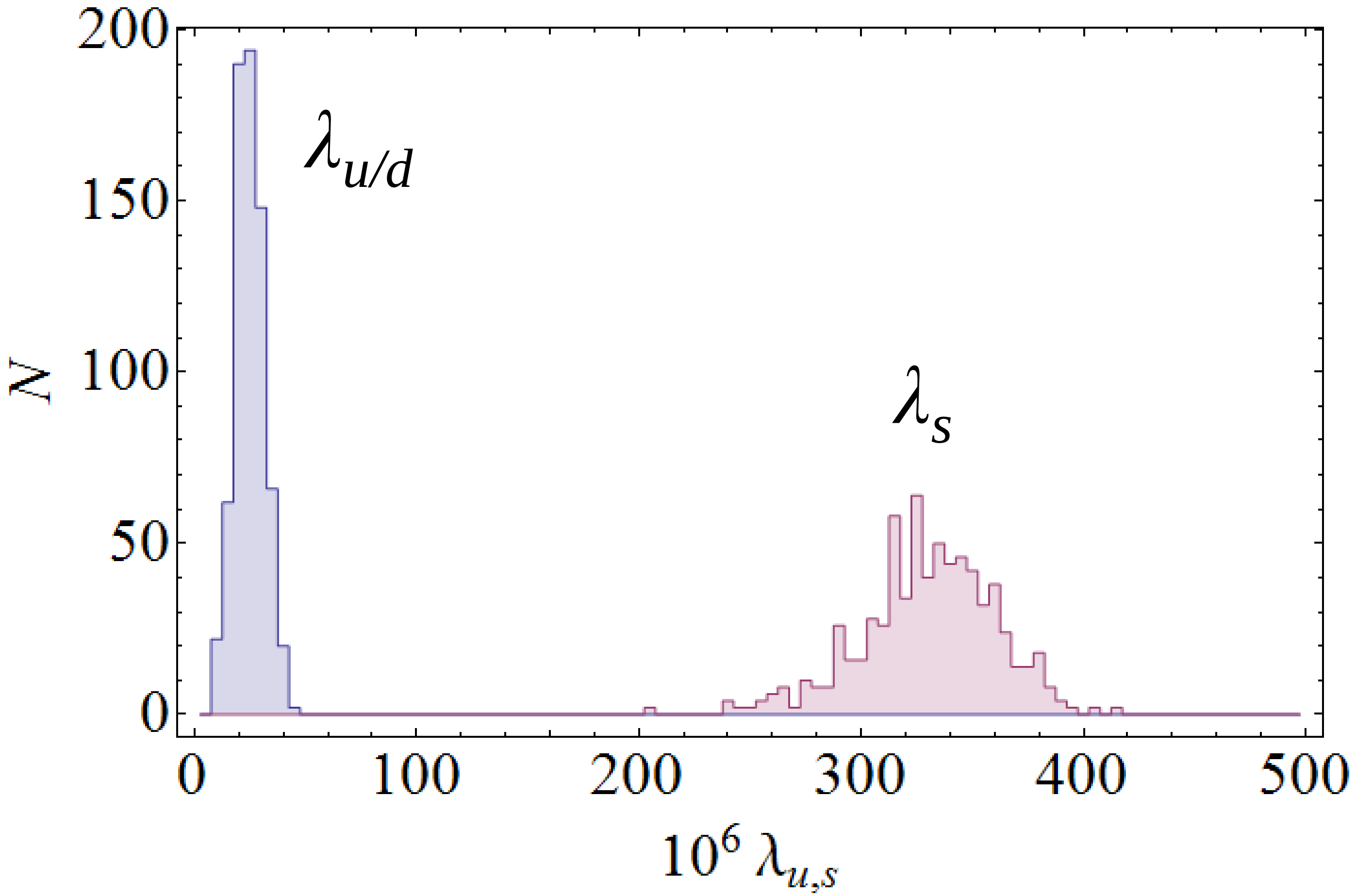


- Autocorrelation



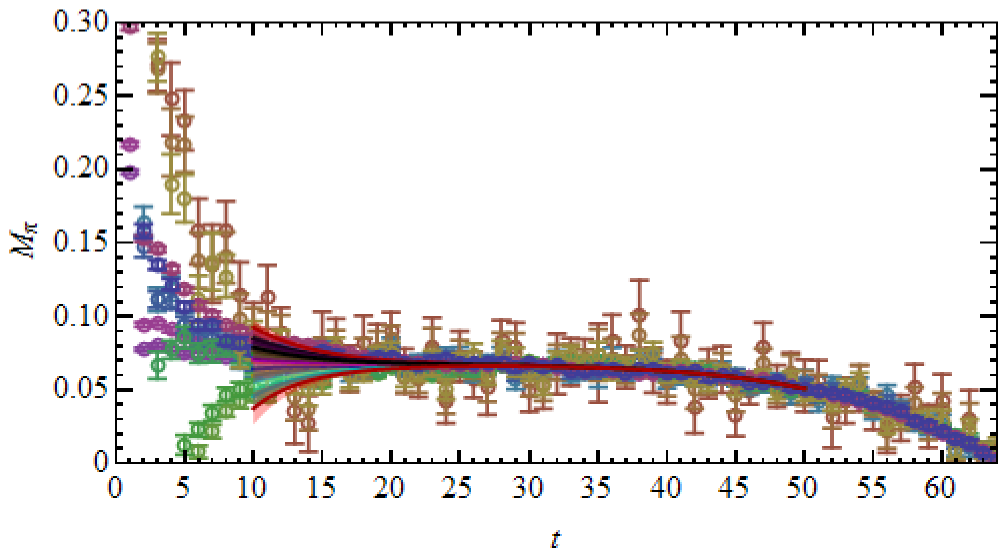
Lowest Eigenvalue

- Example: $24^3 \times 128$ volume, with pion mass 315 MeV
- Histogram distributions



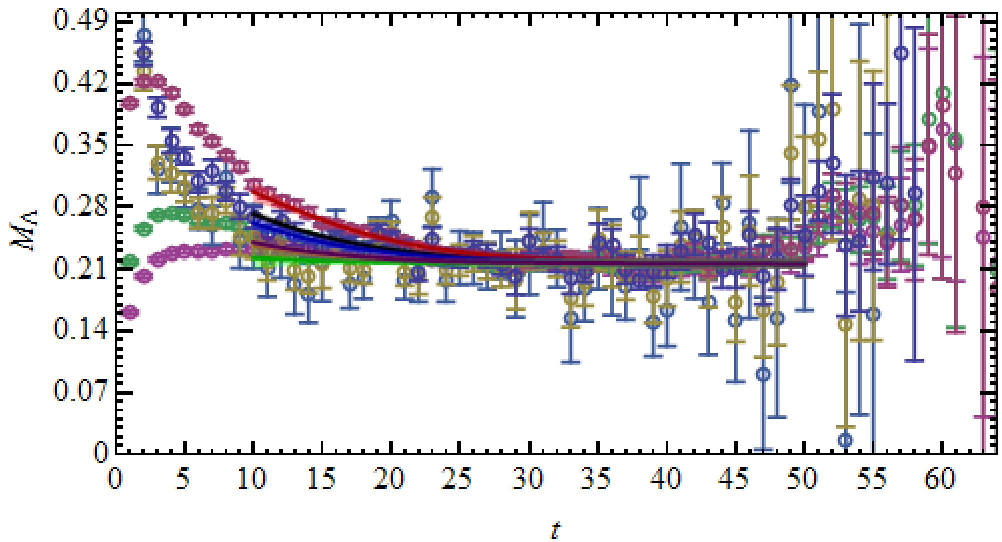
2+1-Flavor Runs

- Preliminary spectroscopic measurements
  - 3 Gaussian smearing parameters + Point/Smeared sink
  - Average over 4 time sources
    (w/ eigcg solver 0707.0131 [hep-lat])
    {0,0,0,0}, {8,8,8,32}, {0,0,0,64}, {8,8,8,128}
  - Ground states obtained from 2-state fits
  - For example: 12 pion correlators



2+1-Flavor Runs

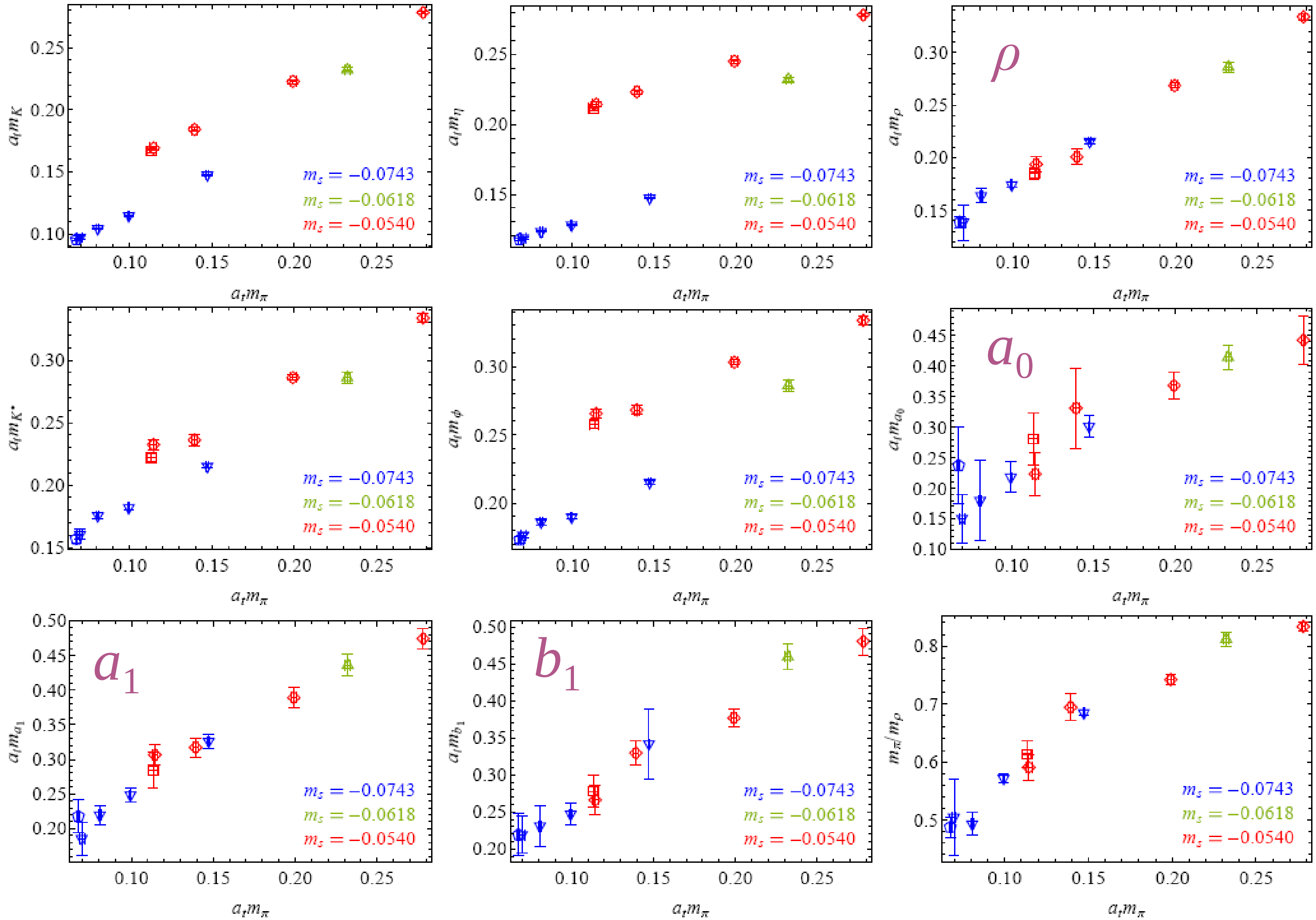
- Preliminary spectroscopic measurements
  - 3 Gaussian smearing parameters + Point/Smeared sink
  - Average over 4 time sources
    (w/ eigcg solver 0707.0131 [hep-lat])
    {0,0,0,0}, {8,8,8,32}, {0,0,0,64}, {8,8,8,128}
  - Ground states obtained from 2-state fits
  - For example: 6 Lambda correlators



More spectroscopy results by Saul Cohen

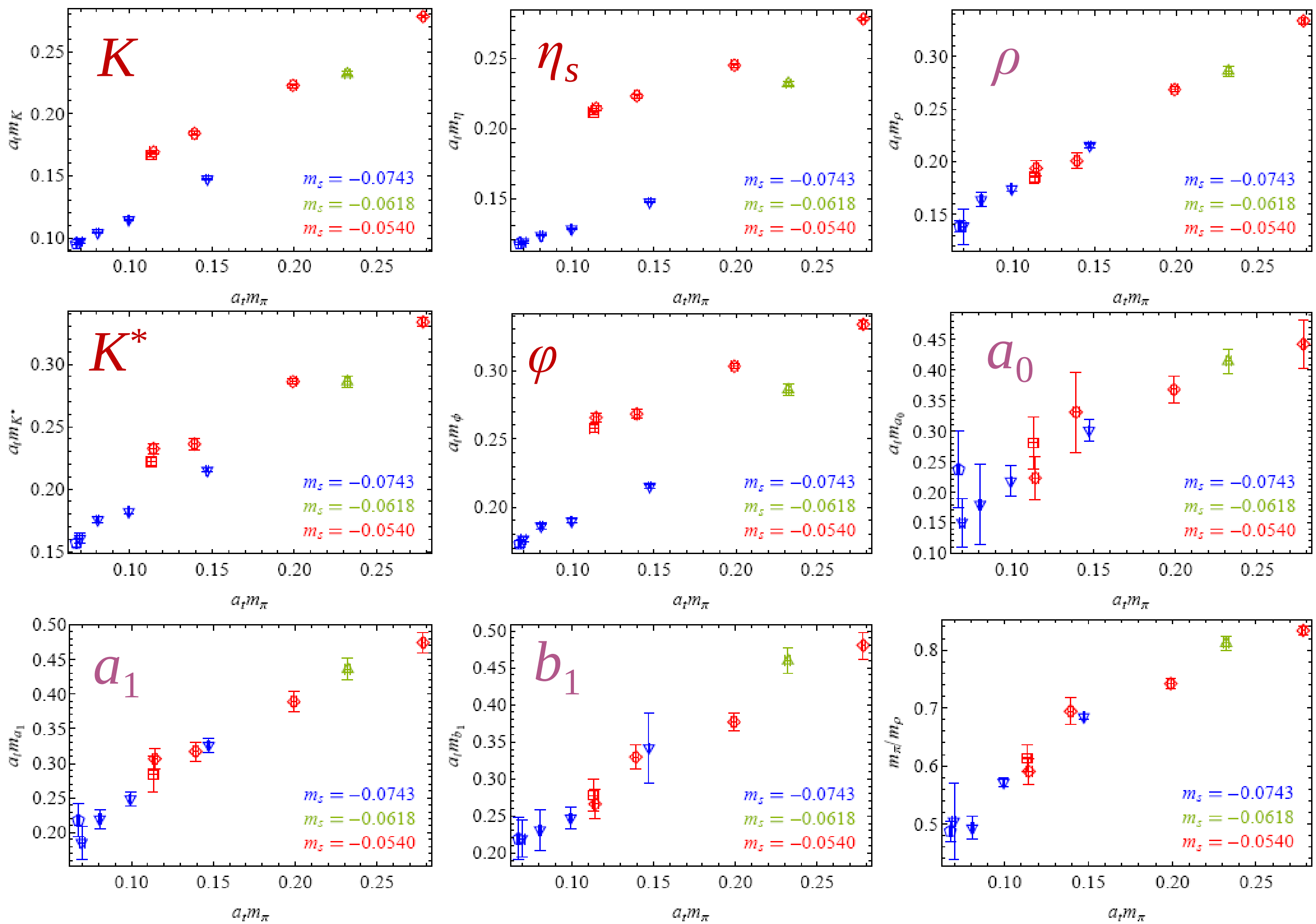
2+1-Flavor Runs

- Meson strange-sea dependence



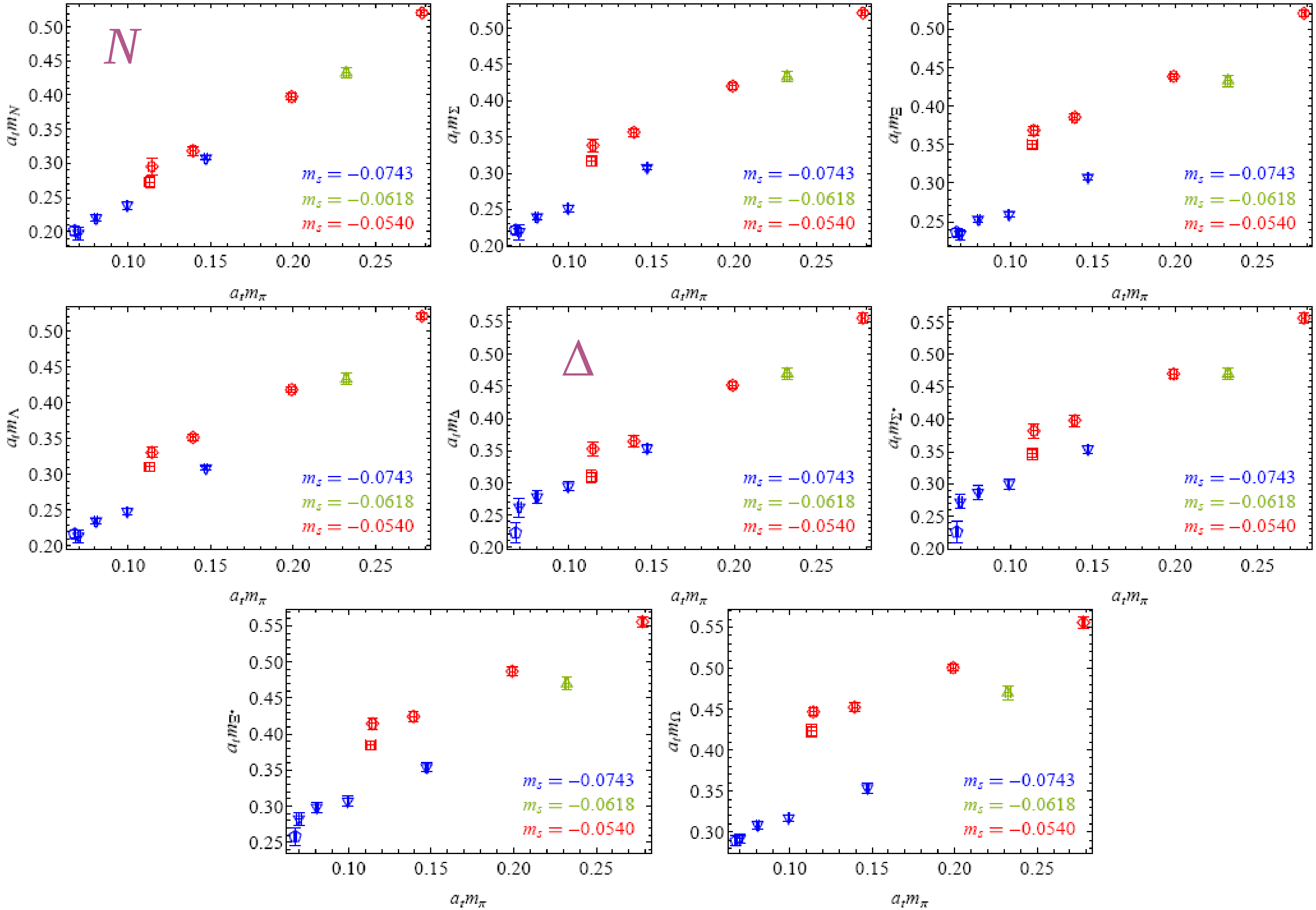
2+1-Flavor Runs

- Meson strange-sea dependence



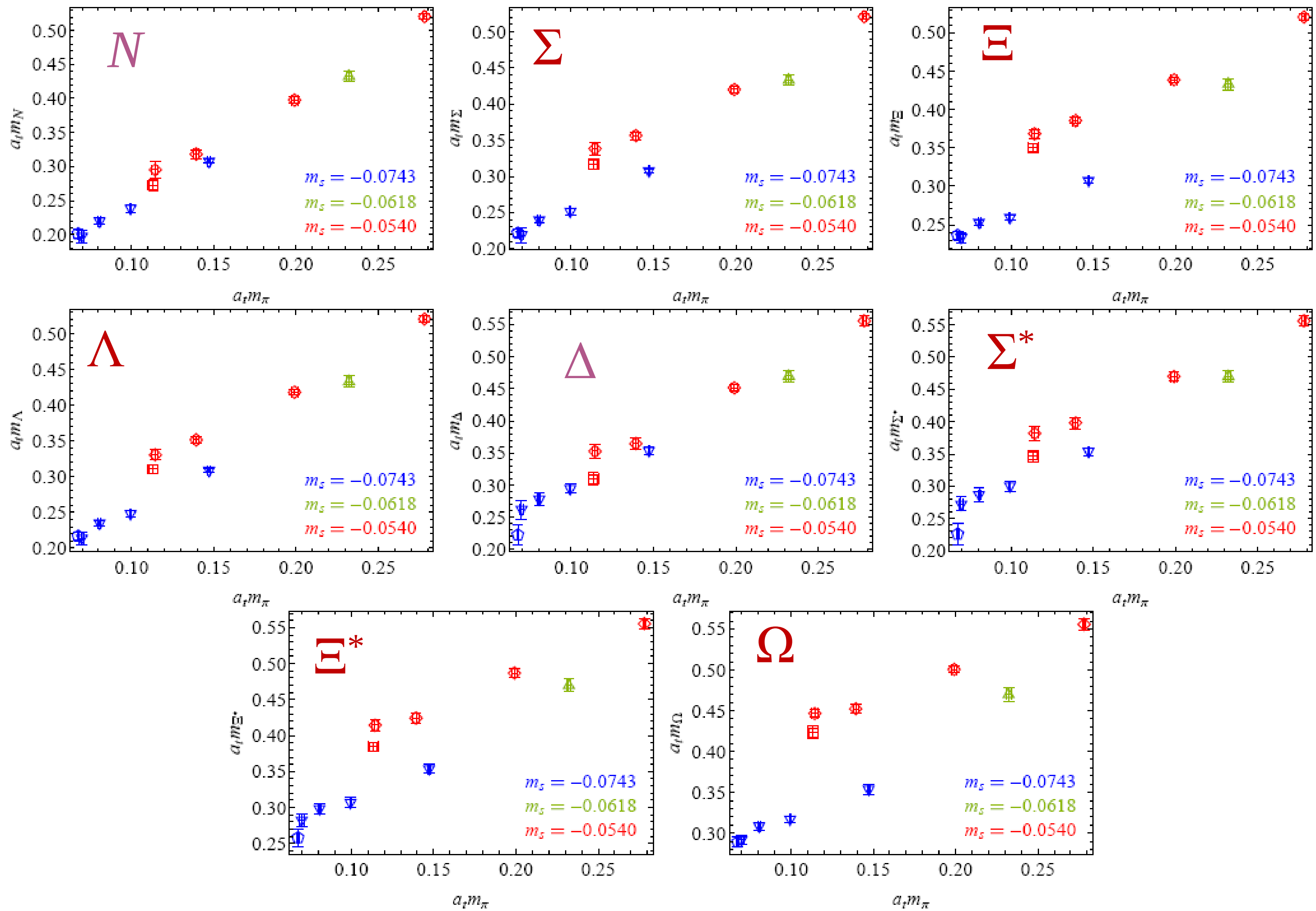
2+1-Flavor Runs

- Baryon strange-sea dependence



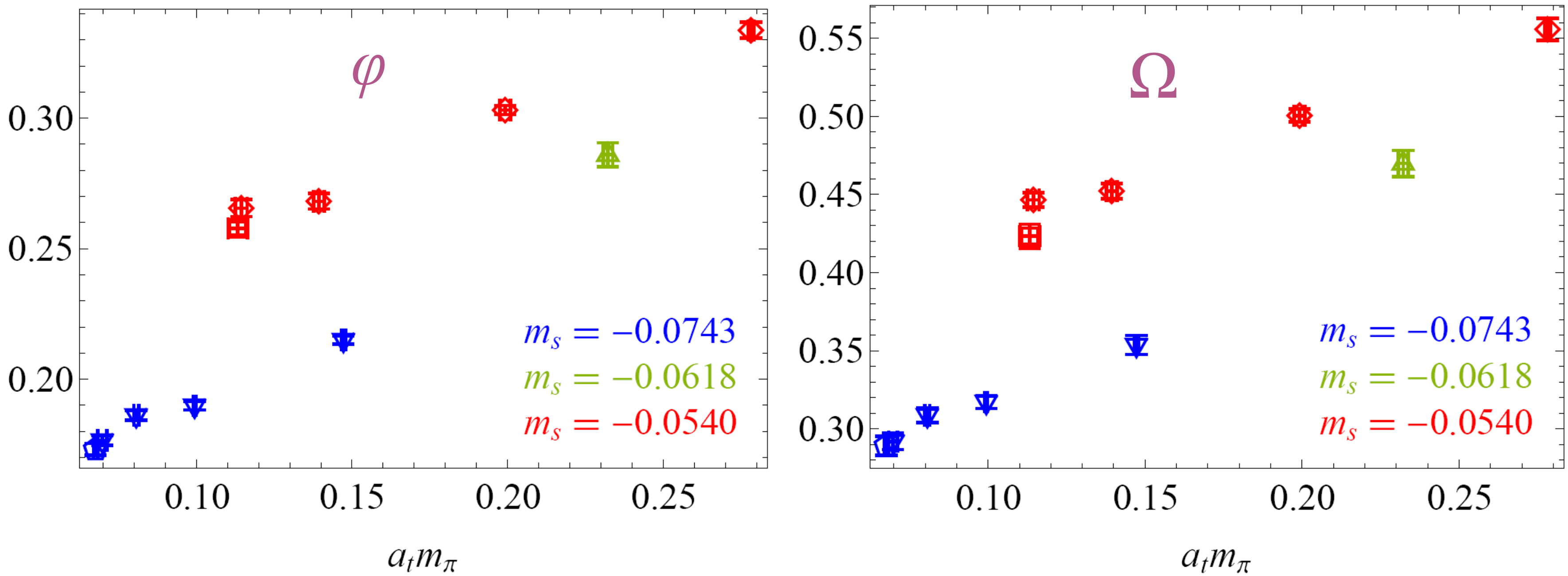
2+1-Flavor Runs

- Baryon strange-sea dependence



Strange-Quark Mass

- Difficult: Chiral extrapolation to obtain m_s and r_0/a_s
- Strange-quark tuning
  - Candidates: kaon, φ, Ω mass, etc.
  - Example: at a fixed m_s, see 30% variation in phi mass



- Need multiple 2+1 runs to obtain reasonable m_s

Newport News Plot

- Better description for *s*-quark tuning
  - Use ratio of hadron masses to eliminate lattice spacing
  - Leading-order XPT

    $l_\Omega = (9/4)\, m_\pi^2/m_\Omega^2$ and

    $s_\Omega = (9/4)\, (2m_K^2 - m_\pi^2)/m_\Omega^2$

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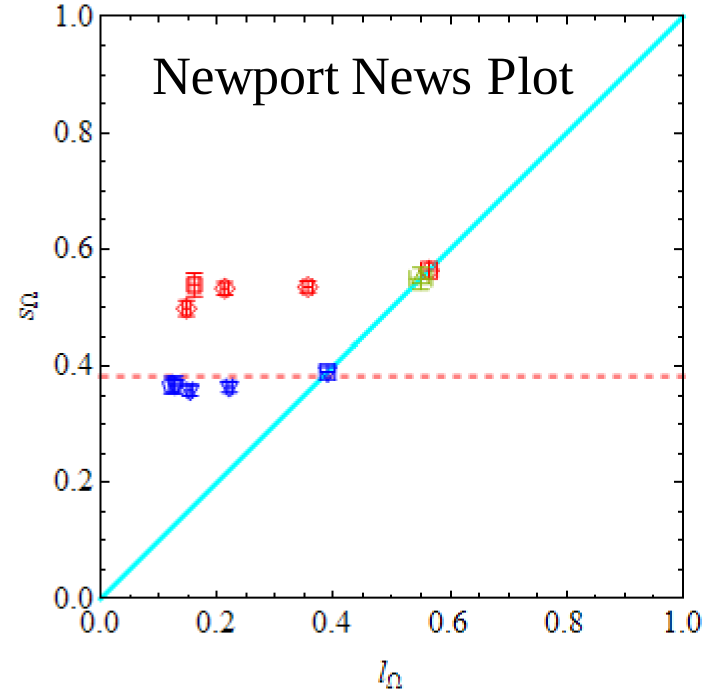

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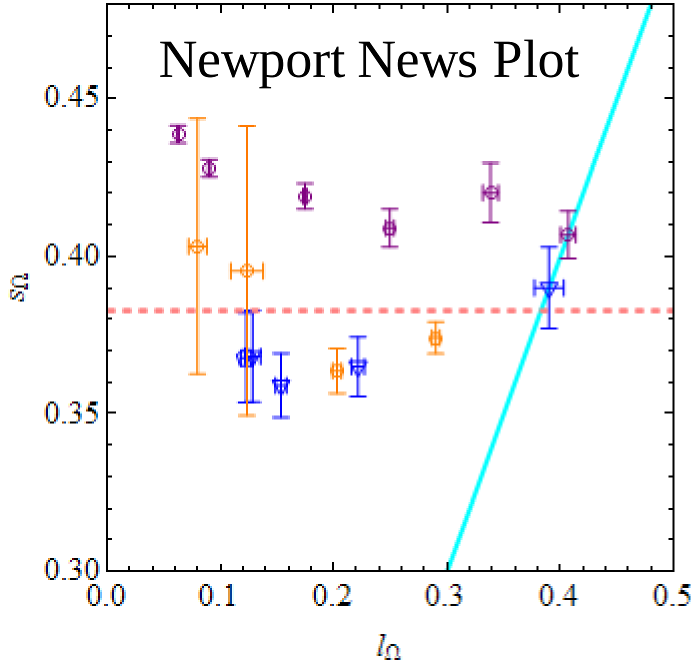
  - 2+1f comparison plot

    Aniso-clover, $a_s = 0.13$ fm

    DWF on asqtad, $a = 0.125$ fm (LHPC)

    DWF on DWF, $a = 0.116$ fm (RBC+UKQCD)



Newport News Plot

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  - Use ratio of hadron masses to eliminate lattice spacing
  - Leading-order XPT
    $l_\Omega = (9/4)\, m_\pi^2/m_\Omega^2$ and
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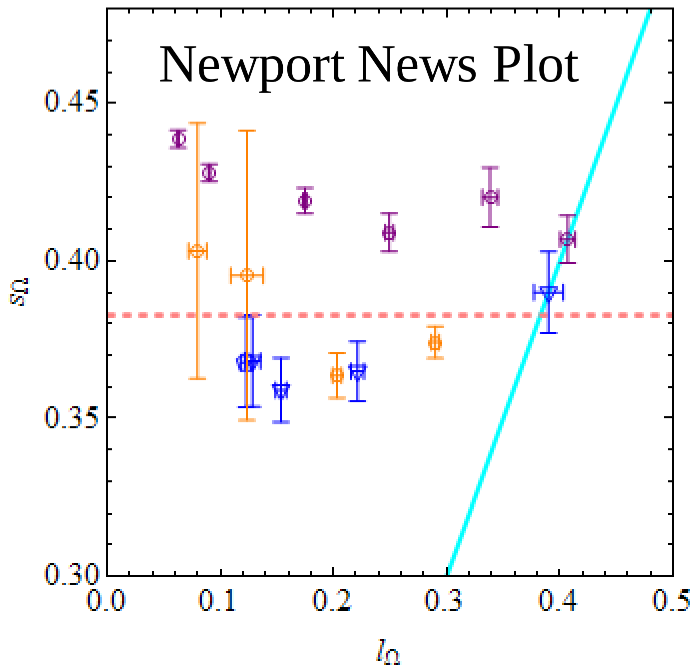
  - 2+1f comparison plot
    Aniso-clover, $a_s \sim 0.13$ fm
    DWF on asqtad, $a = 0.125$ fm (LHPC)
    DWF on DWF, $a = 0.116$ fm (RBC+UKQCD)
  - LO Extrapolation
    Strange is off by 4–6%
  - NLO correction?



Inputs	a_t^{-1}(GeV)	$m_l^{\rm phys}$	$m_s^{\rm phys}$
$m_\pi^2,\ m_k^2,\ m_\Omega$	5.39(8)	−0.08668(11)	−0.0705(4)
$m_\pi^2,\ m_k^2,\ m_\phi$	5.47(5)	−0.08651(8)	−0.0710(2)

Future Dynamical Generation

Where we stand now:

- Scaling based on actual (24^3) runs down to ~170 MeV

$$\text{Cost}_{\text{traj}} = \xi^{1.25}\left(\frac{\text{fm}}{a_s}\right)^6 \cdot \left[\left(\frac{L_s}{\text{fm}}\right)^3\left(\frac{L_t}{\text{fm}}\right)\right]^{5/4} \cdot [C_1 + C_2/m_l]\,.$$

- Currently, ~5k traj @ 875, 580, ~3k @ 456 MeV (16^3): ~6k by July 1
- 315 MeV (24^3), currently 3k traj, get ~1k traj/week
- 24^3 315 MeV ORNL runs underway now
- 24^3 and 32^3 250 MeV for the near future

Future plans:

- < 200 MeV generation possible within next year or two
- Excited single-particle state vs. multi-particle ones
- Multiple lattice spacings

Lattice 2008
July 14-19, 2008
Williamsburg, Virginia, USA
Conference Topics:
• Algorithms and Machines
• Applications beyond QCD
• Chiral Symmetry
• Hadron Spectroscopy
• Hadron Structure
• Nonzero Temperature and Density
• Standard Model Parameters and Renormalization
• Theoretical Developments
• Vacuum Structure and Confinement
• Weak Decays and Matrix Elements
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