$N_f = 2 + 1$ lattice QCD at the physical mass point

Determining the light quark masses

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Work in progress

Special thanks to Dürr, Fodor and Hoelbling

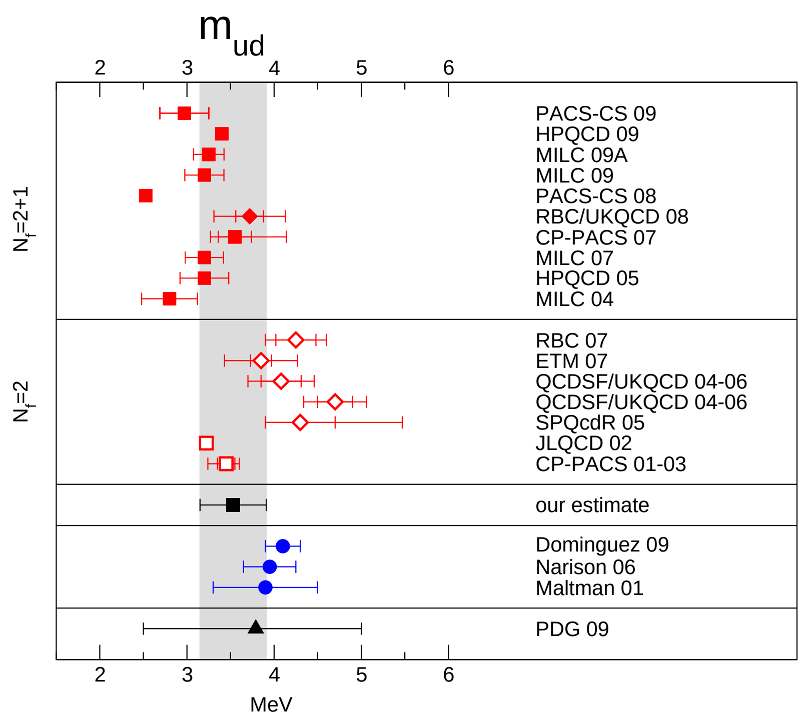
Introduction

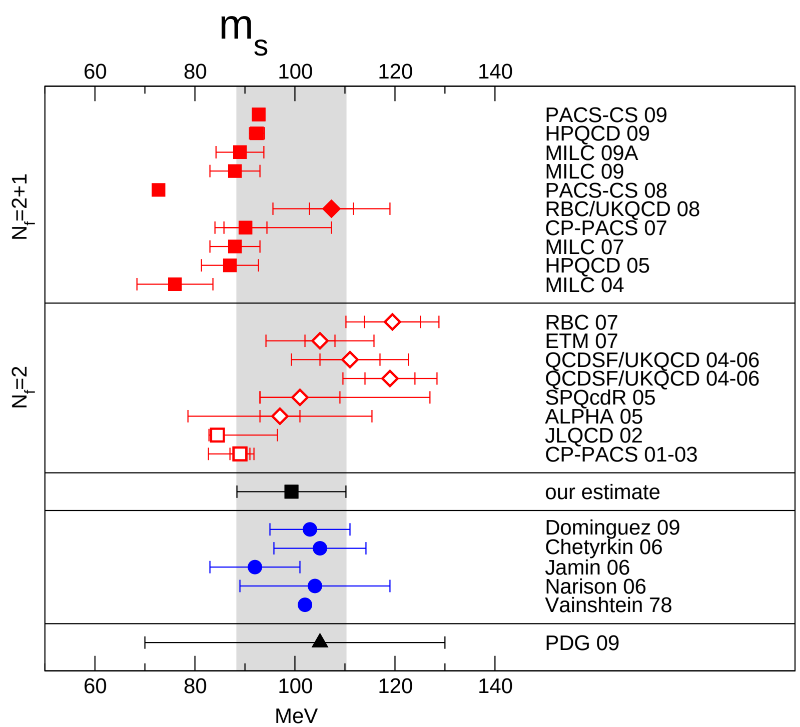
- The masses of the light u, d and s quarks are fundamental parameters of the Standard Model (SM)
- The stability of atoms, the nuclear reactions which power stars, the presence or absence of strong CP violation, etc. depend critically on their precise values
- Their values carry information about the flavor structure of physics beyond the SM
- Quarks are confined w/in hadrons
  $\Rightarrow$ a nonperturbative computation is required to determine them
- The deviation of $m_{ud} \equiv (m_u + m_d)/2$ from zero brings only very small corrections to most hadronic observables
  $\Rightarrow$ its determination is a needle in a haystack problem
- Fortunately, QCD spontaneously breaks chiral symmetry
  $\Rightarrow$ the masses of the resulting Nambu-Goldstone mesons are very sensitive to the light quark masses

$\Rightarrow$ quark masses are an interesting first "measurement" to make w/ physical point LQCD simulations

Current knowledge of the light quark masses

The Flavianet Lattice Averaging Group (FLAG) has performed a detailed analysis of unquenched lattice determinations of the light quark masses





$$m_{ud}^{\overline{MS}}(2\,\mathrm{GeV}) = \begin{cases} 3.53(38)\,\mathrm{MeV} & [11\%] \quad \text{FLAG} \\ 2.5 \div 5.0\,\mathrm{MeV} & [30\%] \quad \text{PDG} \end{cases}$$

$$m_{s}^{\overline{MS}}(2\,\mathrm{GeV}) = \begin{cases} 99.(11)\,\mathrm{MeV} & [11\%] \quad \text{FLAG} \\ 70 \div 130\,\mathrm{MeV} & [30\%] \quad \text{PDG} \end{cases}$$

Even extensive study by MILC does not control all systematics:

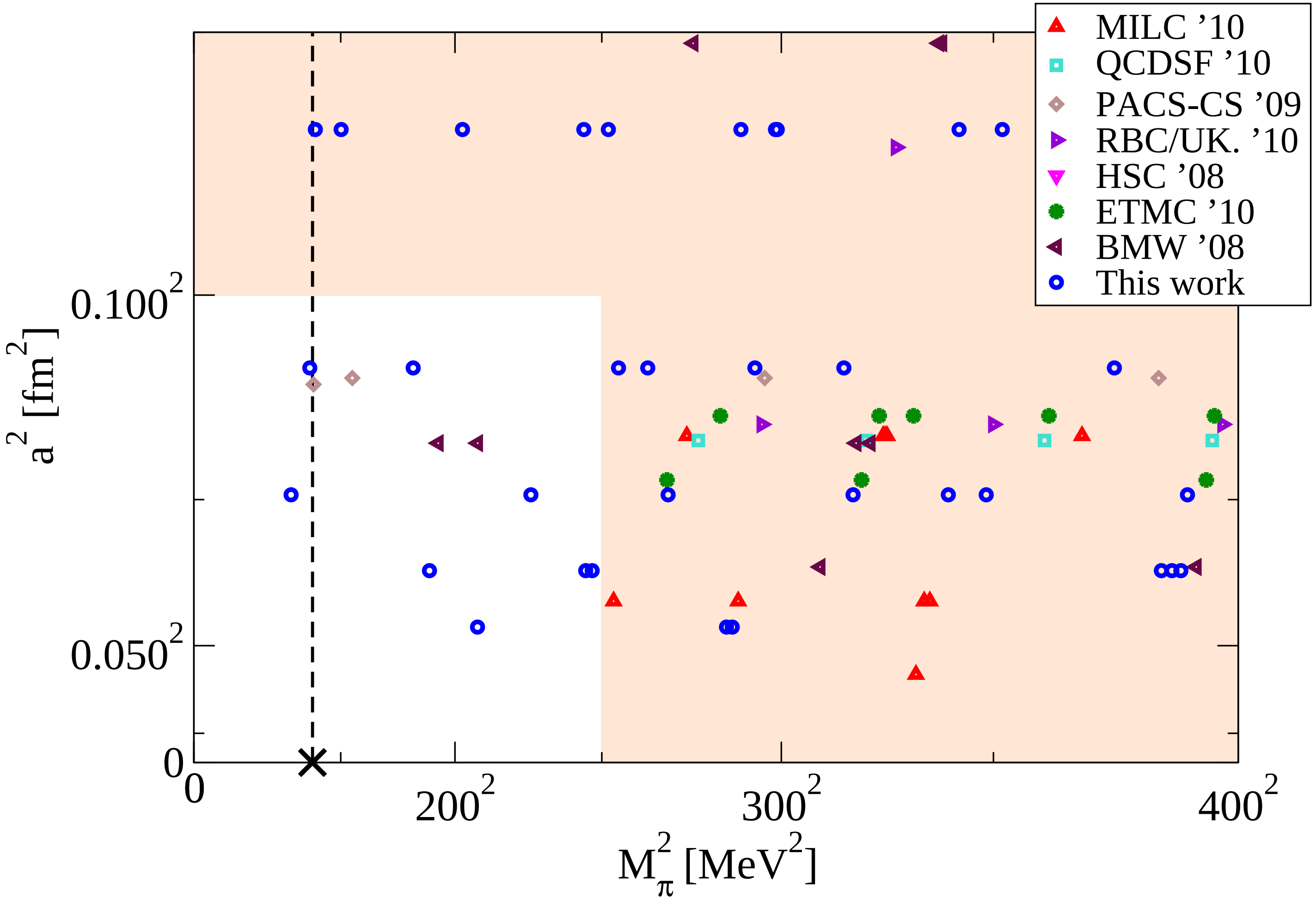
- $M_\pi^{\mathrm{RMS}} \geq 260\,\mathrm{MeV} \quad \Rightarrow \quad m_{ud}^{\mathrm{MILC,eff}} \geq 3.7 \times m_{ud}^{\mathrm{phys}}$
- perturbative renormalization (albeit 2 loops)

The calculation that I have been dreaming of doing

- $N_f = 2 + 1$ all the way down to $M_\pi \lesssim 135\,\mathrm{MeV}$ to allow small interpolation to physical mass point
- Large $L \gtrsim 5\,\mathrm{fm}$ to have sub percent finite V errors
- At least three $a \leq 0.1\,\mathrm{fm}$ for controlled continuum limit
- A reliable determination of the scale w/ a well measured physical observable
- Unitary, local gauge and fermion actions
- Full nonperturbative renormalization and continuum extrapolated running for determining RGI quark masses
- Complete analysis of systematic uncertainties

Where do we stand?

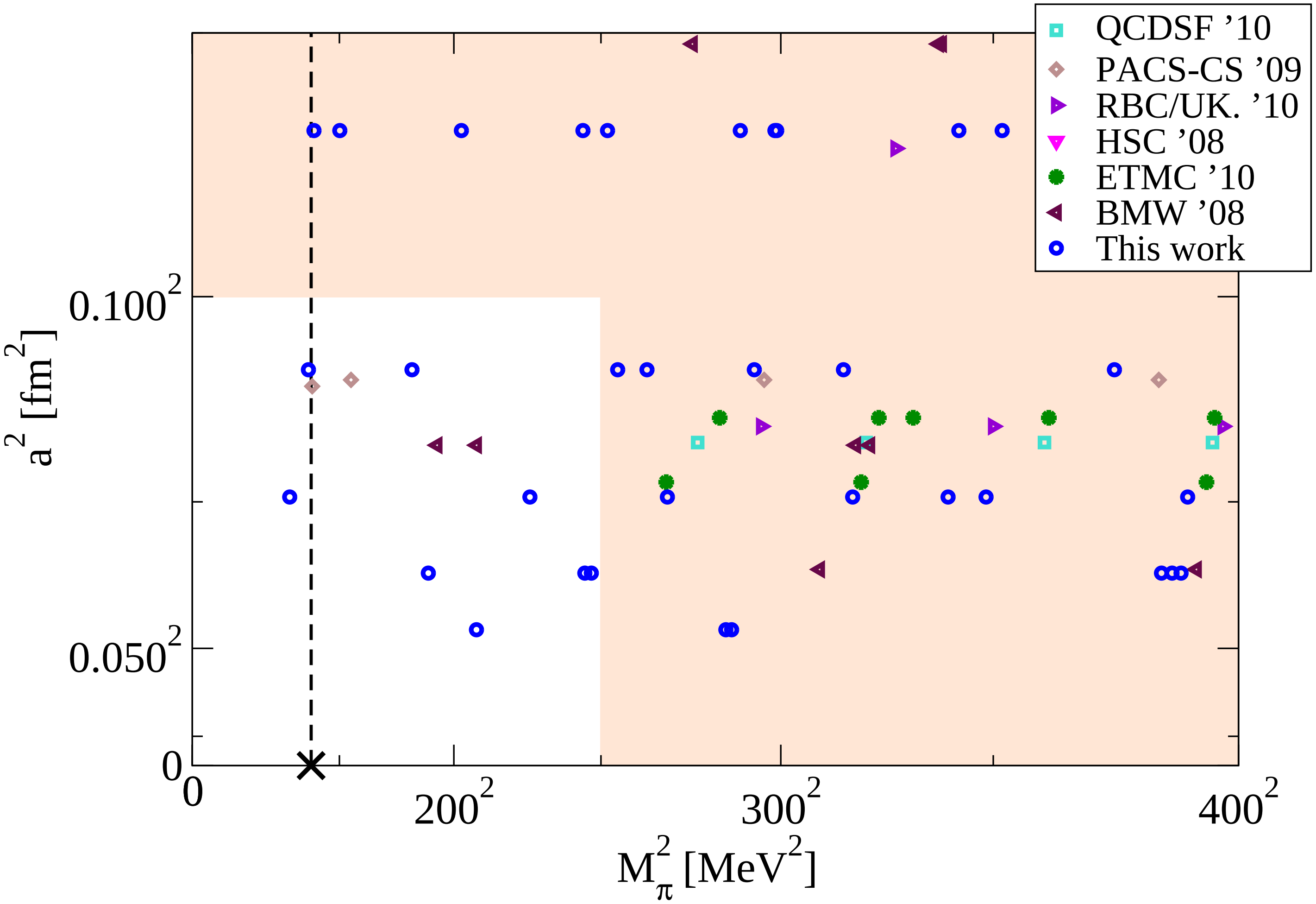
All simulations w/ $N_f \geq 2+1$ and $M_\pi \leq 400\,\mathrm{MeV}$ ... (points for our currently running, next-to-finest simulations at $\beta = 5.7$ are estimates)



(from C. Hoelbling, Lattice 2010)

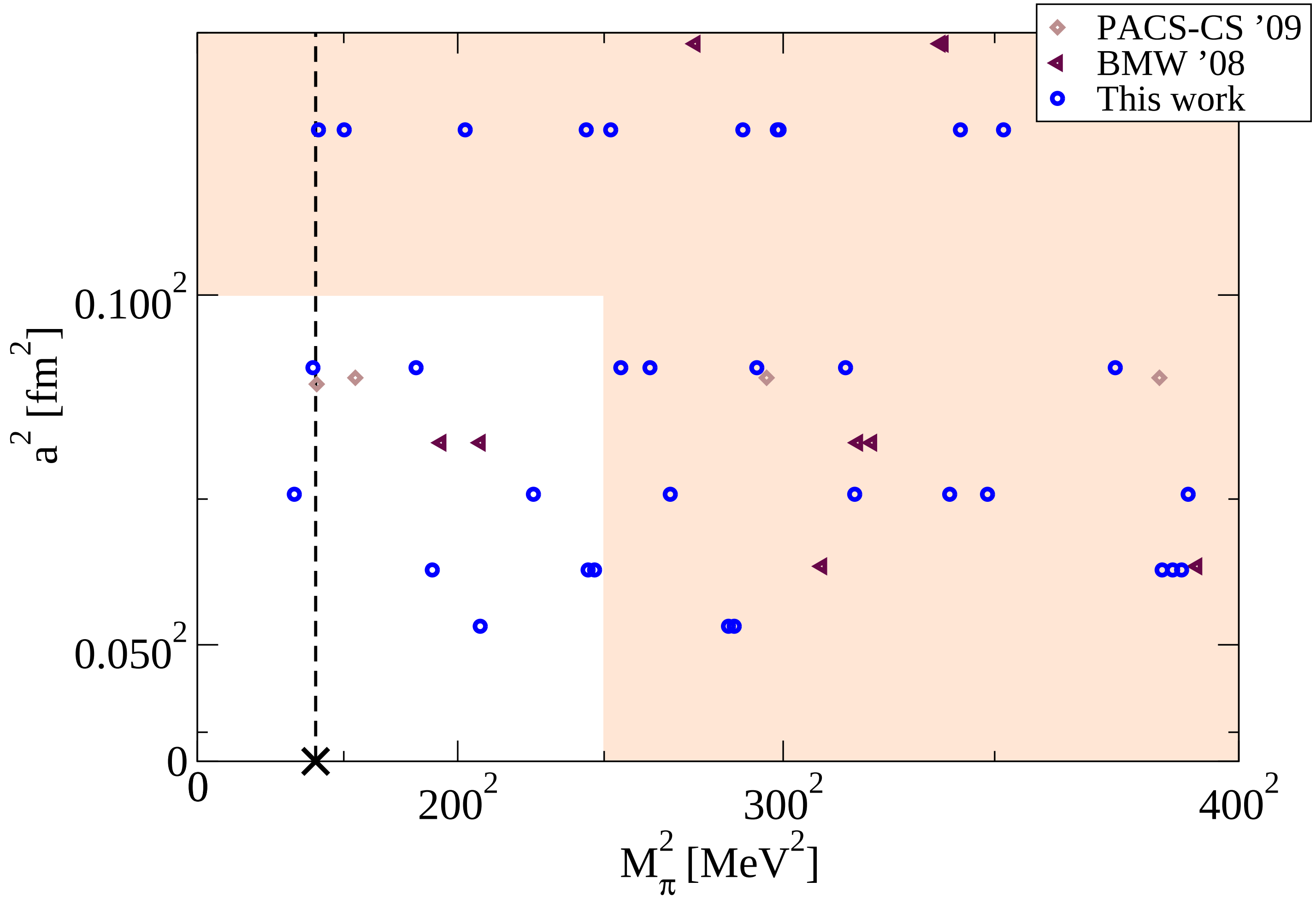
Where do we stand?

... and w/ unitary, local gauge and fermion actions...



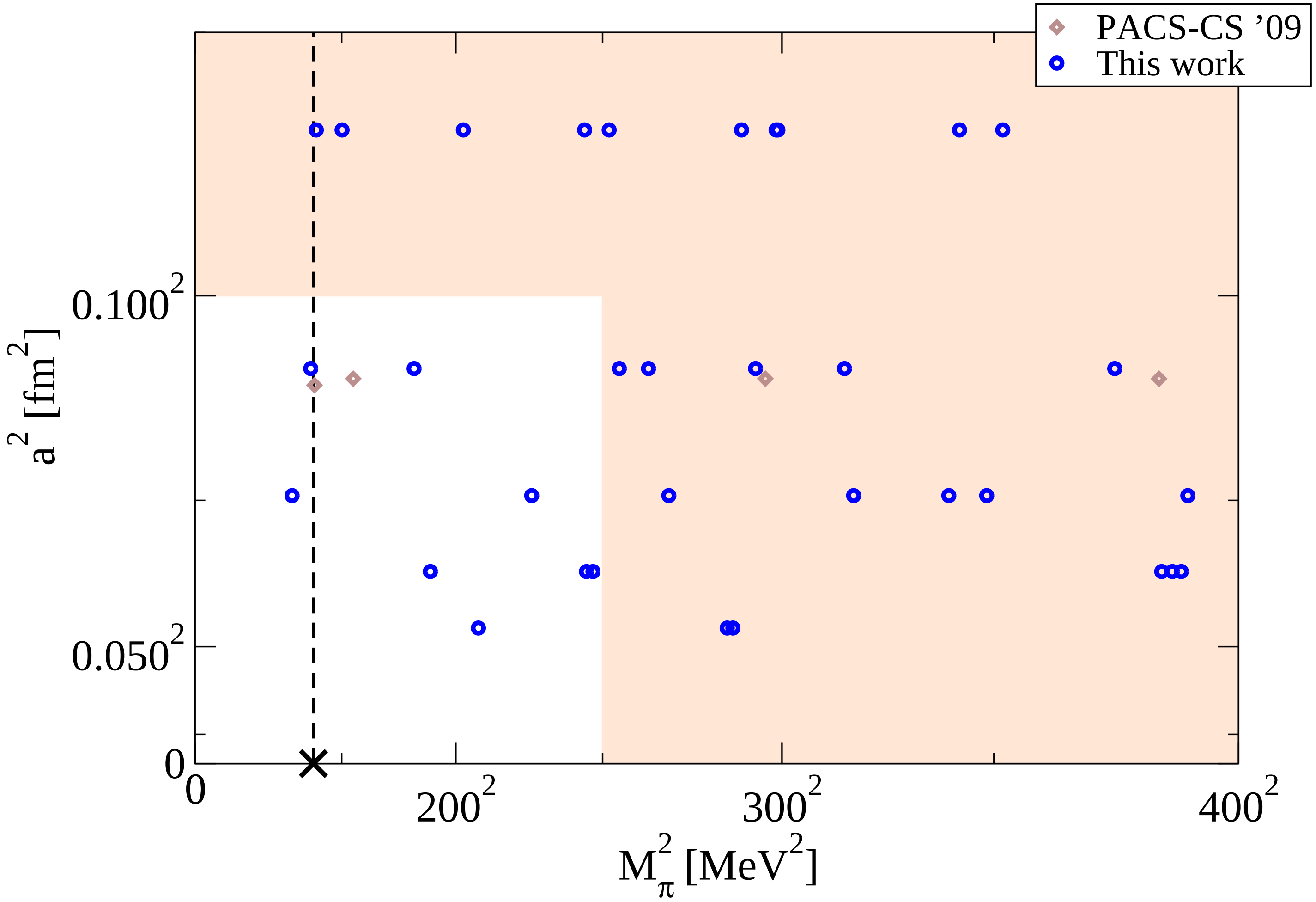
Where do we stand?

... and w/ sea *u* and *d* quarks clearly in the chiral regime, i.e. $M_\pi^{min} \leq 250\,\mathrm{MeV}$...



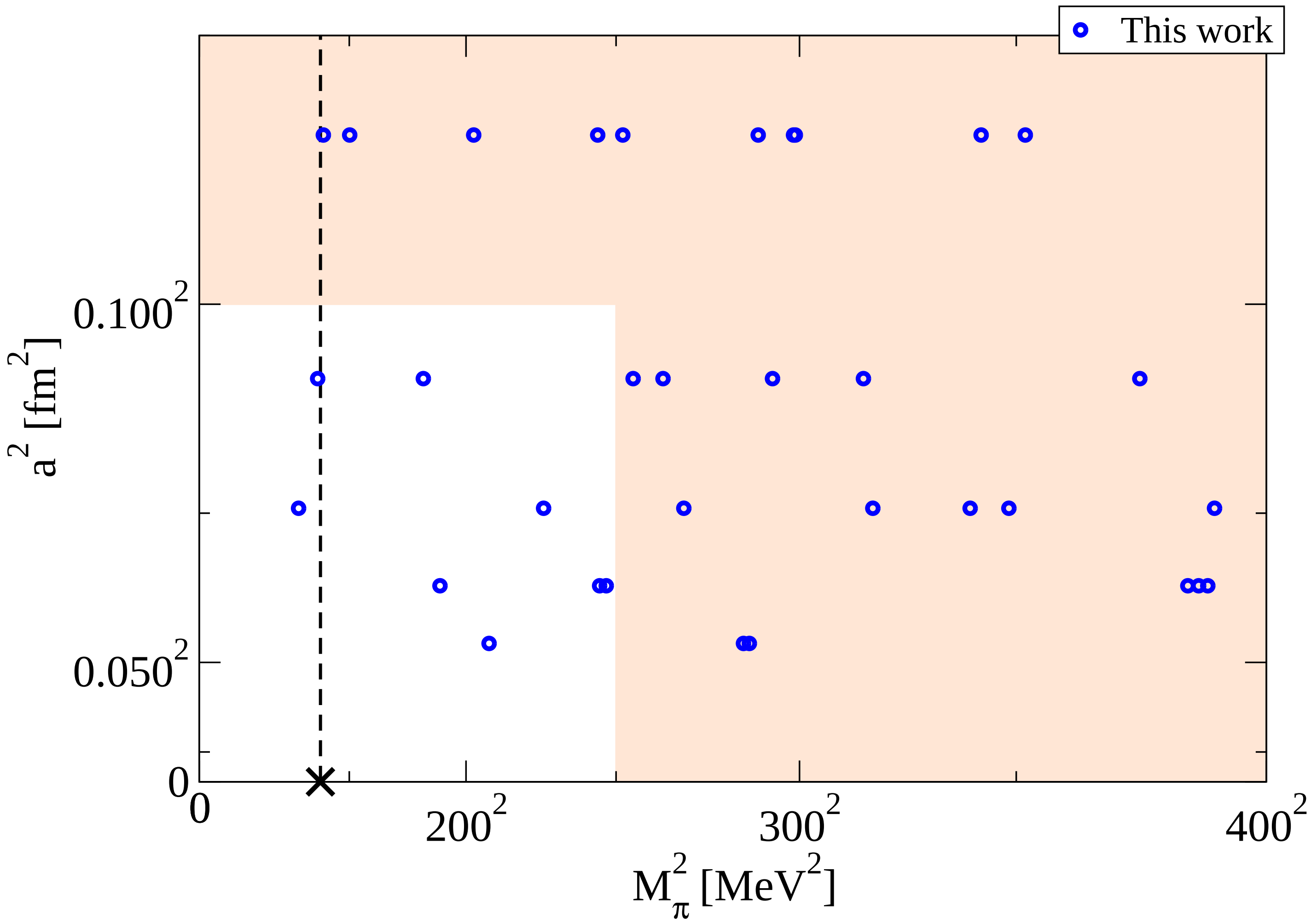
Where do we stand?

. . . and w/ sea *u* and *d* quarks at or below physical mass point . . .



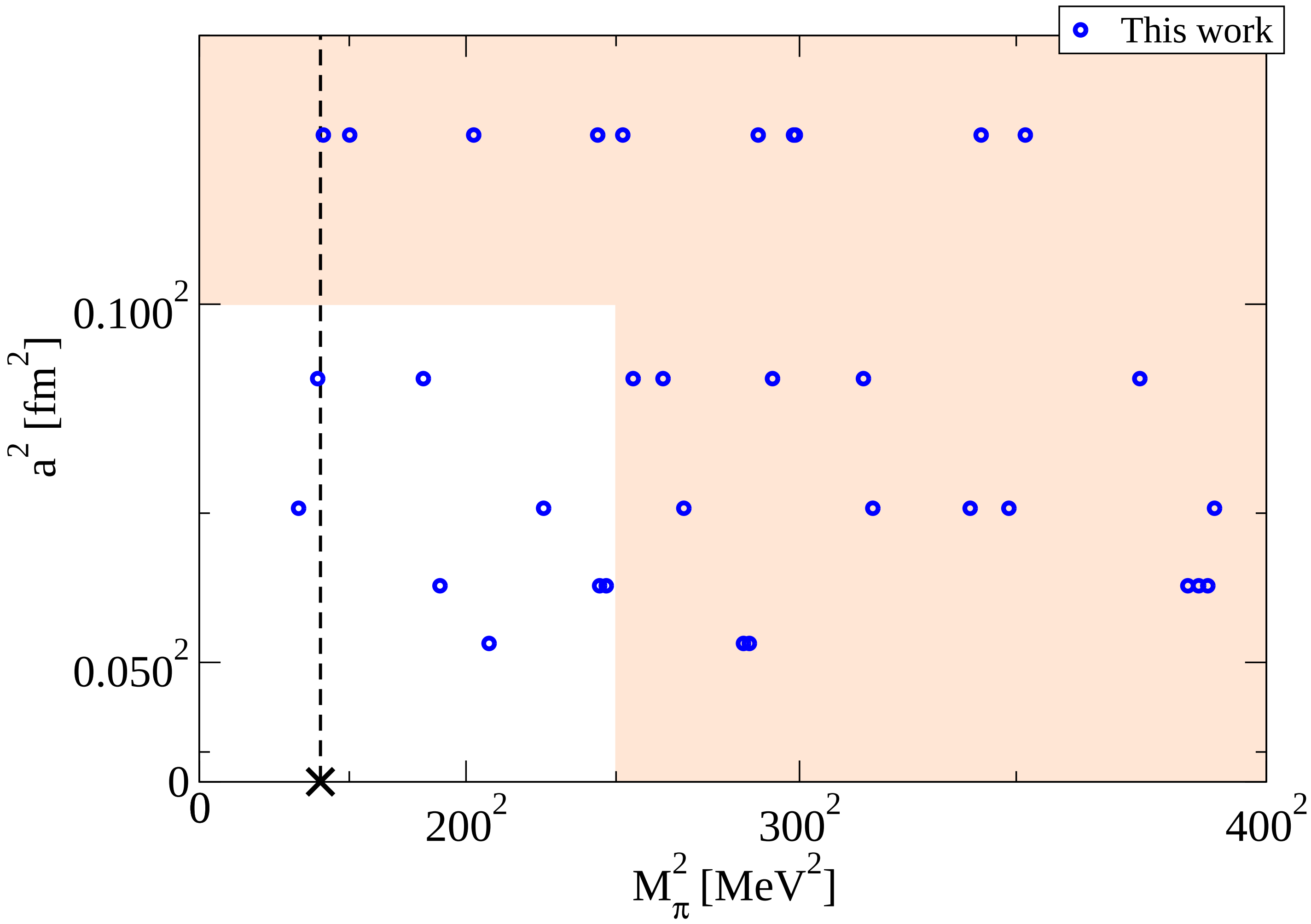
Where do we stand?

... and w/ volumes such that FV errors $\leq 0.5\%$ – PACS-CS has $LM_\pi = 1.97$ ...



Where do we stand?

... and w/ at least three $a \leq 0.1\ fm$ ...



How did we get there?

Dürr et al (BMW), PRD79 2009

$N_f = 2+1$ QCD: degenerate u & d w/ mass m_{ud} and s quark w/ mass $m_s \sim m_s^{\rm phys}$

1) Discretization which balances improvement in gauge/fermionic sector and CPU cost:

- tree-level $O(a^2)$-improved gauge action (Lüscher et al '85)
- tree-level $O(a)$-improved Wilson fermion (Sheikholeslami et al '85) w/ 2 HEX smearing (Morningstar et al '04, Hasenfratz et al '01, Capitani et al '06)

  $\Rightarrow$ approach to continuum is improved ($O(\alpha_s a, a^2)$ instead of $O(a)$)

2) Highly optimized algorithms (see also Urbach et al '06):

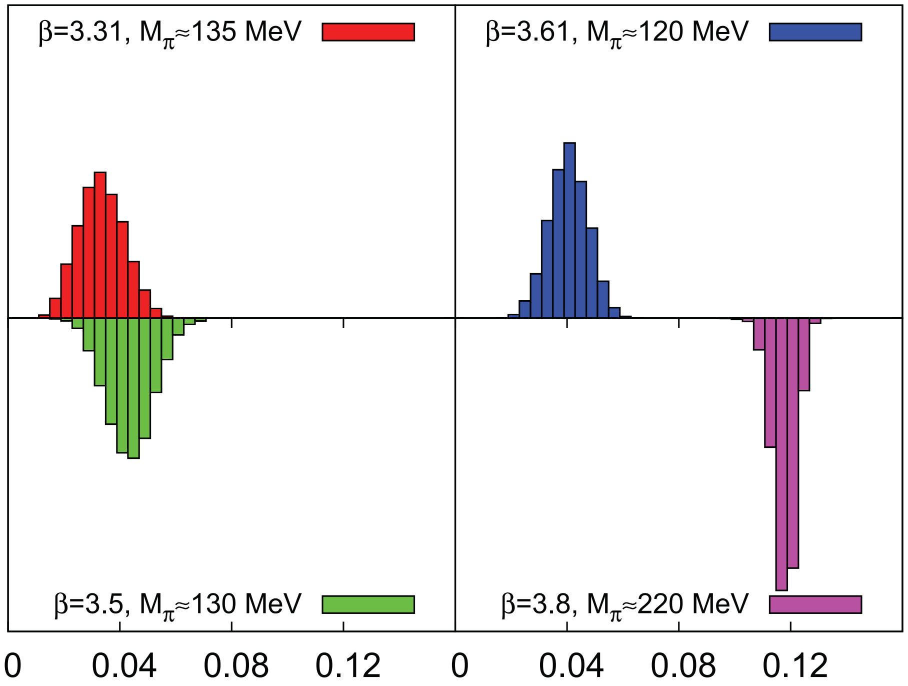
- Hybrid Monte Carlo (HMC) for u and d and Rational HMC (RHMC) for s
- mass preconditioning (Hasenbusch '01)
- multiple timescale integration of molecular dynamics (MD) (Sexton et al '92)
- Higher-order (Omelyan) integrator for MD (Takaishi et al '06)
- mixed precision acceleration of inverters via iterative refinement

3) Highly optimized codes for Blue Gene

How is our setup performing?

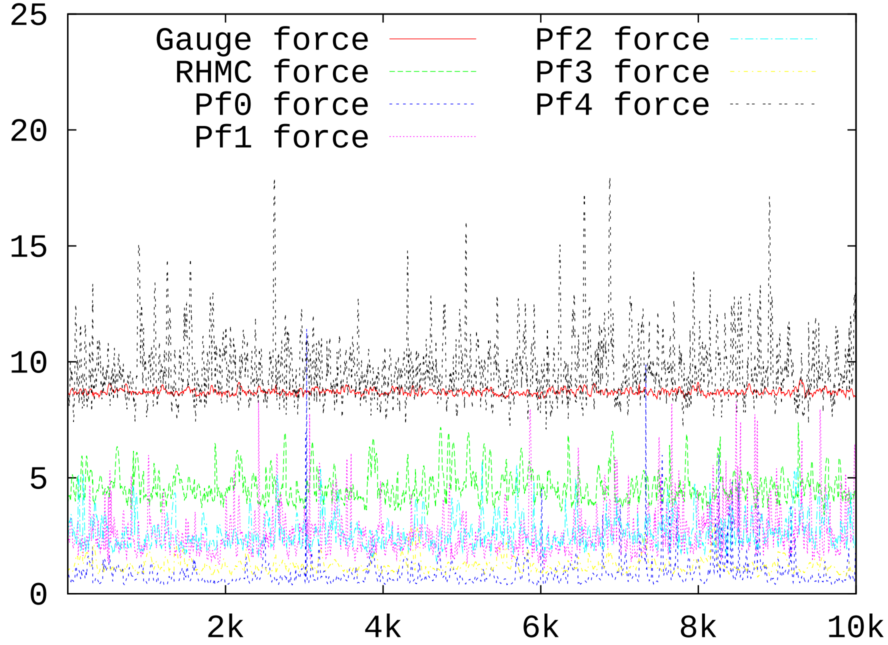
Ensembles w/ smallest m_q per β; lightest pseudofermion

Inverse iteration count ($1/N_{cg}$)



- $10^3/N_{CG}$ distribution is approx. Gaussian
- N_{CG} remains clearly bounded from above

Spacetime max. of MD forces for $\beta = 3.31$ at physical m_{ud}



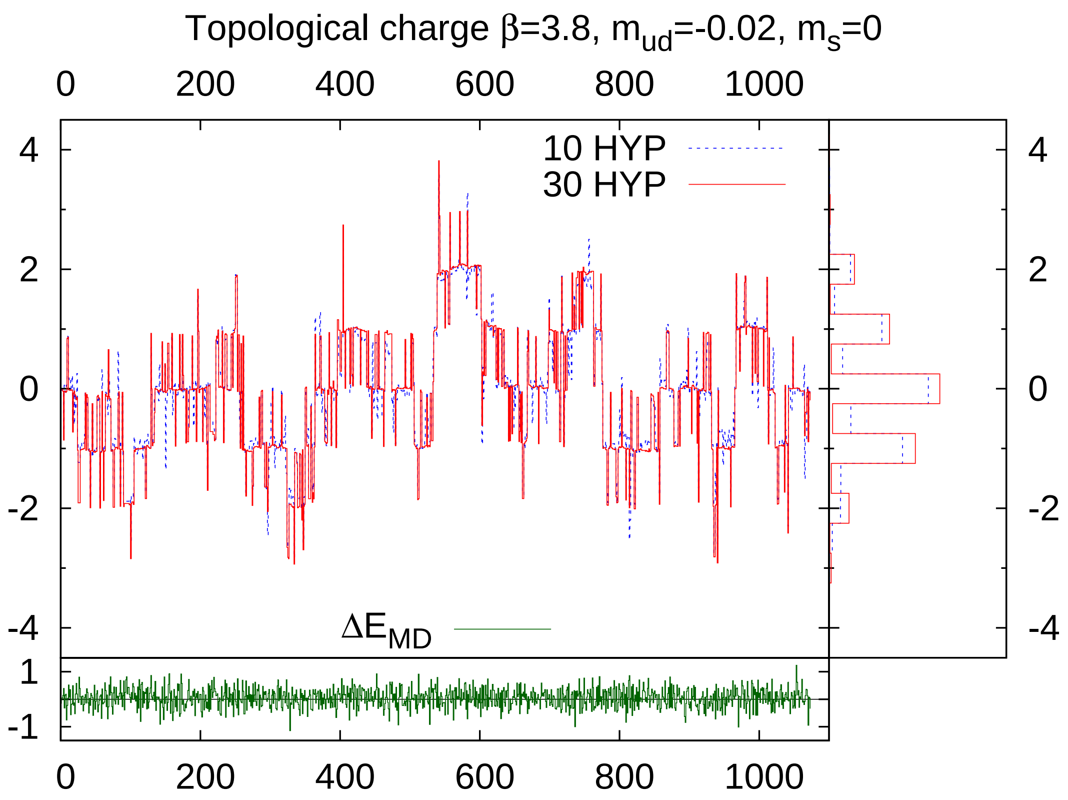
- No killer spikes

$\longrightarrow$ good acceptance $\gtrsim 90\%$

Evolution of topological charge on finest lattice

$a \simeq 0.054\,\mathrm{fm}$ and $M_\pi \simeq 280\,\mathrm{MeV}$ on $48^3 \times 64$ lattice

$$Q = \frac{a^4}{(4\pi)^2} \sum_x \mathrm{Tr}[F_{\mu\nu}^{\mathrm{HYP}}(x)\tilde{F}_{\mu\nu}^{\mathrm{HYP}}]$$

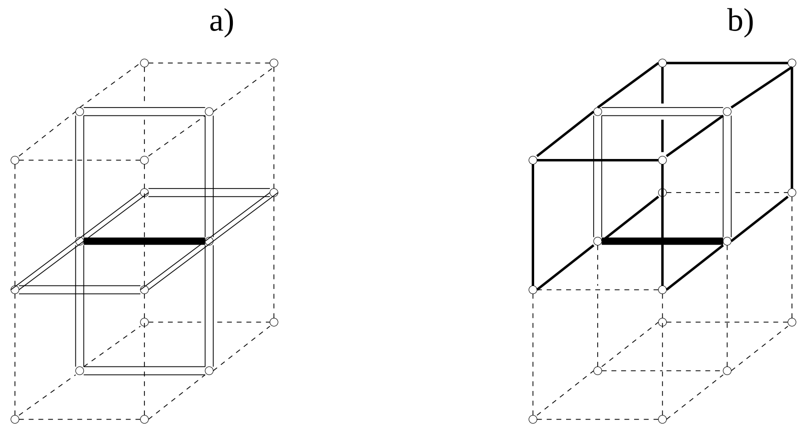


- Q fluctuates and evolves: integrated autocorrelation time $\sim O(10)$
- Q falls into integer centered bins
- Q distribution is reasonably symmetric
- No obvious ergodicity problem

What is 2 HEX smearing?

2 HEX smearing:

- Elementary smearing algorithm is stout (EXponential) smearing (Morningstar et al '04)
- Embedded into 2 steps of HYPercubic smearing (Hasenfratz et al '01)



- Couples $q(x)$ to $A_\mu(x + (3.5a)\hat{e})$ ($\hat{e}.\hat{e} = 1$) w/ weight $\sim 3 \times 10^{-5}$

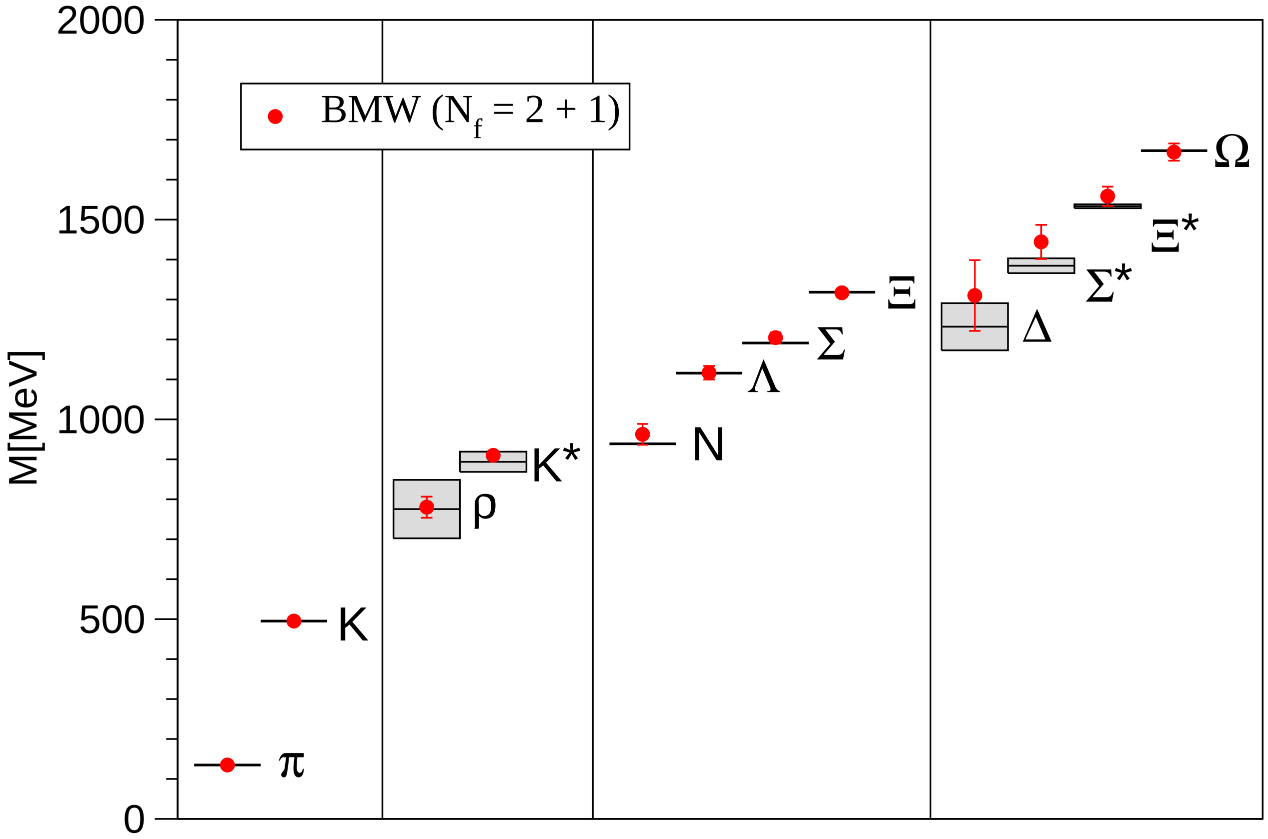
$\rightarrow$ effective range: $\sqrt{\langle r^2 \rangle} = 1.1a$

- Ultralocal and effectively extends barely more than nearest neighbor
- Only differs from regular improved Wilson fermions by $O(\alpha_s a)$
- More local than previously used 6 stout smearing (Dürr et al, Science 322 (2008))

Is smearing a problem?

Dürr et al (BMW), Science 322 (2008) 1224

With 6 stout smearing and $M_\pi \gtrsim 190\,\mathrm{MeV}$, light hadron spectrum is correctly reproduced

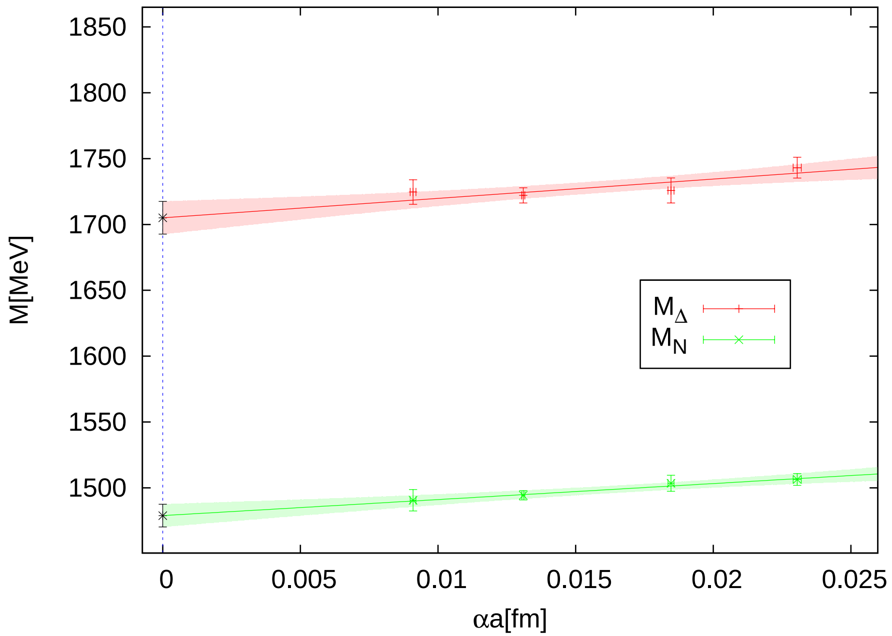


Does our smearing enhance discretization errors?

$\Rightarrow$ scaling study: $N_f = 3$ w/ 2 HEX action, 4 lattice spacings ($a \simeq 0.06 \div 0.15\,\mathrm{fm}$), $M_\pi L > 4$ fixed and

$$M_\pi / M_\rho = \sqrt{2(M_K^{ph})^2 - (M_\pi^{ph})^2} / M_\phi^{ph} \sim 0.67$$

i.e. $m_q \sim m_s^{ph}$



- M_N and M_Δ are linear in $\alpha_s a$ out to $a \sim 0.15\,\mathrm{fm}$

$\Rightarrow$ very good scaling: discret. errors $\lesssim 2\%$ out to $a \sim 0.15\,\mathrm{fm}$

- Continuum limit results perfectly consistent w/ analogous 6 stout analysis in Dürr et al (BMW), PRD79 (2009)

Does our smearing enhance discretization errors?

Perhaps 2 HEX works for spectral quantities but not for short distance dominated quantities
$\Rightarrow$ repeat ALPHA's quenched milestone determination of $r_0(m_s + m_{ud})^{\overline{\rm MS}}(2\,{\rm GeV})$

Perform quenched calculation w/ Wilson glue and 2 HEX fermions

- $5\ \beta$ w/ $a \sim 0.06 \div 0.15\,{\rm fm}$
- At least $4\ m_q$ per β w/ $M_\pi L > 4$ and fixed $L \simeq 1.84{\rm fm}$
- Calculate

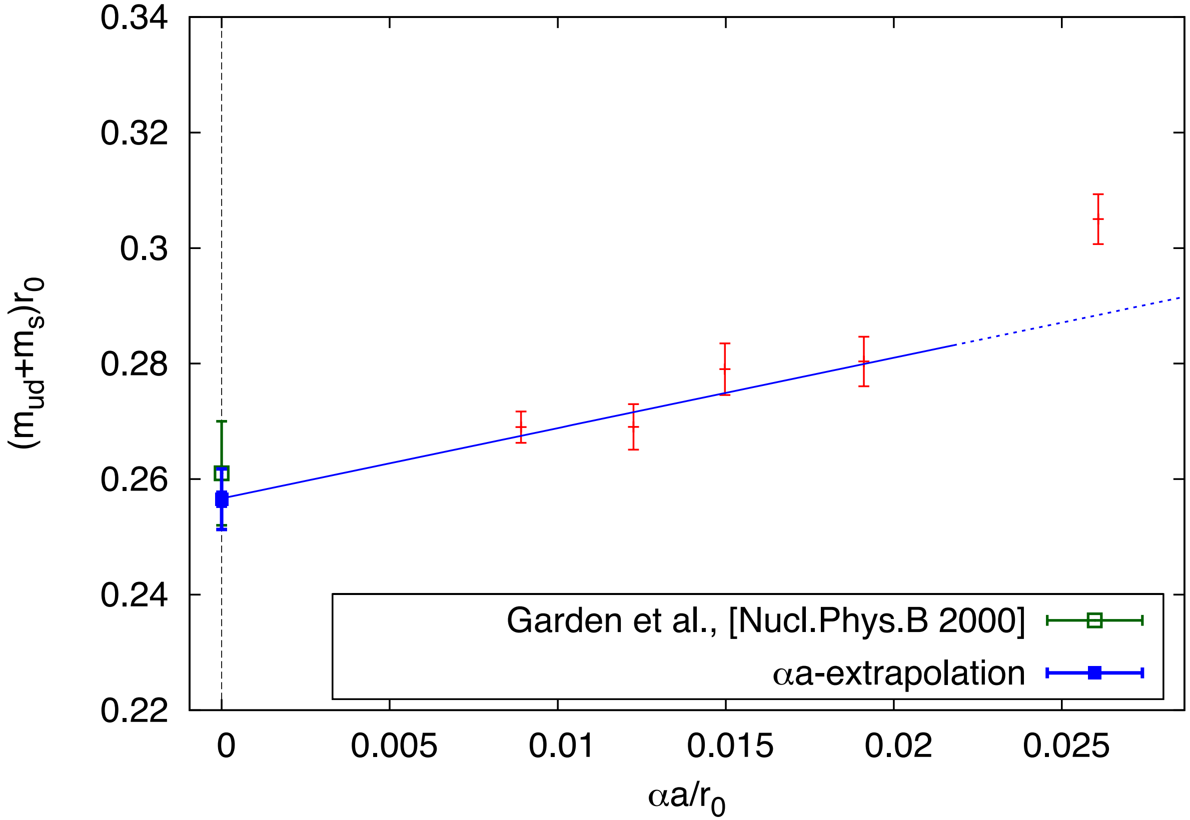
$$m(\mu) = \frac{(1 - am^W/2)m^W}{Z_S(\mu)}$$

w/ $m^W = m^{\rm bare} - m^{\rm crit}$

- Determine $Z_S(\mu)$ using RI/MOM NPR (Martinelli et al '95) and run *nonperturbatively in continuum* to $\mu = 3.5\,{\rm GeV}$ (see below)
- Interpolate in $r_0 M_{PS}$ to $r_0 M_K^{\rm phys}$
- $m^{\rm RI}(3.5\,{\rm GeV}) \longrightarrow m^{\overline{\rm MS}}(2\,{\rm GeV})$ perturbatively

Quenched check: determination of $r_0(m_s + m_{ud})$

Perform continuum extrapolation of $r_0(m_s + m_{ud})^{\overline{\rm MS}}(2\,{\rm GeV})$ **(preliminary)**



With full systematic analysis

$$r_0(m_s + m_{ud})^{\overline{\rm MS}}(2\,{\rm GeV}) = 0.261(4)(4)$$

Perfect agreement w/ ALPHA $r_0(m_s + m_{ud})^{\overline{\rm MS}}(2\,{\rm GeV}) = 0.261(9)$

$N_f = 2 + 1$ simulation parameters

$38 + 9$, $N_f = 2 + 1$ phenomenological runs:

- 5 $a \simeq 0.054 \div 0.116\,\mathrm{fm}$
- $M_\pi^{min} \simeq 135, 130, 120, 190, 220\,\mathrm{MeV}$
- L up to 6 fm and such that $\delta_{\mathrm{FV}} \leq 0.5\%$ on M_π for all runs
- $10 + 3$ different values of m_s around m_s^{phys}
- Determine lattice spacing using M_Ω

$17 + 4$, $N_f = 3$ RI/MOM runs at same β as phenomenological runs:

- At least 4 $m_q \in [m_s^{\mathrm{phys}}/3, m_s^{\mathrm{phys}}]$ per β for chiral extrapolation
- $L \geq 1.7\,\mathrm{fm}$ in all runs

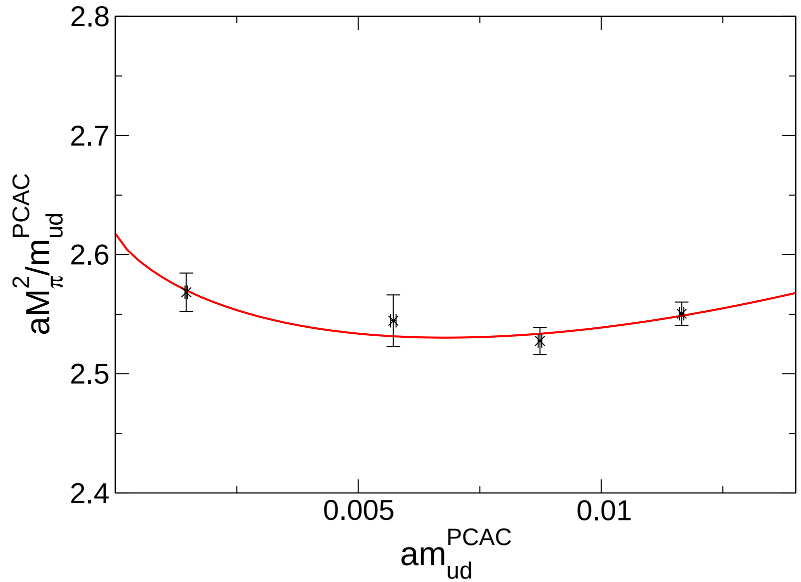
Do we see chiral logs?

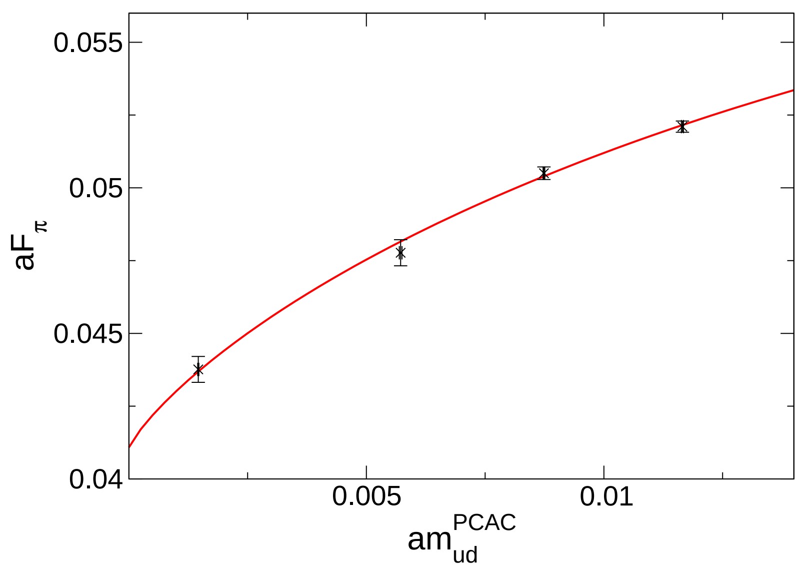
Simultaneous fit of M_π^2 and F_π vs m_{ud} to NLO $SU(2)$ χPT expressions (Gasser et al, '84)

$$M_\pi^2 = M^2\left[1 - \frac{1}{2}x\log\left(\frac{\Lambda_3^2}{M^2}\right)\right] \qquad F_\pi^2 = F\left[1 + x\log\left(\frac{\Lambda_4^2}{M^2}\right)\right]$$

w/ $M^2 = 2Bm_{ud}$ and $x = M^2/(4\pi F)^2$

Fixed $a \simeq 0.09\,\mathrm{fm}$ and $M_\pi \simeq 130 \to 400\,\mathrm{MeV}$ **(preliminary)**





Consistent w/ NLO χPT ...

VWI and AWI masses: ratio-difference method

With $N_f = 2+1$, $O(a)$-improved Wilson fermions, can construct the following renormalized, $O(a)$-improved quantities (using Bhattacharya et al '06)

$$(m_s - m_{ud})^{\mathrm{VWI}} = (m_s^{\mathrm{bare}} - m_{ud}^{\mathrm{bare}})\frac{1}{Z_S}\left[1 - \frac{b_S}{2}\,a(m_{ud}^{\mathrm{W}} + m_s^{\mathrm{W}}) - \bar{b}_S\,a(2m_{ud}^{\mathrm{W}} + m_s^{\mathrm{W}})\right] + O(a^2)$$

w/ $m^{\mathrm{W}} = m^{\mathrm{bare}} - m^{\mathrm{crit}}$ and

$$\frac{m_s^{\mathrm{AWI}}}{m_{ud}^{\mathrm{AWI}}} = \frac{m_s^{\mathrm{PCAC}}}{m_{ud}^{\mathrm{PCAC}}}\left[1 + (b_A - b_P)\,a(m_s^{\mathrm{bare}} - m_{ud}^{\mathrm{bare}})\right]$$

w/

$$m^{\mathrm{PCAC}} \equiv \frac{1}{2}\frac{\sum_{\vec{x}}\langle\bar{\partial}_\mu\,[A_\mu(x) + ac_A\partial_\mu P(x)]\,P(0)\rangle}{\sum_{\vec{x}}\langle P(x)P(0)\rangle}$$

and $b_{A,P,S} = 1 + O(\alpha_s)$, $\bar{b}_{A,P,S} = O(\alpha_s^2)$, $c_A = O(\alpha_s)$

Ratio-difference method (cont'd)

Define

$$d \equiv am_s^{\rm bare} - am_{ud}^{\rm bare}\,, \qquad r \equiv \frac{m_s^{\rm PCAC}}{m_{ud}^{\rm PCAC}}$$

and subtracted bare masses

$$am_{ud}^{\rm sub} \equiv \frac{d}{r-1}\,, \qquad am_s^{\rm sub} \equiv \frac{rd}{r-1}$$

Then, with our tree-level $O(a)$-improvement, renormalized masses can be written

$$m_{ud} = \frac{m_{ud}^{\rm sub}}{Z_S}\left[1 - \frac{a}{2}(m_{ud}^{\rm sub} + m_s^{\rm sub})\right] + O(\alpha_s a)$$

$$m_s = \frac{m_s^{\rm sub}}{Z_S}\left[1 - \frac{a}{2}(m_{ud}^{\rm sub} + m_s^{\rm sub})\right] + O(\alpha_s a)$$

Benefits:

- Only Z_S (non-singlet) is required and difficult RI/MOM Z_P is circumvented
- No need to determine $m^{\rm crit}$

Improved RI/MOM for Z_S

Determine $Z_S^{\mathrm{RI}}(\mu, a)$ nonperturbatively in RI/MOM scheme, from truncated, forward quark two-point functions in Landau gauge (Martinelli et al '95), computed on specifically generated $N_f = 3$ gauge configurations

Use $S(p) \rightarrow \bar{S}(p) = S(p) - \mathrm{Tr}_D[S(p)]/4$ (Becirevic et al '00)

- $\Rightarrow$ tree-level $O(a)$ improvement
- $\Rightarrow$ significant improvement in S/N
- $\Rightarrow$ recover usual massless RI/MOM scheme for $m^{\mathrm{RGI}} \rightarrow 0$

For controlled errors, require:

(a) $\mu \ll 2\pi/a$ for $a \rightarrow 0$ extrapolation

(b) $\mu \gg \Lambda_{\mathrm{QCD}}$ if masses are to be used in perturbative context

i.e. the window problem, which we solve as follows

Ad (a): RI/MOM at sufficiently low scale

Controlled continuum extrapolation of renormalized mass

$\Rightarrow$ renormalize at μ where RI/MOM $O(\alpha_s a)$ errors are *small for all* β

- For coarsest $(\beta = 3.31)$ lattice, $2\pi/a \simeq 11\,\mathrm{GeV}$
- Restrict study of $Z_S^{\mathrm{RI}}(\mu, a)$ to $\mu \lesssim \pi/2a \simeq 2.7\,\mathrm{GeV}$ $(\beta = 3.31)$
- Pick $\mu \in [1.2,\ 1.8]\,\mathrm{GeV}$ as common renormalization point for all β
- Can take $a \to 0$

  $\Rightarrow$ continuum $m^{\mathrm{RI}}(\mu)$ determined fully nonperturbatively . . .
- . . . but at $\mu \gtrsim \Lambda_{\mathrm{QCD}}$

  $\Rightarrow$ not very useful for phenomenology since perturbative error large at such μ

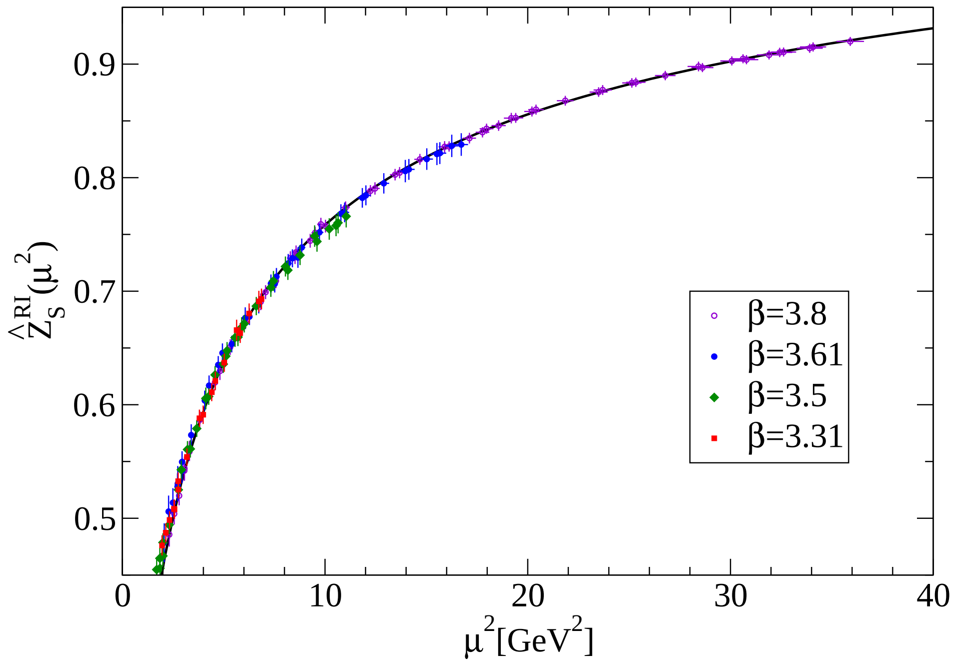
Ad (b): nonperturbative continuum running to 4.2 GeV

To make result useful, run nonperturbatively in *continuum limit* up to perturbative scale

For μ : $1.2 \to 4.2\,\mathrm{GeV}$, always have at least 3 a (including the $\beta = 3.7$ results to come) w/ $\mu \lesssim \pi/2a$

$\Rightarrow$ can determine nonperturbative running in continuum limit

$$R^{\mathrm{RI}}(\mu, 4.2\,\mathrm{GeV}) = \lim_{a\to 0} \frac{Z_S^{\mathrm{RI}}(4.2\,\mathrm{GeV}, a)}{Z_S^{\mathrm{RI}}(\mu, a)}$$



Rescaled $Z_S^{\mathrm{RI}}(\mu, a_\beta)$ for $\beta < 3.8$ to $\sim$ match $Z_S^{\mathrm{RI}}(\mu, a_{\beta=3.8})$

Preliminary

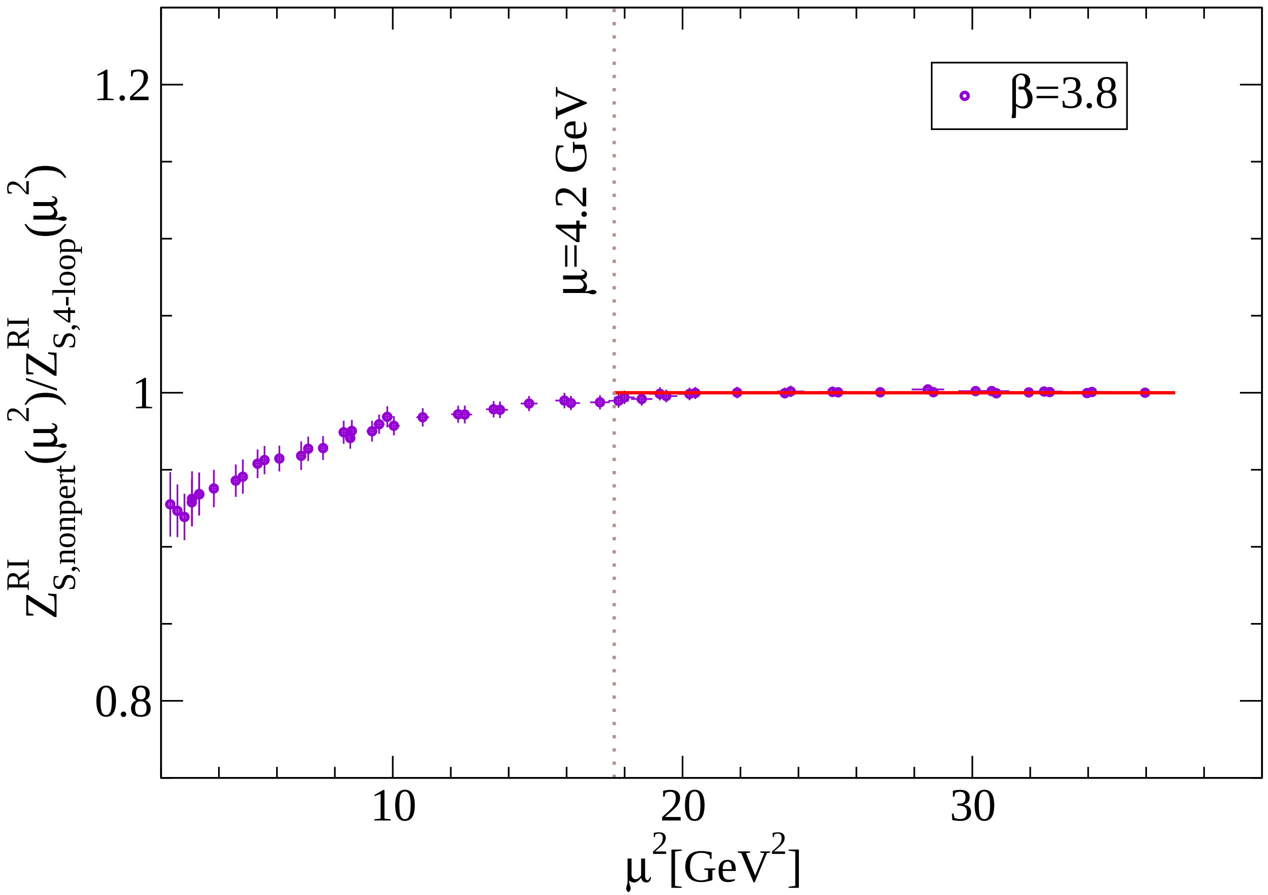
Running is very similar at all 4 β

$\Rightarrow$ flat $a \to 0$ extrapolation

Ad (b): running above 4.2 GeV

For $\mu > 4.2\,\mathrm{GeV}$, 4-loop perturbative running agrees w/ nonperturbative running on our finer lattices

Preliminary

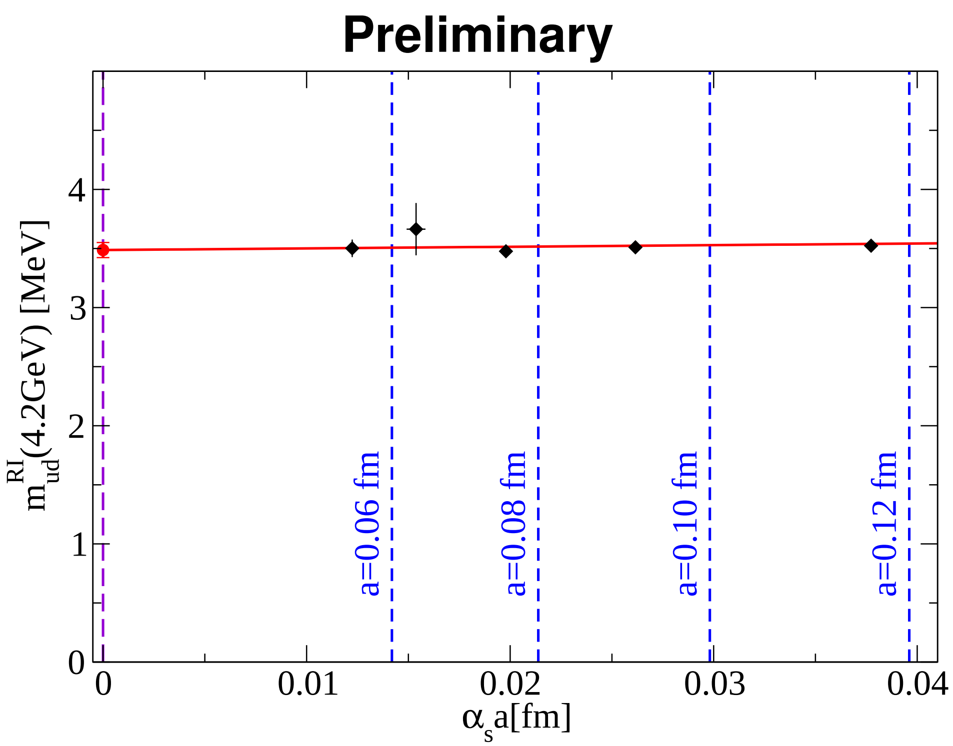


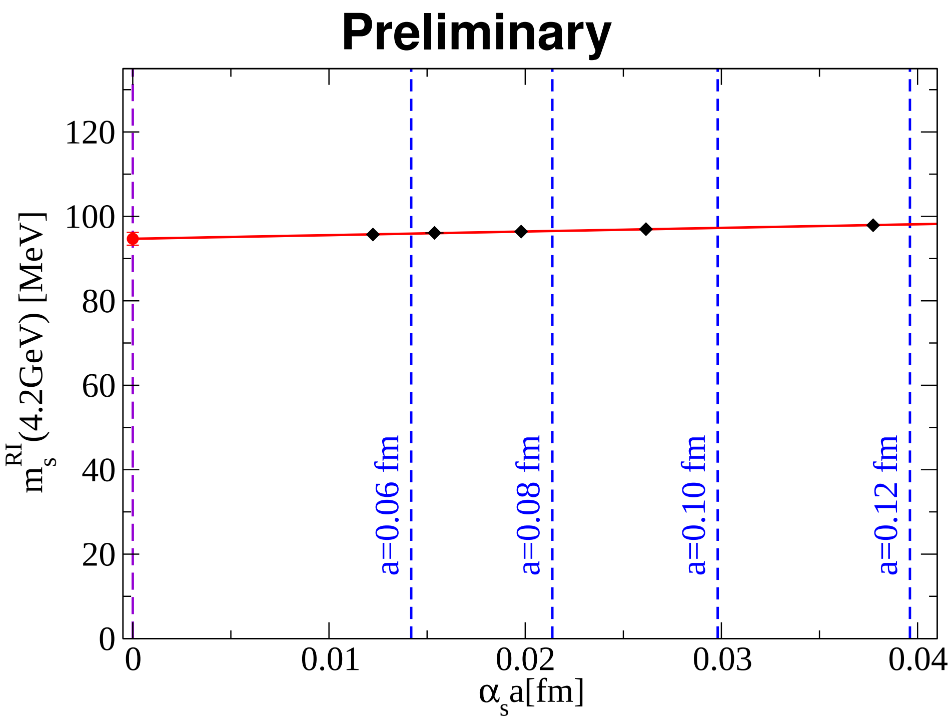
Continuum extrapolation of renormalized masses

Renormalized quark masses **interpolated** in M_π^2 & M_K^2 to physical point using:

- $SU(2)$ χPT
- or low-order polynomial anszätze
- w/ cuts on pion mass $M_\pi < 340, 400\,\mathrm{MeV}$

Example of continuum extrapolations (statistical errors shown here)





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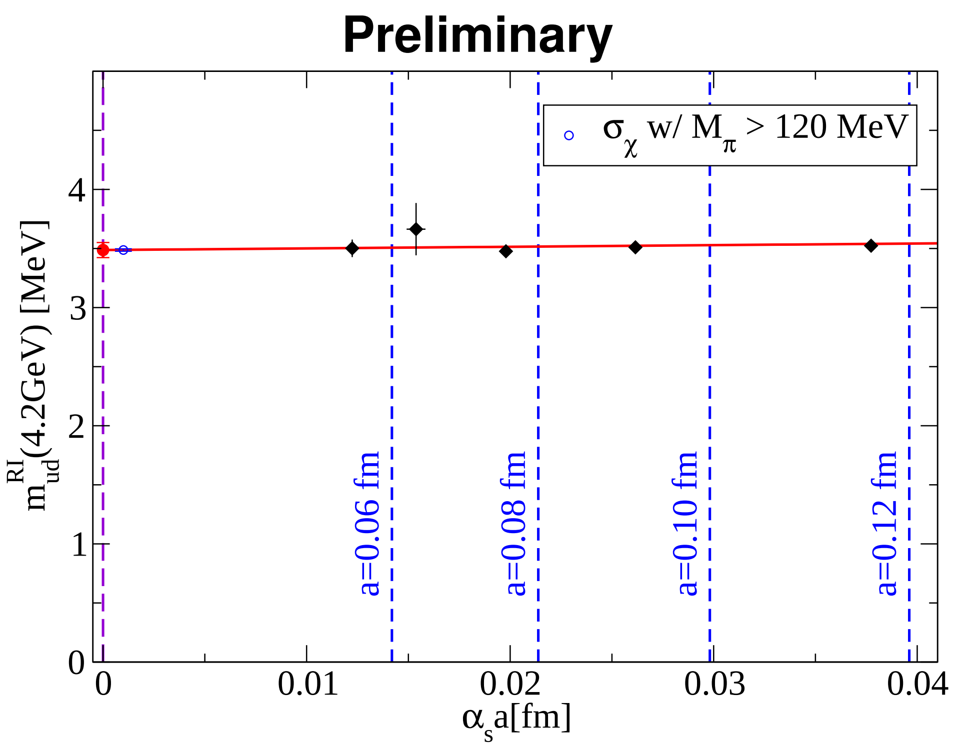
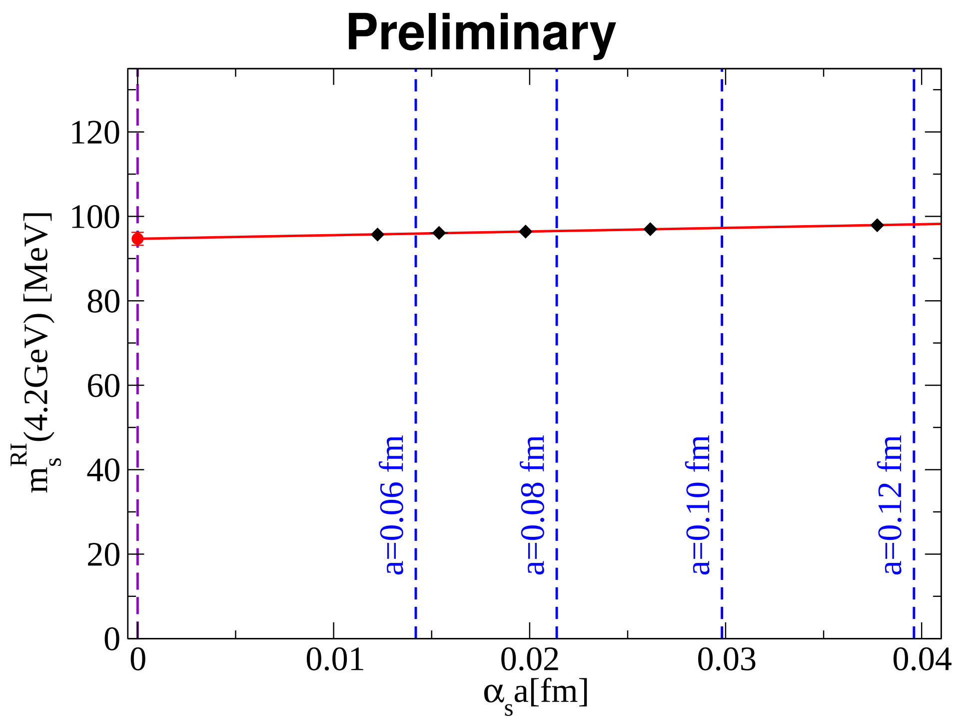
... and syst. error due to chiral interp.





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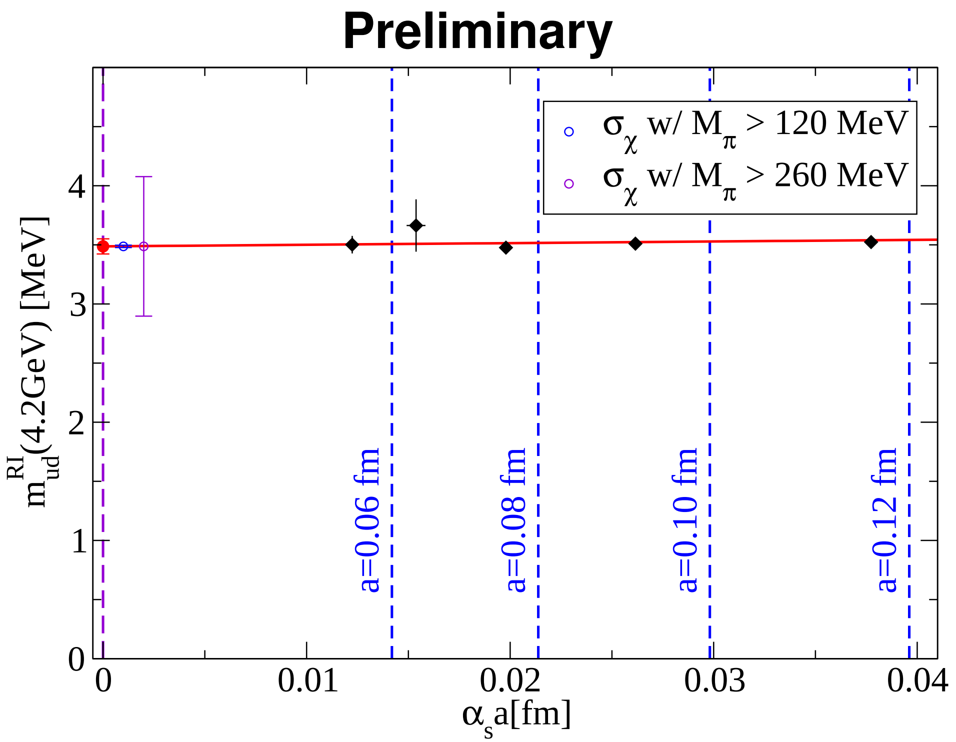
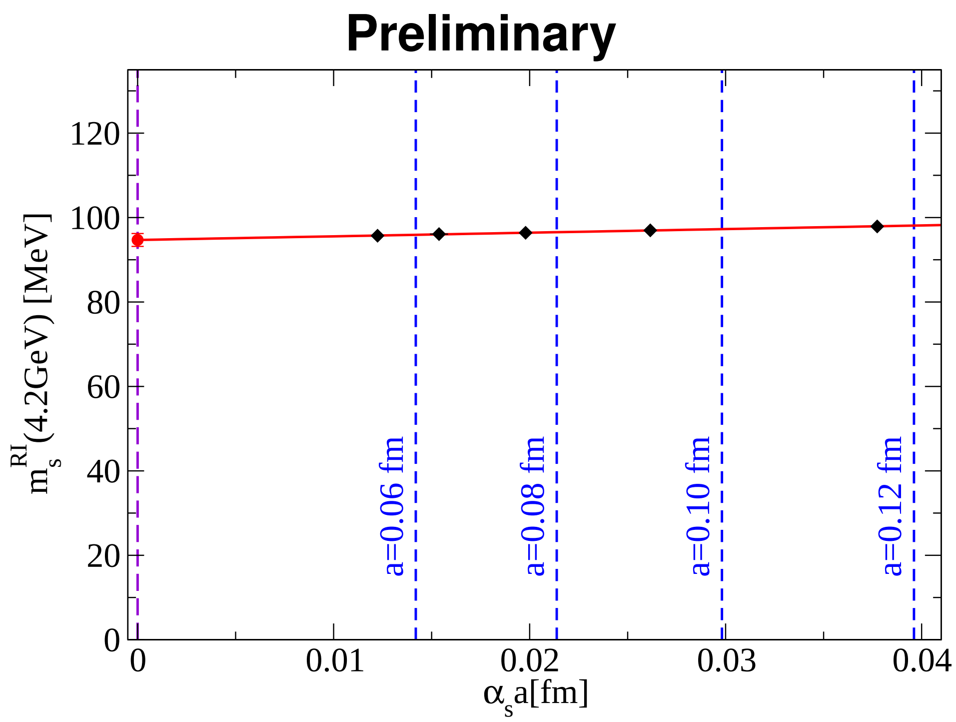
Example of continuum extrapolations (statistical errors shown here)

... and syst. error due to chiral extrap. if $M_\pi \leq M_\pi^{\mathrm{RMS}}|_{\mathrm{MILC}}^{\mathrm{min}} \simeq 260\,\mathrm{MeV}$ data are excluded





Conclusions

- $N_f = 2+1$ simulations have been performed all the way down to $m_{ud}^{\rm phys}$ and below w/ $m_s \simeq m_s^{\rm phys}$:
  - 5 $a \simeq 0.054 \div 0.116\,\mathrm{fm}$
  - $M_\pi^{min} \simeq 135,\ 130,\ 120,\ 190,\ 220\,\mathrm{MeV}$
  - L up to 6 fm and such that $\delta_{\rm FV} \leq 0.5\%$ on M_π for all runs

$\longrightarrow$ eliminates large systematic error associated w/ reaching $m_{ud}^{\rm phys}$

- Described an RI/MOM procedure which includes continuum limit, nonperturbative running

$\longrightarrow$ eliminates large systematic error associated w/ the "window" problem

- Currently finalizing analysis of light quark masses
- Systematic error will be estimated following an extended frequentist approach (Dürr et al, Science '08)

  $\longrightarrow$ expect total uncertainty on m_{ud} and m_s to be of order $2 \div 3\%$

$\Rightarrow$ will significantly improve knowledge of m_{ud} and m_s whose errors are, at present, 11% [FLAG] $\div$ 30% [PDG]

Conclusions

- MILC and HPQCD claim results w/ similar uncertainties, but these are obtained from simulations w/ $M_\pi^{\mathrm{RMS}} \geq 260\,\mathrm{MeV}$
- Imposing the cut $M_\pi \geq 260\,\mathrm{MeV}$ on our results

  $\Rightarrow \delta_\chi m_{ud} \sim 0.3\% \longrightarrow \delta_\chi m_{ud} \sim 15\%$

  $\Rightarrow$ assumptions on mass dependence of results, which go beyond NLO $SU(2)$ χPT, must be made
- Fully controlled LQCD calculations can now be envisaged w/out any assumptions on light quark mass dependence of results
- The dream of simulating QCD w/ no ifs nor buts is finally becoming a reality