News from the lattice

Laurent Lellouch

CPT Marseille

with

Dürr, Fodor, Frison, Hoelbling, Katz, Krieg, Kurth, Lellouch, Lippert, Portelli, Ramos, Szabo, Vulvert
(Budapest-Marseille-Wuppertal Collaboration)

Some of the questions that we would like to answer

- Can one show that the mass of ordinary matter comes from QCD?
- What are the masses of the light u, d (and s) quarks which are the building blocks of ordinary matter?
- Is our understanding of quark flavor mixing and the fundamental asymmetry between matter and antimatter, which it leads to, correct?
- Does dark matter couple strongly enough to ordinary matter to make it visible with current detectors?
- Can one show that QCD and QED explain why the proton is lighter than the neutron? (If $M_p > M_N$, there would be no atoms . . .)
- Heisenberg's uncertainty principle allows the creation of particle-antiparticle pairs which can induce the decay of other particles (e.g. vac. $\to \bar{u}u \Rightarrow \rho \to \pi\pi$)

  Does QCD describe $\rho \to \pi\pi$ correctly?
- Can a confining gauge theory such as QCD explain electroweak symmetry breaking and the masses of elementary particles? (Technicolor at LHC?)
  $\to$ ask C.-J. David Lin!

All require quantitative understanding of nonperturbative strong interaction effects

$\Rightarrow$ only known ab initio approach is Lattice QCD

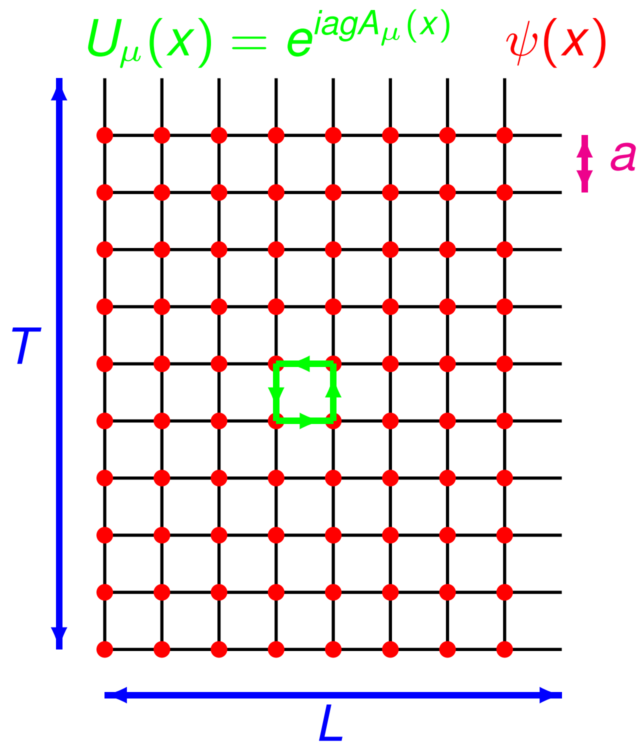
What is Lattice QCD (LQCD)?

Lattice gauge theory $\longrightarrow$ mathematically sound definition of NP QCD:

- UV (and IR) cutoffs and a well defined path integral in Euclidean spacetime:

$$\langle O \rangle = \int \mathcal{D}U\mathcal{D}\bar{\psi}\mathcal{D}\psi\, e^{-S_G - \int \bar{\psi}D[M]\psi}\, O[U,\psi,\bar{\psi}]$$
$$= \int \mathcal{D}U\, e^{-S_G} \det(D[M])\, O[U]_{\rm Wick}$$

- $\mathcal{D}Ue^{-S_G}\det(D[M]) \geq 0$ and finite # of dof's $\to$ evaluate numerically using stochastic methods



NOT A MODEL: LQCD is QCD when $a \to 0$, $V \to \infty$ and stats $\to \infty$

In practice, limitations . . .

Limitations: statistical and systematic errors

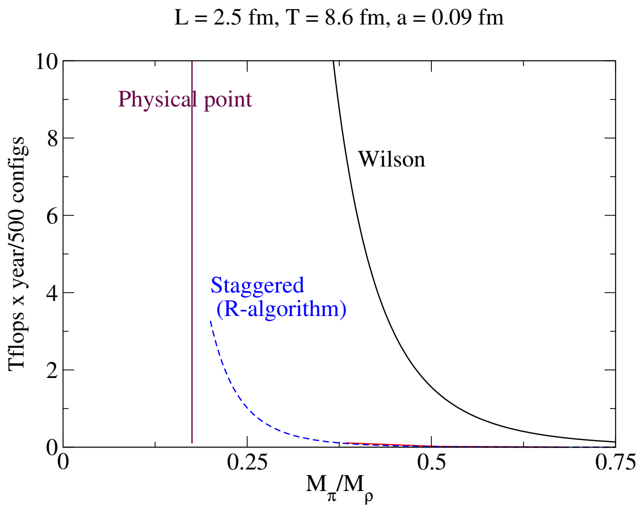
Limited computer resources $\to$ a, L and m_q are compromises and statistics finite

- **Quenching:** in past, $\det(D[M]) \to \mathrm{cst}$
  Being removed w/ difficult $2{+}1$ calculations
- **Statistical:** $1/\sqrt{N_{conf}}$
  Eliminate w/ $N_{conf} \to \infty$
- **Discretization:** $a\Lambda_{QCD},\ am_q,\ a|\vec{p}|$, with $a^{-1} \sim 2-4\,\mathrm{GeV}$

  Eliminate w/ $a \to 0$: need at least three a's
- **Chiral extrapolation:** m_{ud}^{ph} barely reachable $\Rightarrow m_q[> m_{ud}^{ph}] \to m_{ud}^{ph}$
  Difficult calculations w/ $M_\pi \lesssim 350\,\mathrm{MeV} + \chi$PT or Taylor expansions
  Better: simulate directly at m_{ud}^{ph}
- **Finite volume:** simple quantities $\sim \left(\frac{M_\pi}{\pi F_\pi}\right)^2 \frac{e^{-M_\pi L}}{(M_\pi L)^{3/2}} \to M_\pi L \gtrsim 4$ usually safe
  Resonant states more complicated
  Eliminate with $L \to \infty$ ($+\ \chi$PT)
- **Renormalization:** in all field theories must renormalize;
  Can be done in PT, best done nonperturbatively

Why is LQCD so numerically difficult?

- # of d.o.f. $\sim \mathcal{O}(10^9)$ and large overhead for $\det(D[M])$ ($\sim 10^9 \times 10^9$ matrix)
- cost of simulations increases rapidly when $m_{u,d} \to m_{u,d}^{\rm phys}$ & $a \to 0$



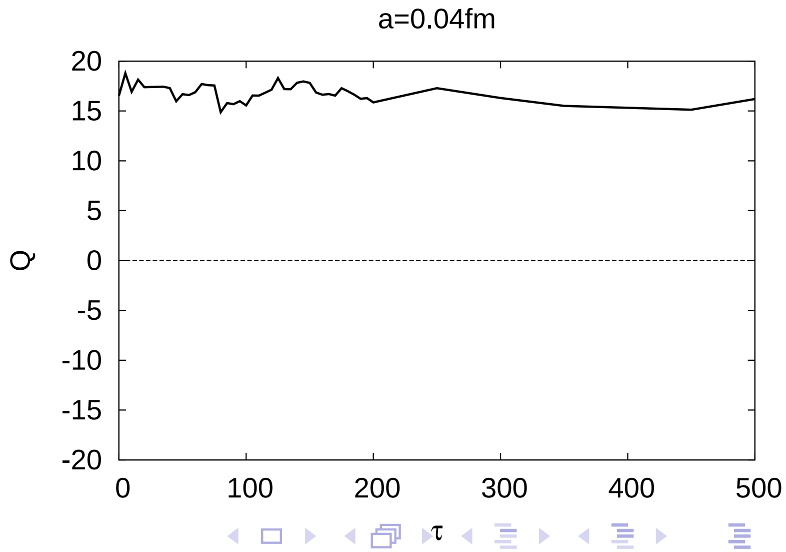
Wilson fermions ($\lesssim$ 2004)

- cost $\sim N_{\rm conf} V^{5/4} m_{u,d}^{-3} a^{-7}$ (Ukawa '02)
- Serious cost wall

$\Rightarrow$ can physical $m_{u,d}$ ever be reached?

Observe very long-lived autocorrelations of topological charge vs MC time (Schaefer et al '09, quenched)

$\Rightarrow$ $a \to 0$ may be even harder than anticipated



How we overcome these problems

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:

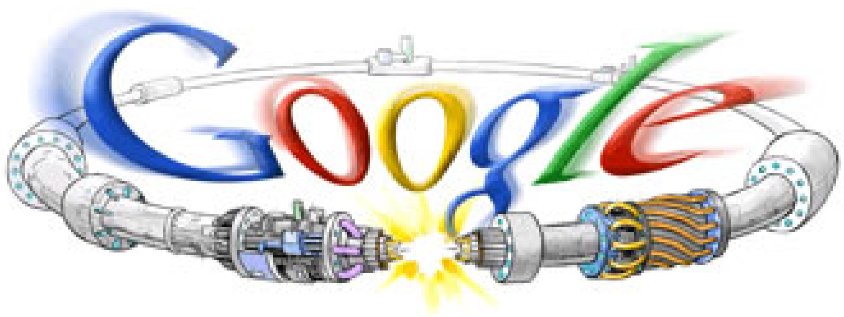
- tree-level $O(a^2)$-improved gauge action (Lüscher et al '85)
- tree-level $O(a)$-improved Wilson fermion (Sheikholeslami et al '85) w/ 6-stout or 2-HEX smearing (Morningstar et al '04, Hasenfratz et al '01, Capitani et al '06)
  $\Rightarrow$ approach to continuum is improved ($O(\alpha_s a, a^2)$ 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

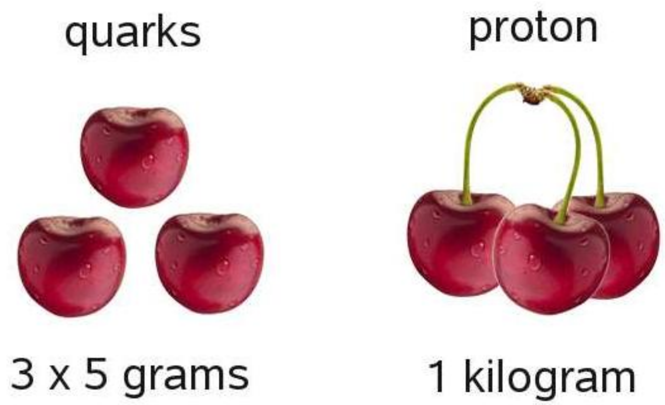
3) Highly optimized codes

Where does the mass of ordinary matter come from?



$\rightarrow$ Higgs? SEWSB? . . . ?
$\Rightarrow$ mass of fundamental particles
$\not\Rightarrow$ mass of ordinary matter

- $> 99\%$ of mass of visible universe is in the form of p & n
- Mass of object usually sum of mass of constituents: not true for light hadrons



- Light hadron masses are generated by QCD through energy imparted to q & g via:

$$m = E/c^2$$

Ab initio calculation of the light hadron spectrum

Dürr et al, Science 322 (2008) 1224

Aim: determine light hadron spectrum, at few percent level, directly in QCD in calculation w/ all sources of systematic errors under control

⇒ **i.** Inclusion of $N_f = 2 + 1$ sea quark effects w/ an exact algorithm and w/ a unitary, local action whose universality class is known to be QCD ($\rightarrow$ see above)

⇒ **ii.** 3 parameters of $N_f{=}2 + 1$ QCD (m_{ud}, m_s & $\Lambda_{\rm QCD}$) by observables w/ small undisputed errors, transparent connection to experiment and no hidden assumptions

⇒ **iii.** Complete spectrum for the light mesons and octet and decuplet baryons

⇒ **iv.** Large volumes to guarantee negligible finite-size effects ($\rightarrow$ check)

⇒ **v.** Controlled interpolations to m_s^{ph} (straightforward) and extrapolations to m_{ud}^{ph} (difficult)

Of course, simulating directly around m_{ud}^{ph} would be better!

⇒ **vi.** Controlled extrapolations to the continuum limit
$\rightarrow$ at least 3 a's in the scaling regime

⇒ **vii.** Complete analysis of systematic uncertainties

Simulation parameters: BMW '08

β, a [fm]	am_{ud}	M_π [GeV]	am_s	$L^3 \times T$	# traj.
3.3	-0.0960	0.65	-0.057	$16^3 \times 32$	10000
	-0.1100	0.51	-0.057	$16^3 \times 32$	1450
$\sim$ 0.125	-0.1200	0.39	-0.057	$16^3 \times 64$	4500
	-0.1233	0.33	-0.057	$16^3 \times 64$ | $24^3 \times 64$ | $32^3 \times 64$	5000 | 2000 | 1300
	-0.1265	0.27	-0.057	$24^3 \times 64$	700
3.57	-0.03175	0.51	0.0	$24^3 \times 64$	1650
	-0.03175	0.51	-0.01	$24^3 \times 64$	1650
$\sim$ 0.085	-0.03803	0.42	0.0	$24^3 \times 64$	1350
	-0.03803	0.41	-0.01	$24^3 \times 64$	1550
	-0.044	0.31	0.0	$32^3 \times 64$	1000
	-0.044	0.31	-0.07	$32^3 \times 64$	1000
	-0.0483	0.20	0.0	$48^3 \times 64$	500
	-0.0483	0.19	-0.07	$48^3 \times 64$	1000
3.7	-0.007	0.65	0.0	$32^3 \times 96$	1100
	-0.013	0.56	0.0	$32^3 \times 96$	1450
$\sim$ 0.065	-0.02	0.43	0.0	$32^3 \times 96$	2050
	-0.022	0.39	0.0	$32^3 \times 96$	1350
	-0.025	0.31	0.0	$40^3 \times 96$	1450

- # of trajectories given is after thermalization
- autocorrelation times (plaquette, n_{CG}) less than $\approx$ 10 trajectories
- 2 runs with 10000 and 4500 trajectories $\longrightarrow$ no long-range correlations found

ad ii, iii: QCD parameters and light hadron masses

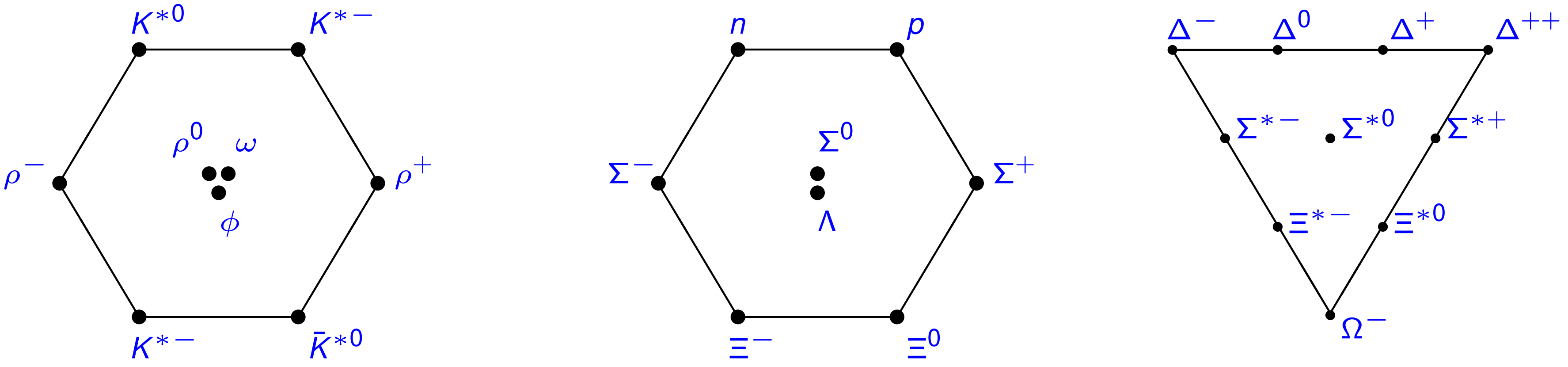
N_f=2+1 QCD in isospin limit has 3 parameters which have to be fixed w/ expt:

- $\Lambda_{\rm QCD}$: fixed w/ Ω or Ξ mass
  - don't decay through the strong interaction
  - have good signal
  - have a weak dependence on m_{ud}

  $\to$ 2 separate analyse and compare

- (m_{ud}, m_s): fixed using M_π and M_K

Determine masses of remaining non-singlet light hadrons in

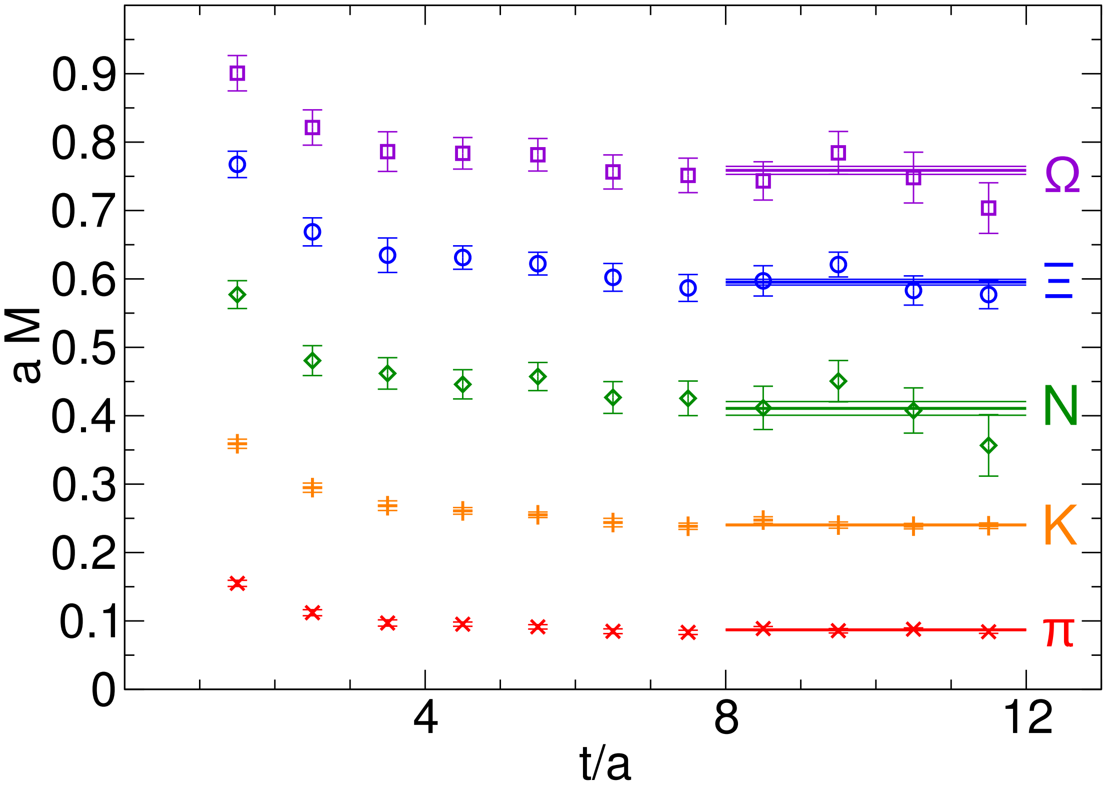


ad iii: fits to 2-point functions in different channels

e.g. in pseudoscalar channel, M_π from correlated fit

$$C_{PP}(t) \equiv \frac{1}{(L/a)^3} \sum_{\vec{x}} \langle [\bar{d}\gamma_5 u](x)[\bar{u}\gamma_5 d](0)\rangle \overset{0\ll t\ll T}{\longrightarrow} \frac{\langle 0|\bar{d}\gamma_5 u|\pi^+(\vec{0})\rangle\langle\pi^+(\vec{0})|\bar{u}\gamma_5 d|0\rangle}{2M_\pi} e^{-M_\pi t}$$

Effective mass $aM(t+a/2) = \log[C(t)/C(t+a)]$

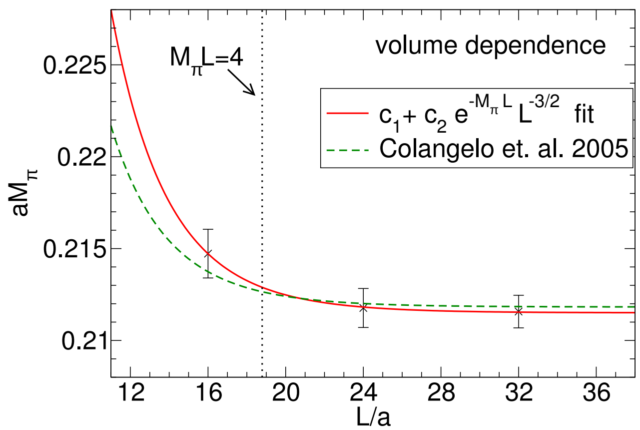


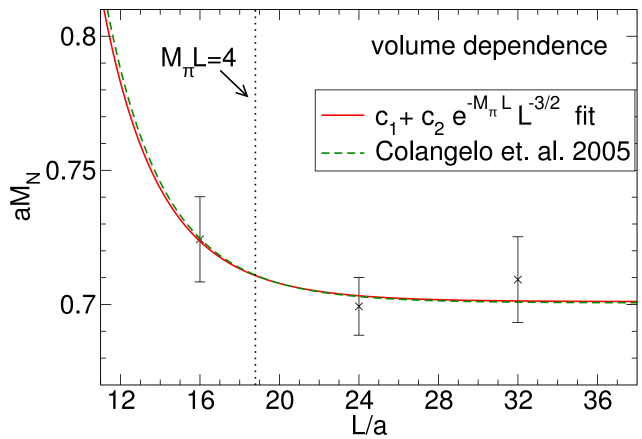
Effective masses for simulation at $a \approx 0.085\,\mathrm{fm}$ and $M_\pi \approx 0.19\,\mathrm{GeV}$

Gaussian sources and sinks with $r \sim 0.32\,\mathrm{fm}$ (BMW '08)

ad iv: (I) Virtual pion loops around the world

- In large volumes $\text{FVE} \sim e^{-M_\pi L}$
- $M_\pi L \gtrsim 4$ expected to give $L \to \infty$ masses within our statistical errors
- For $a \approx 0.125\,\text{fm}$ and $M_\pi \approx 0.33\,\text{GeV}$, perform FV study $M_\pi L = 3.5 \to 7$





Well described by (Dürr and Colangelo et al, 2005)

$$\frac{M_X(L) - M_X}{M_X} = C \left(\frac{M_\pi}{\pi F_\pi} \right)^2 \frac{1}{(M_\pi L)^{3/2}} e^{-M_\pi L}$$

Though very small, we fit them out

ad iv: (II) Finite volume effects for resonances

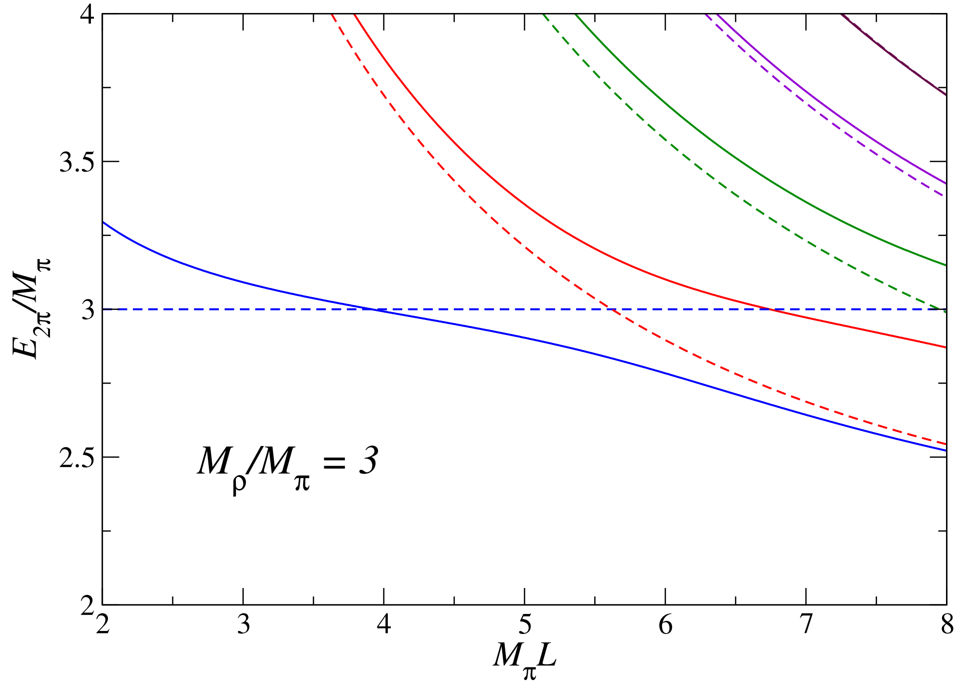
Important since 5/12 of hadrons studied are resonances

Systematic treatment of resonant states in finite volume (Lüscher, '85-'91)

e.g., the $\rho \leftrightarrow \pi\pi$ system in the COM frame

- Non-interacting:
  $E_{2\pi} = 2(M_\pi^2 + k^2)^{1/2}$, $\vec{k} = 2\pi\vec{n}/L$, $\vec{n} \in Z^3$
- Interacting case: k solution of

  $$n\pi - \delta_{11}(k) = \phi(q), \; n \in Z, \; q = kL/2\pi$$



Know L and lattice gives $E_{2\pi}$ and M_π

$\Rightarrow$ infinite volume mass of resonance and coupling to decay products

- in this calculation, low sensitivity to width (compatible w/ expt w/in large errors)
- small but dominant FV correction for resonances

ad v: extrapolation to m_{ud}^{ph} and interpolation to m_s^{ph}

Consider two approaches to the physical QCD limit for a hadron mass M_X:

1. Mass-independent scale setting
2. Simulation-by-simulation normalization

For both normalization procedures, use parametrization

$$M_X = M_X^{(0)} + \alpha_K M_K^2 + \alpha_\pi M_\pi^2 + \mathrm{h.o.t.}$$

- linear term in M_K^2 is sufficient for interpolation to m_s^{ph}
- curvature in M_π^2 is visible in extrapolation to m_{ud}^{ph} in some channels

→ two options for h.o.t.:

  - ChPT: expansion about $M_\pi^2 = 0$ and $\mathrm{h.o.t.} \propto M_\pi^3$ (Langacker et al '74)
  - Flavor: expansion about center of M_π^2 interval considered and $\mathrm{h.o.t.} \propto M_\pi^4$

- Further estimate of contributions of neglected h.o.t. by restricting fit interval: $M_\pi \leq 650 \to 550 \to 450\,\mathrm{MeV}$

→ use $2 \times 2 \times 3$ combinations of options for error estimate

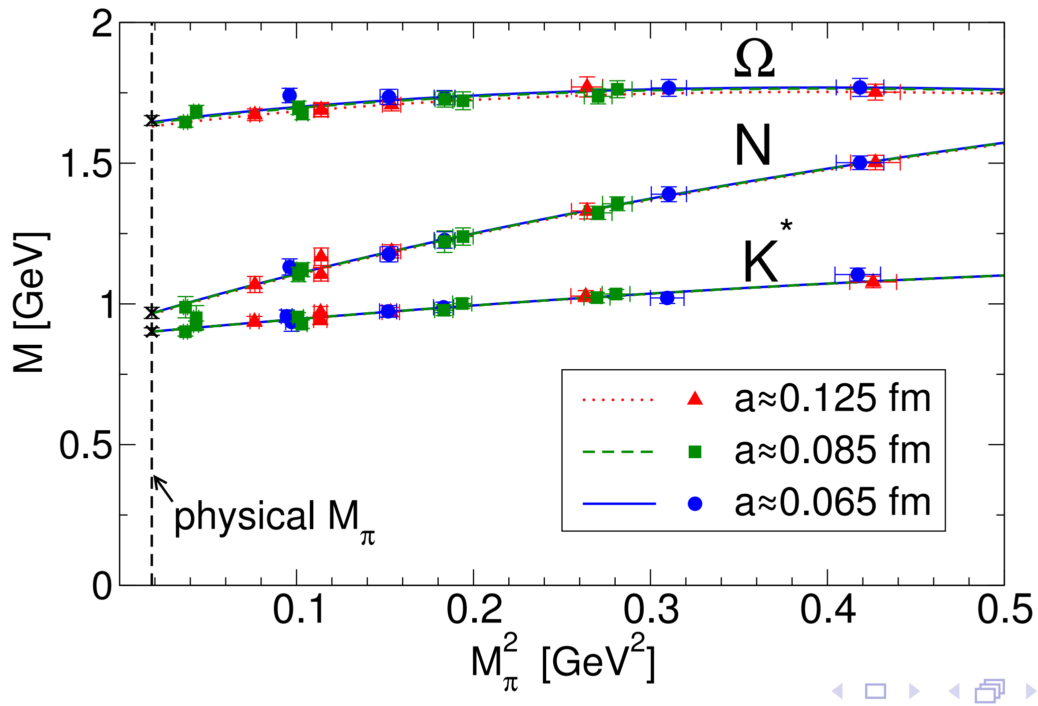
ad vi: including the continuum extrapolation

- Cutoff effects formally $O(\alpha_s a)$ and $O(a^2)$
- Small and cannot distinguish a and a^2
- Include through

$$M_X^{ph} \to M_X^{ph}[1+\gamma_X\, a] \quad \text{or} \quad M_X^{ph}[1+\gamma_X\, a^2]$$

$\to$ difference used for systematic error estimation

- not sensitive to am_s or am_{ud}



ad vii: systematic and statistical error estimate

Uncertainties associated with:

- *Continuum extrapolation* $\rightarrow O(a)$ vs $O(a^2)$
- *Extrapolation to physical mass point*

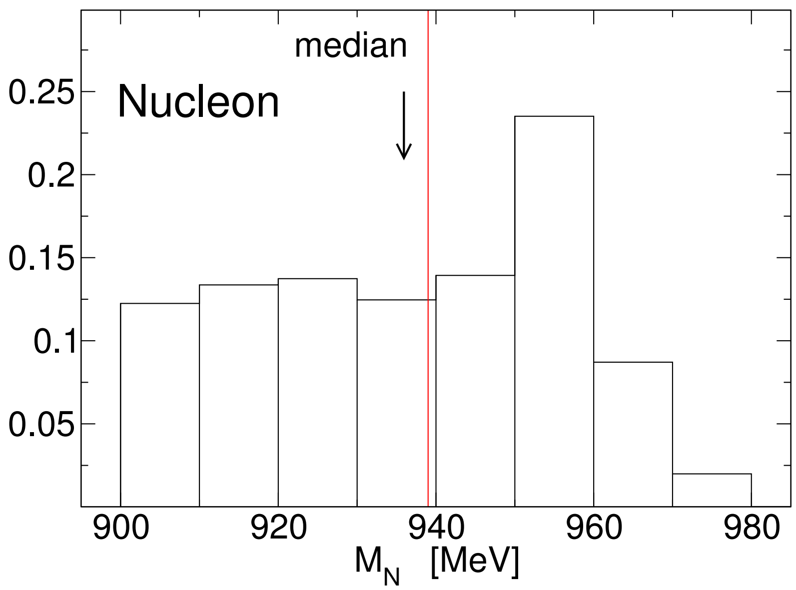
  $\rightarrow$ ChPT vs Taylor expansion
  $\rightarrow$ 3 M_π ranges $\leq 650\,\mathrm{MeV}, 550\,\mathrm{MeV}, 450\,\mathrm{MeV}$

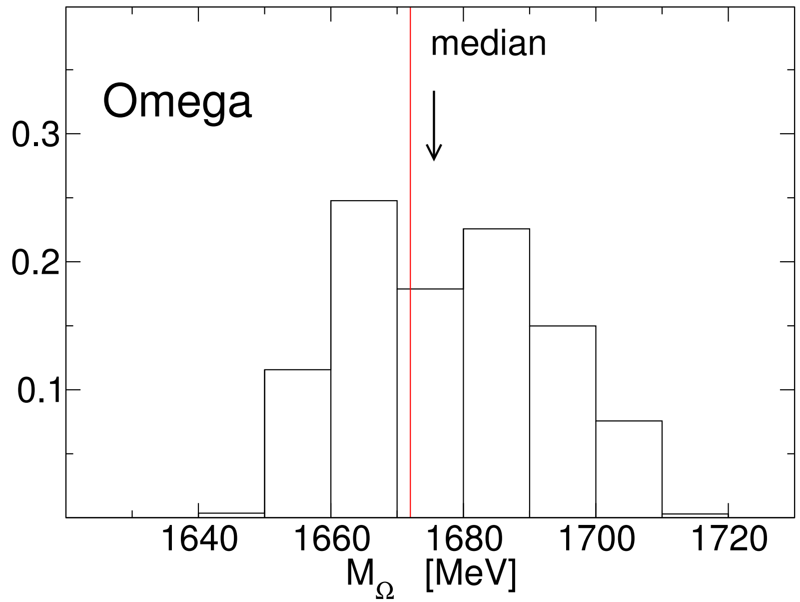
- *Normalization* $\rightarrow M_X$ vs R_X
  $\Rightarrow$ contributions to *physical mass point extrapolation* (and *continuum extrapolation*) uncertainties
- *Excited state contamination* $\rightarrow$ 18 time fit ranges for 2pt fns
- *Volume extrapolation* $\rightarrow$ include or not leading exponential correction

$\Rightarrow$ 432 procedures which are applied to 2000 bootstrap samples, for each of Ξ and Ω scale setting

ad vii: systematic and statistical error estimate

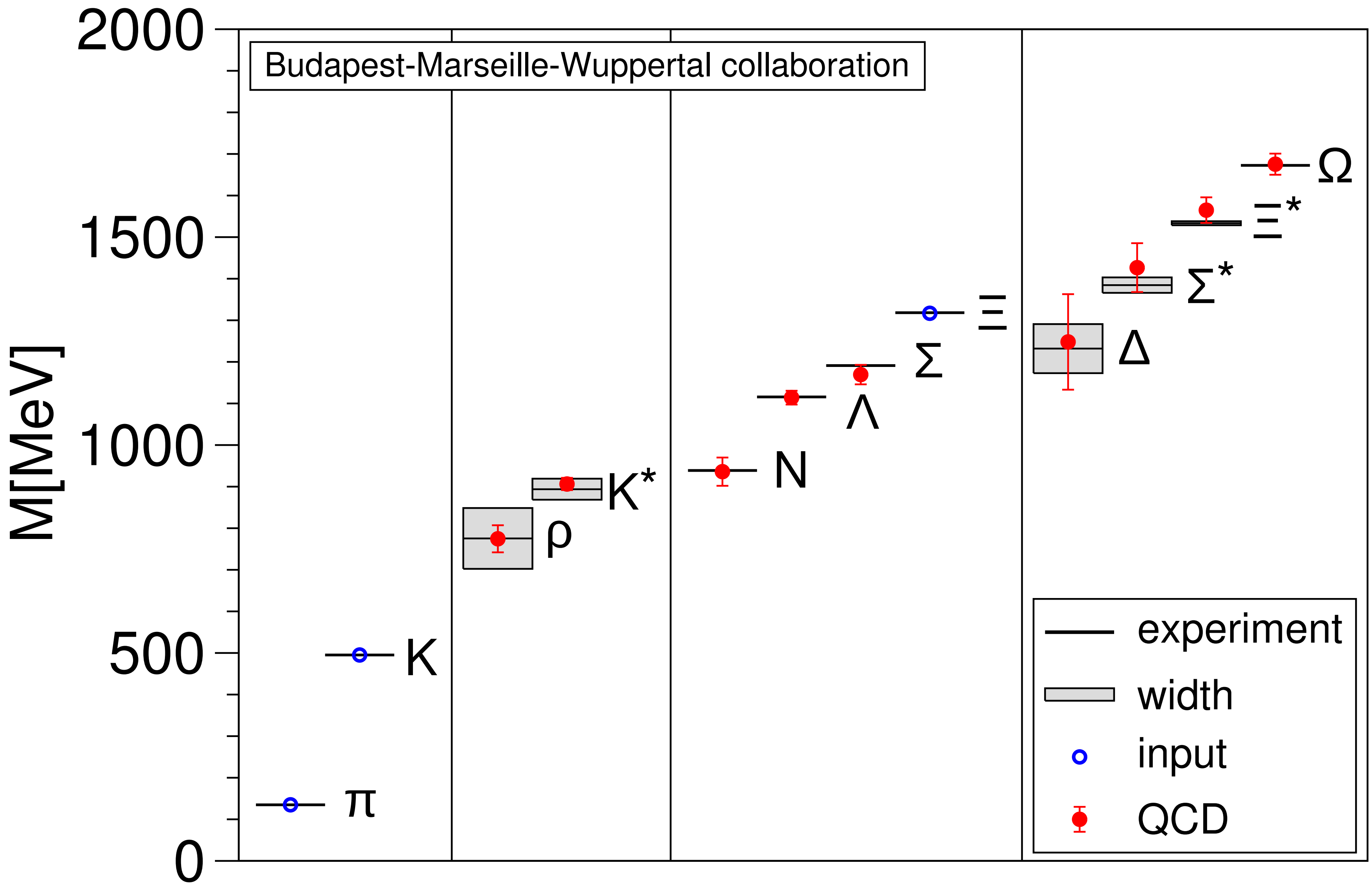
→ distribution for M_X: weigh each of the 432 results for M_X in original bootstrap sample by fit quality





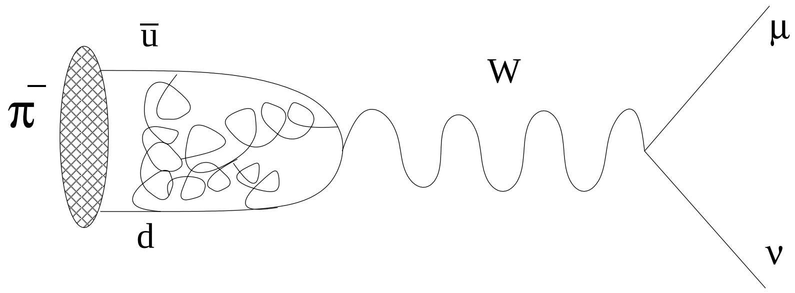
- Median → central value
- Central 68% CI → systematic error
- Central 68% CI of bootstrap distribution of medians → statistical error

Post-dictions for the light hadron spectrum



$|V_{us}/V_{ud}|$ from $K,\pi \to \mu\bar{\nu}(\gamma)$

In experiment see



$$\propto \quad V_{ud}\,\langle 0|\bar{u}\gamma_\mu\gamma_5 d|\pi^-\rangle \propto V_{ud}\,F_\pi$$

Have (Marciano '04, Flavianet '08)

$$\frac{\Gamma(K\to\mu\bar{\nu}(\gamma))}{\Gamma(\pi\to\mu\bar{\nu}(\gamma))} \longrightarrow \frac{|V_{us}|}{|V_{ud}|}\frac{F_K}{F_\pi} = 0.2760(6)\ [0.22\%]$$

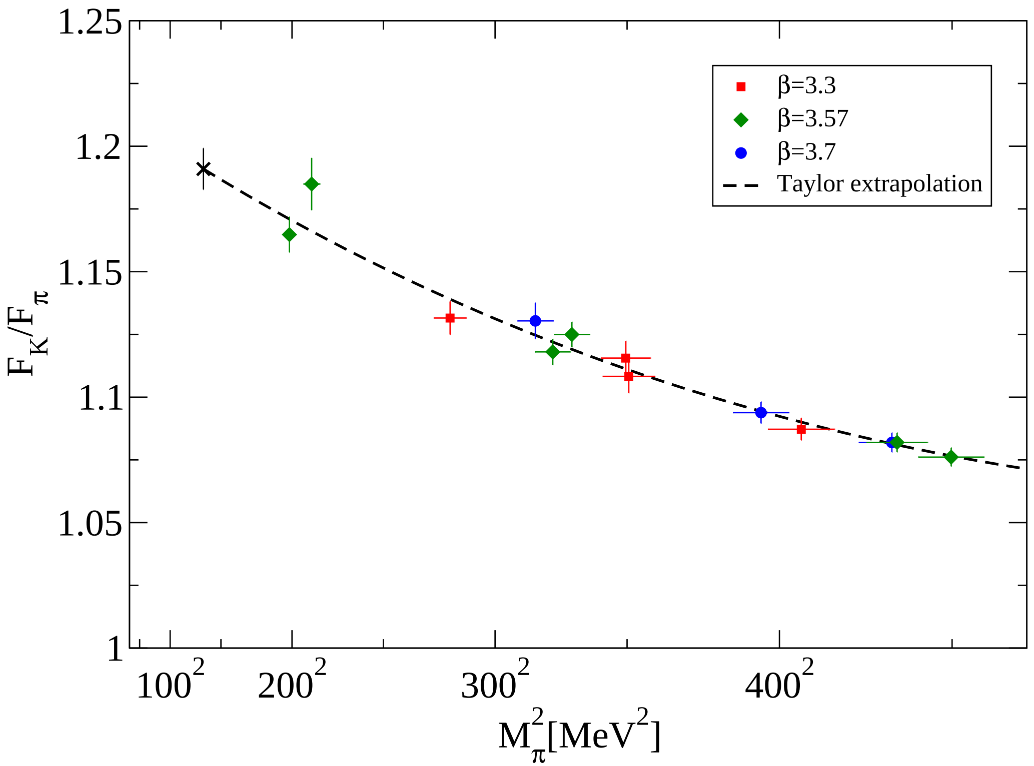
$\Rightarrow$ need high precision nonperturbative calculation of F_K/F_π

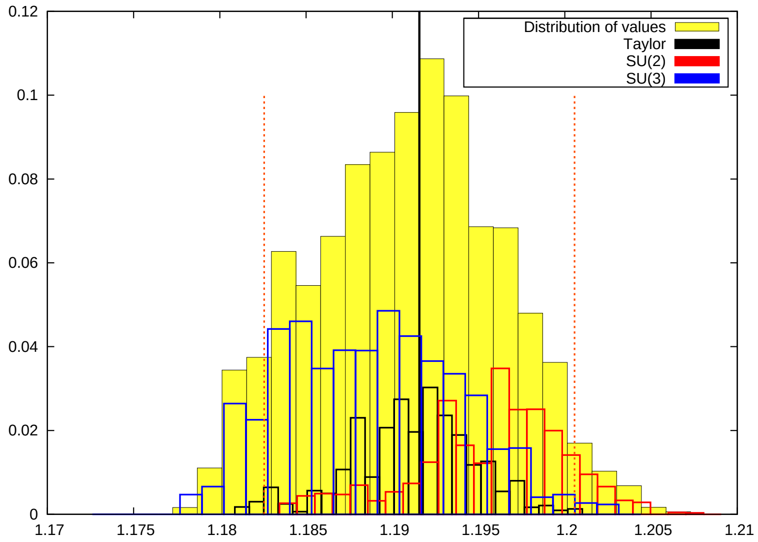
- Use our '08 data sets ($M_\pi \to 190\,\mathrm{MeV}$, $a \approx 0.065 \div 0.125\,\mathrm{fm}$, $L \to 4\,\mathrm{fm}$) to compute F_K/F_π
- Perform 1512 independent full analyses of our data

  $\Rightarrow$ systematic error distribution for F_K/F_π (as above)
- Get statistical error from bootstrap analysis on 2000 samples

F_K/F_π in QCD

Dürr et al, PRD81 '10

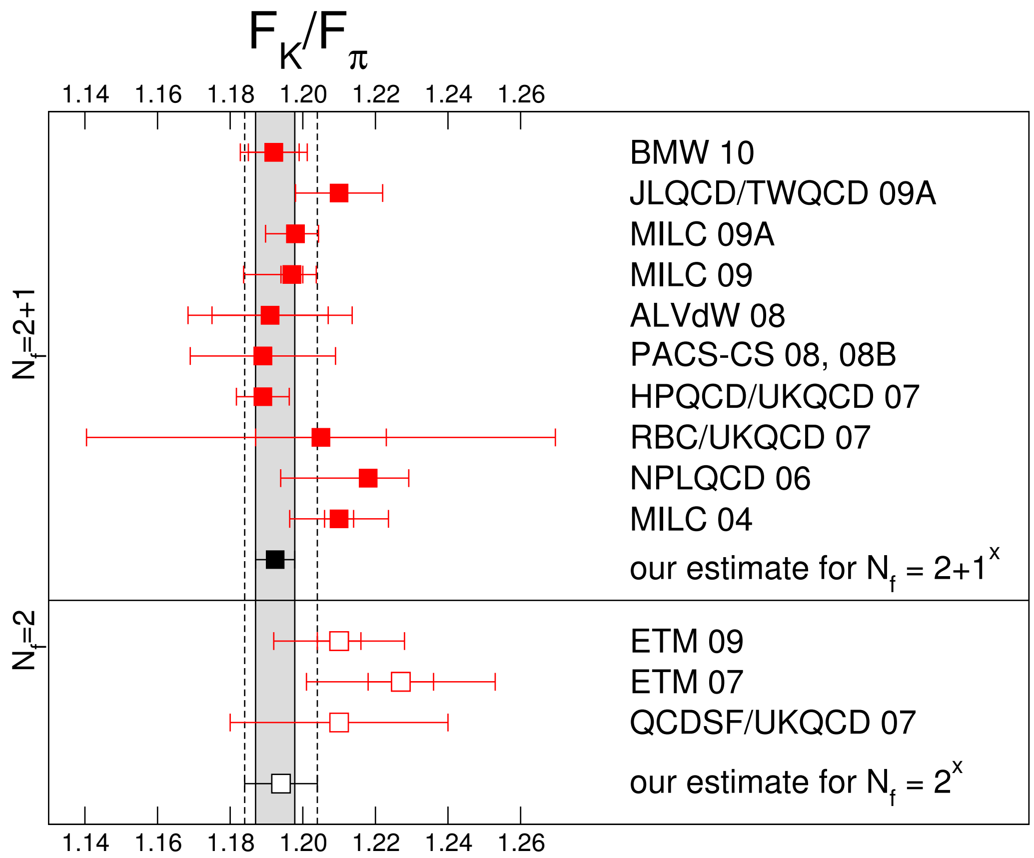




$$\frac{F_K}{F_\pi} = 1.192(7)_{\rm stat}(6)_{\rm syst}\ [0.8\%]$$

Main source of sytematic error: extrapolation $m_{ud} \to m_{ud}^{\rm phys}$; then $a \to 0$

F_K/F_π summary and CKM unitarity



(Flavianet Lattice Averaging Group (FLAG) '10)

FLAG '10 estimates (direct)

$$\frac{F_K}{F_\pi} = 1.193(6) \qquad N_f = 2+1$$

$$\frac{F_K}{F_\pi} = 1.210(6)(17) \qquad N_f = 2$$

(x) FLAG determinations assuming the SM: expt for $\Gamma_{K\ell_2}$, $\Gamma_{K\ell_3}$ and $|V_{ub}|$ (neglible contribution), plus SM universality and CKM unitarity ($|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 1$)

$\Rightarrow F_K/F_\pi$, $|V_{ud}|$ and $|V_{us}|$ in terms of lattice $f_+(0)$

Find

$$\frac{G_q^2}{G_\mu^2}|V_{ud}|^2\left[1+|V_{us}/V_{ud}|^2+|V_{ub}/V_{ud}|^2\right] = 1.0001(9)\ [0.09\%]$$

If assume true result within 2σ then, naively, $\Lambda_{NP} \geq 1.9\,\mathrm{TeV}$

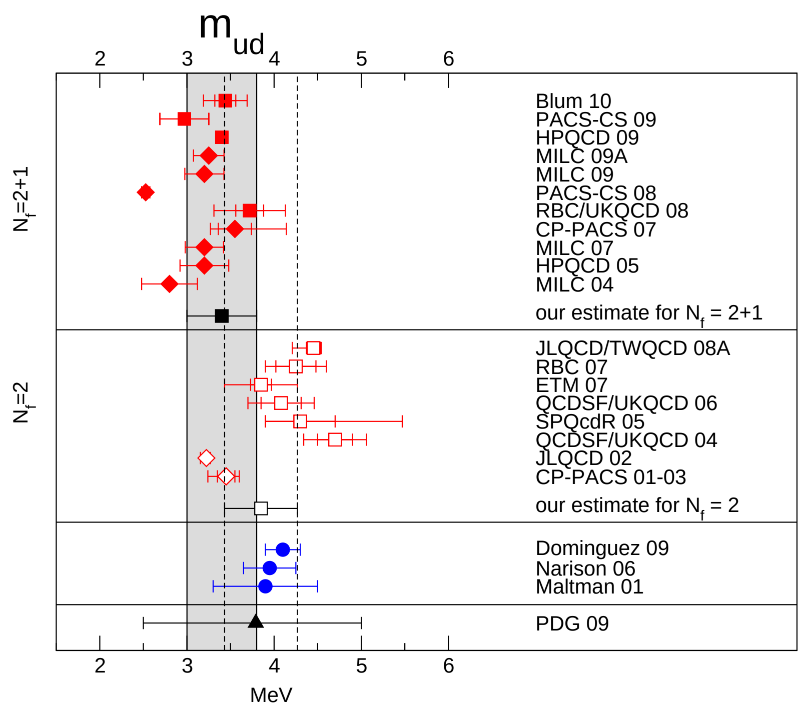
Light quark masses at the physical mass point

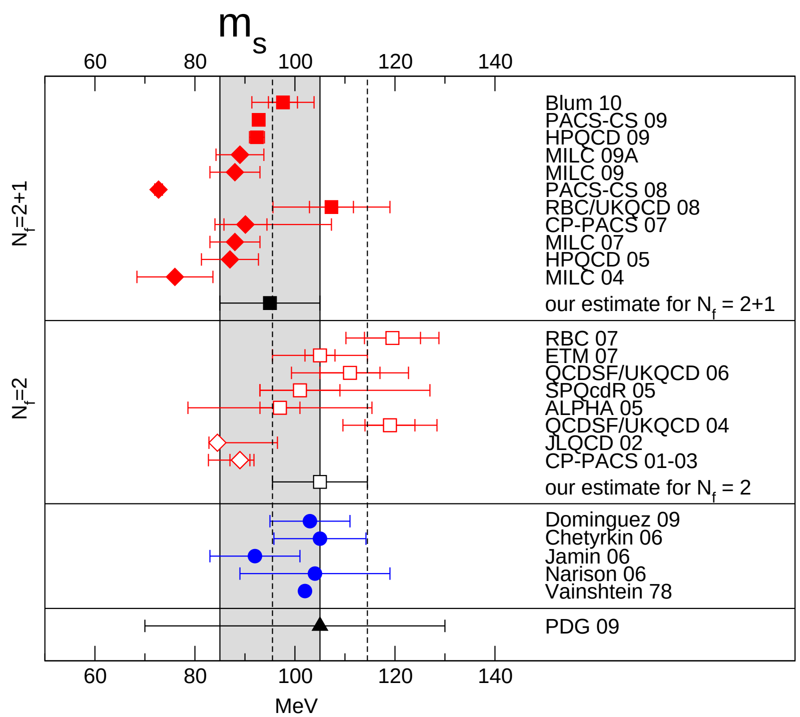
- Masses of light u, d and s quarks $\rightarrow$ fundamental parameters of the Standard Model (SM)
- Stability of atoms, nuclear reactions which power stars, presence or absence of strong CP violation, etc. depend critically on precise values
- Values carry information about flavor structure of BSM physics
- Quarks are confined w/in hadrons
  $\Rightarrow$ a nonperturbative computation is required
- 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 haystack problem
- Fortunately, QCD spontaneously breaks chiral symmetry
  $\Rightarrow$ masses of resulting Nambu-Goldstone mesons very sensitive the light quark masses
  $\Rightarrow$ presence of chiral logs near physical point
  $\Rightarrow$ must get very close to m_{ud}^{ph} to control mass dependence precisely

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

Current knowledge of the light quark masses

FLAG has performed a detailed analysis of unquenched lattice determinations of the light quark masses ("our estimate" = FLAG estimate)





$$m_{ud}^{\overline{MS}}(2\,\mathrm{GeV}) = \begin{cases} 3.4(4)\,\mathrm{MeV} & [12\%] \quad \text{FLAG} \\ 2.5 \div 5.0\,\mathrm{MeV} & [30\%] \quad \text{PDG} \end{cases}$$

$$m_{s}^{\overline{MS}}(2\,\mathrm{GeV}) = \begin{cases} 95.(10)\,\mathrm{MeV} & [11\%] \quad \text{FLAG} \\ 70 \div 130\,\mathrm{MeV} & [30\%] \quad \text{PDG} \end{cases}$$

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)

My dream calculation

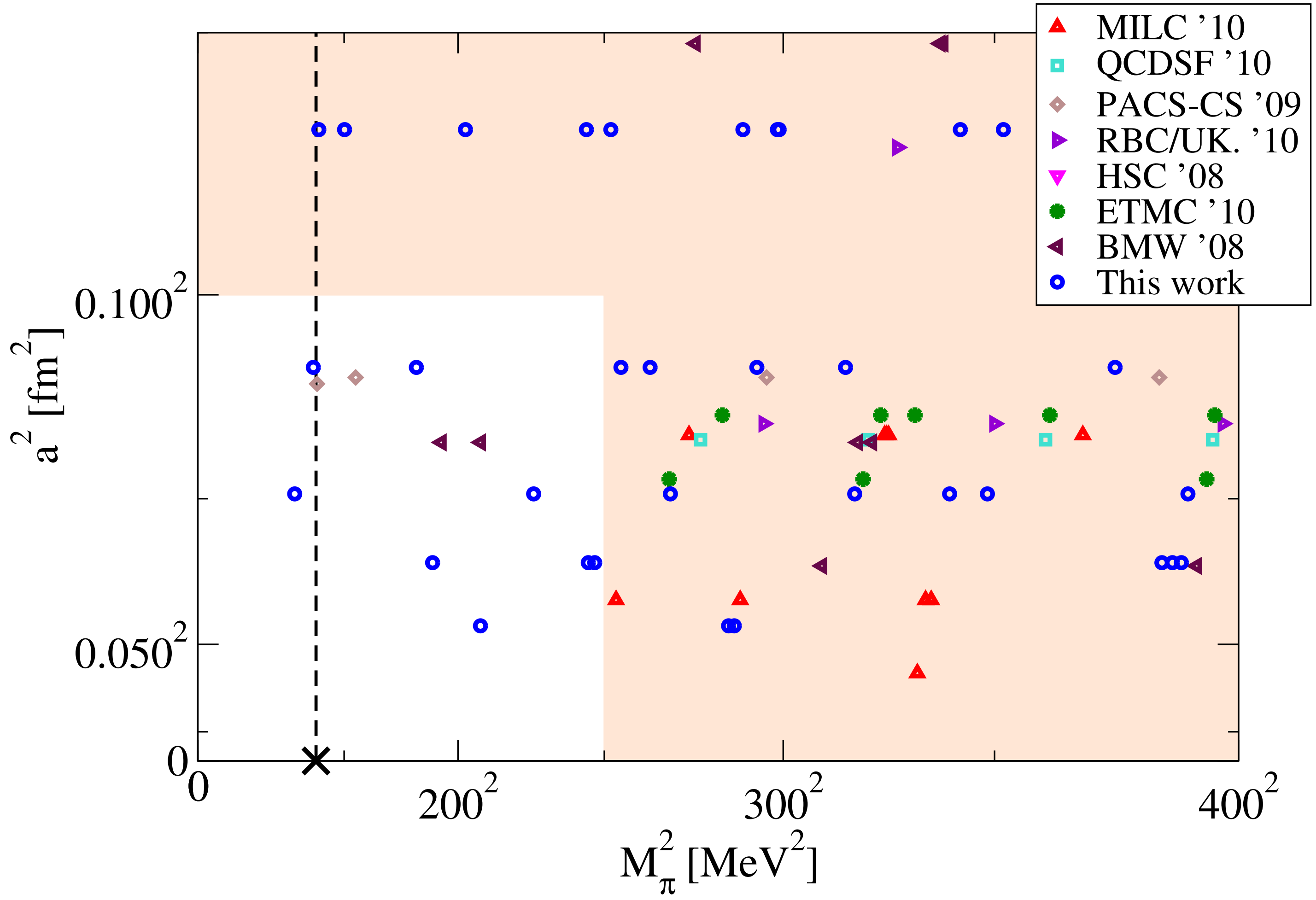
Requirements for ab initio calculations (i-vii) given earlier

$+ 2$ ingredients which guarantee added precision:

- $N_f = 2 + 1$ calculations **all the way down to** $M_\pi \sim 130\,\mathrm{MeV}$ to allow small interpolation to physical mass point ($M_\pi = 134.8(3)\,\mathrm{MeV}$)
- Full **nonperturbative renormalization** and **nonperturbative continuum extrapolated running** for determining renormalization group invariant (RGI) quark masses

Where do we stand?

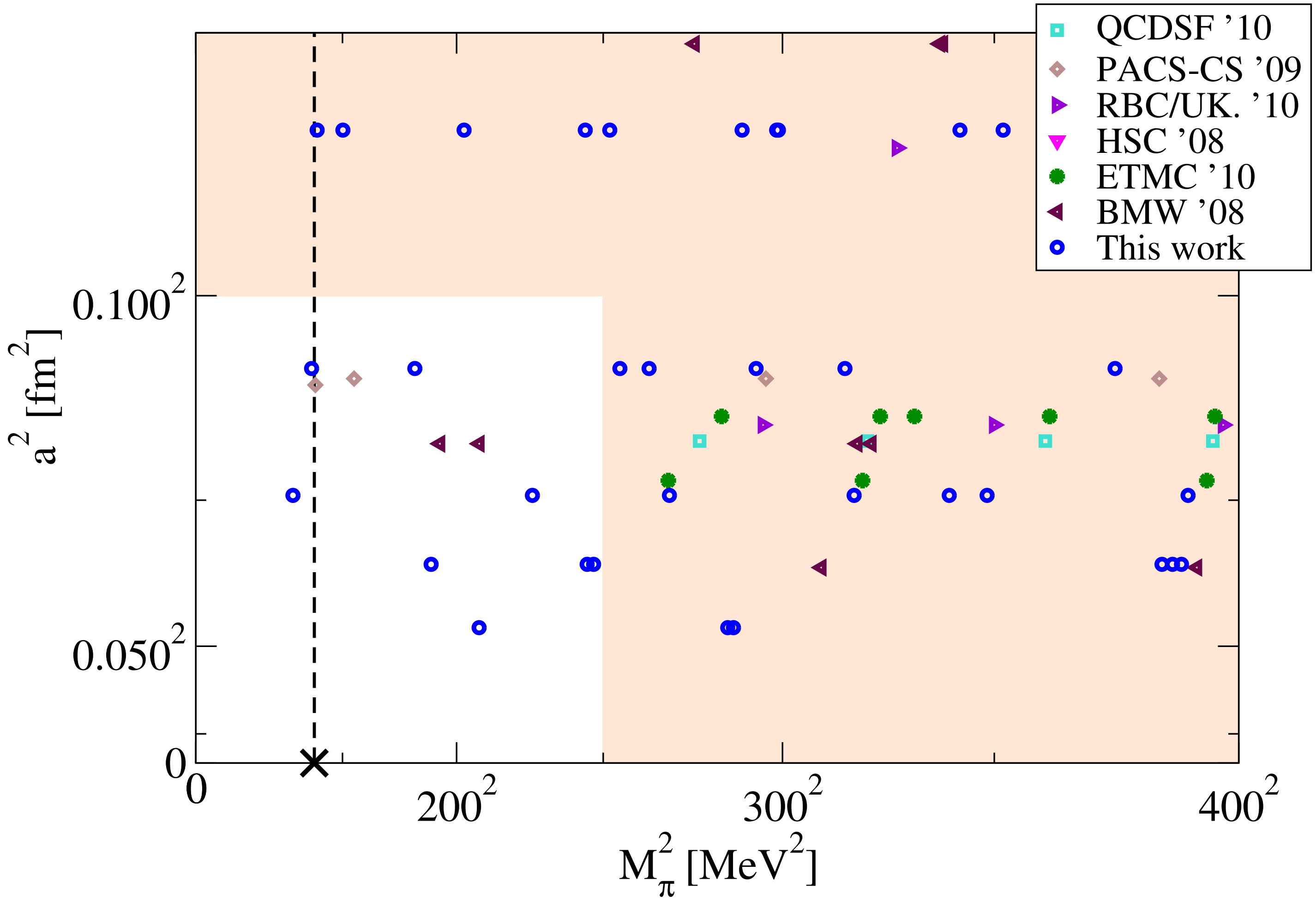
All simulations w/ $N_f \geq 2+1$ and $M_\pi \leq 400\,\mathrm{MeV}$ ... (points for our currently running, next-to-finest simulations at $\beta = 3.7$ are estimates)



(from C. Hoelbling, Lattice 2010)

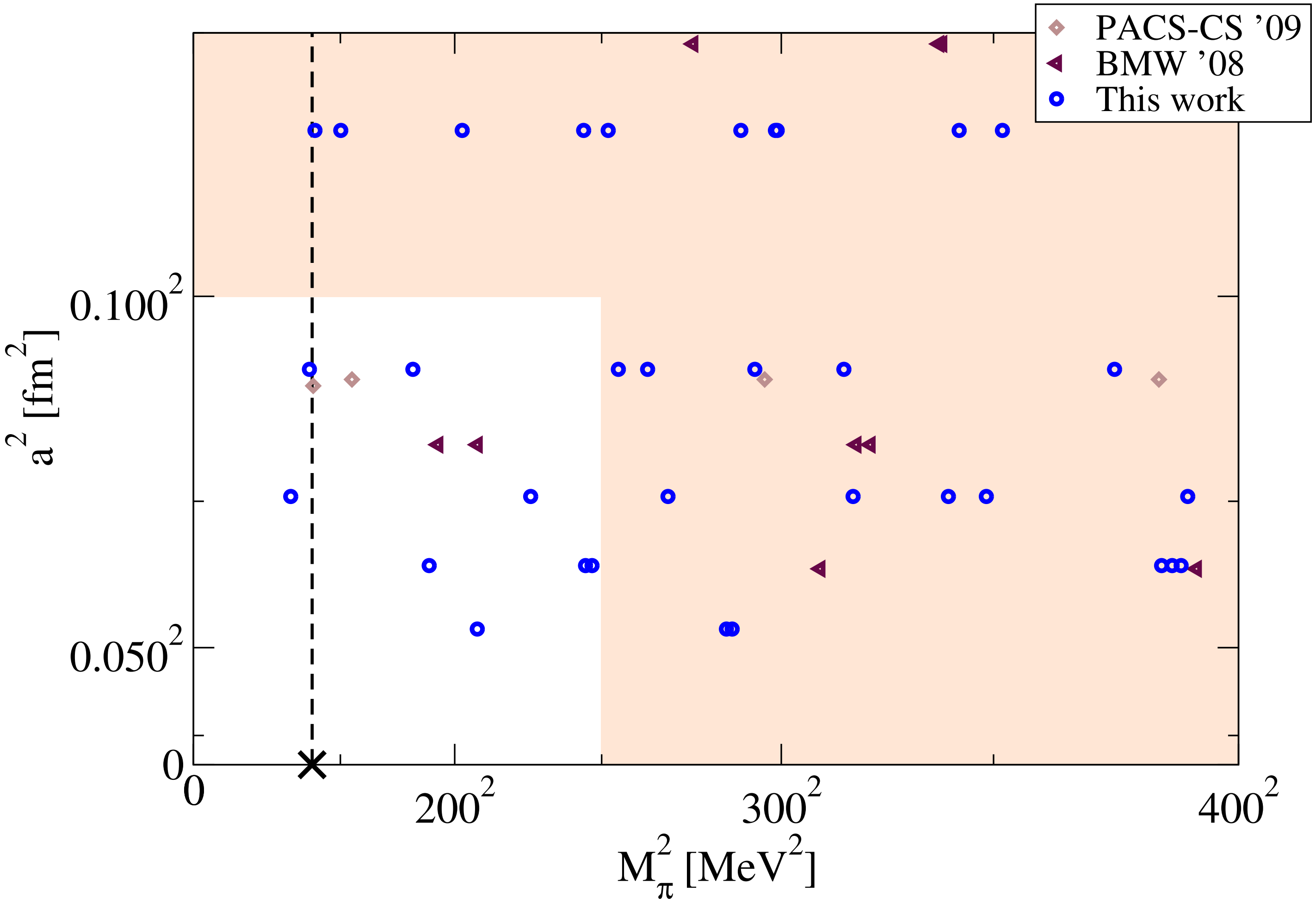
Where do we stand?

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



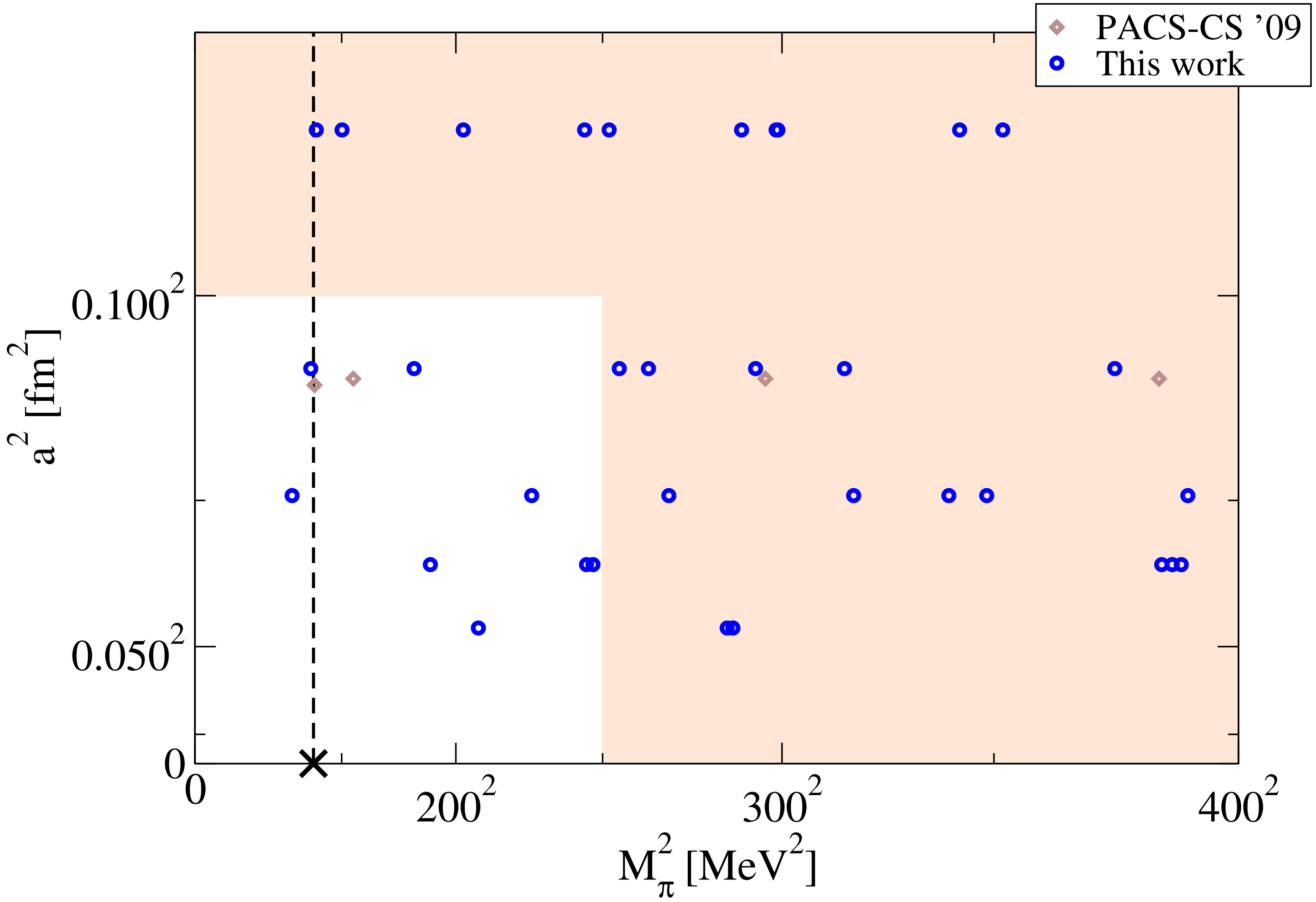
Where do we stand?

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



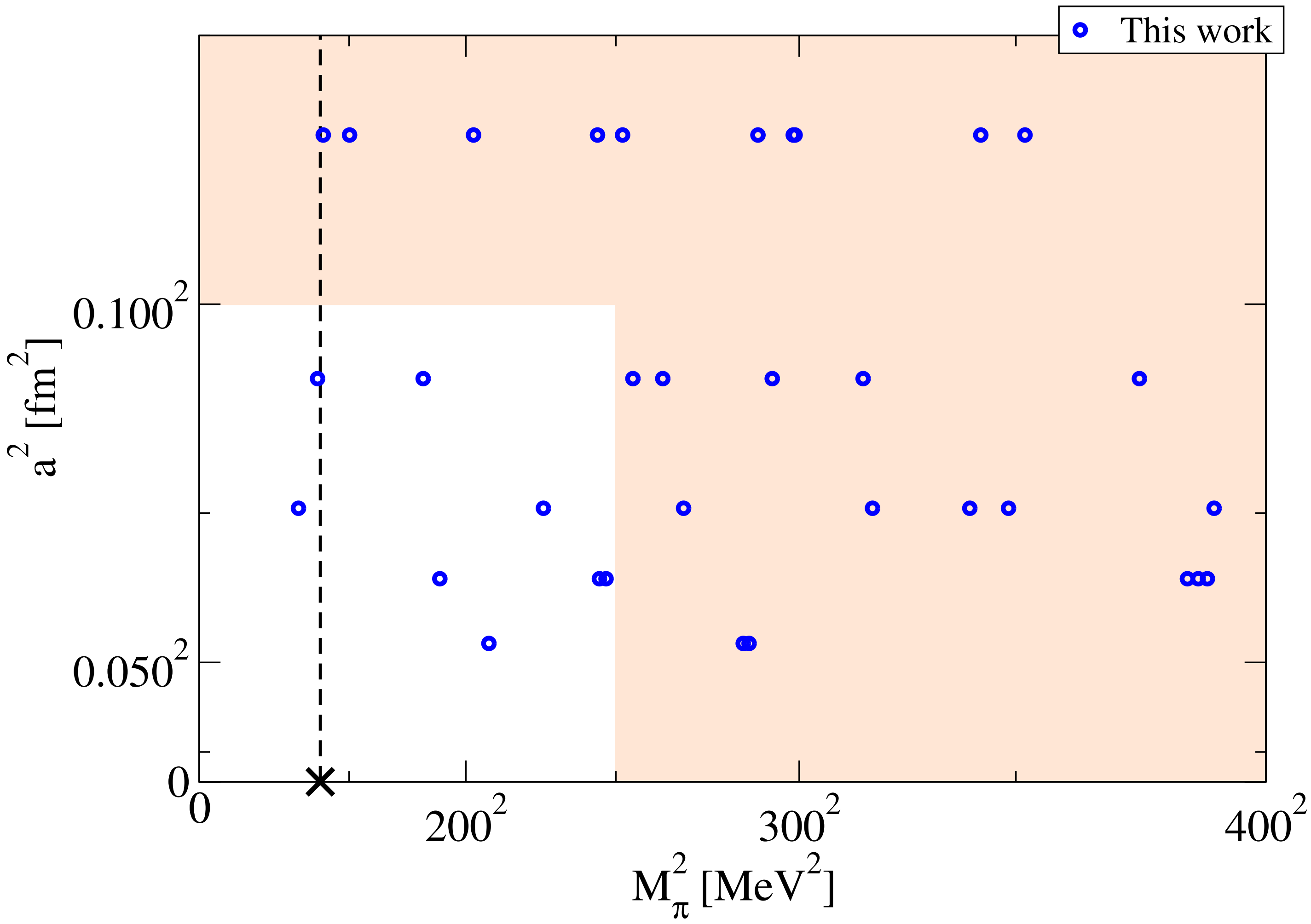
Where do we stand?

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



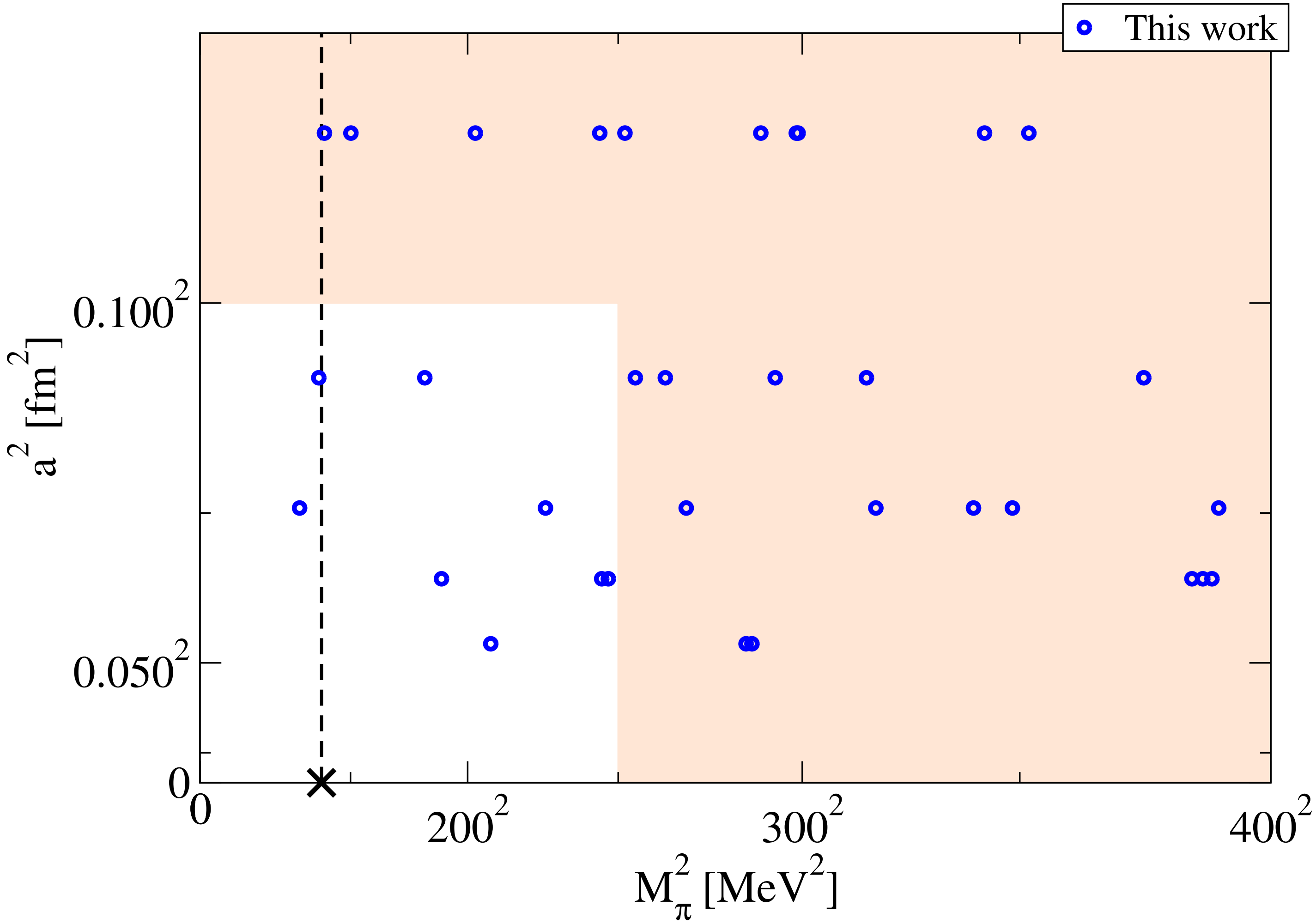
Where do we stand?

. . . 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* – PACS-CS has only 1 $a \sim 0.09\,\mathrm{fm}$

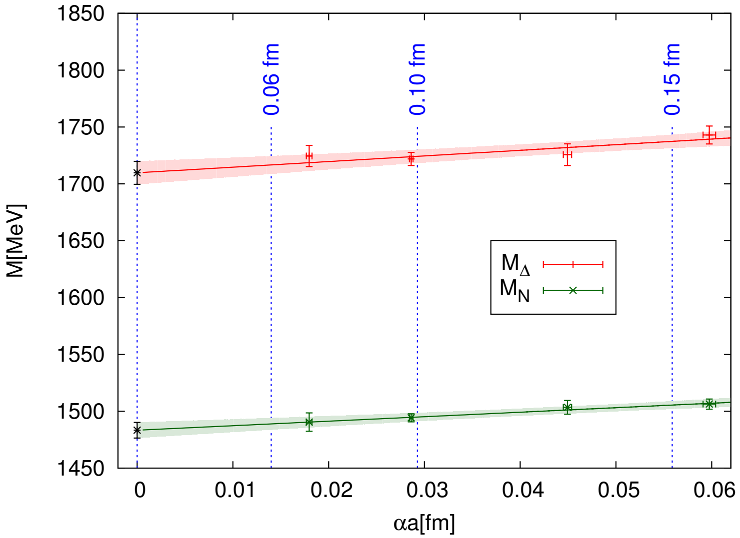


Does our smearing enhance discretization errors?

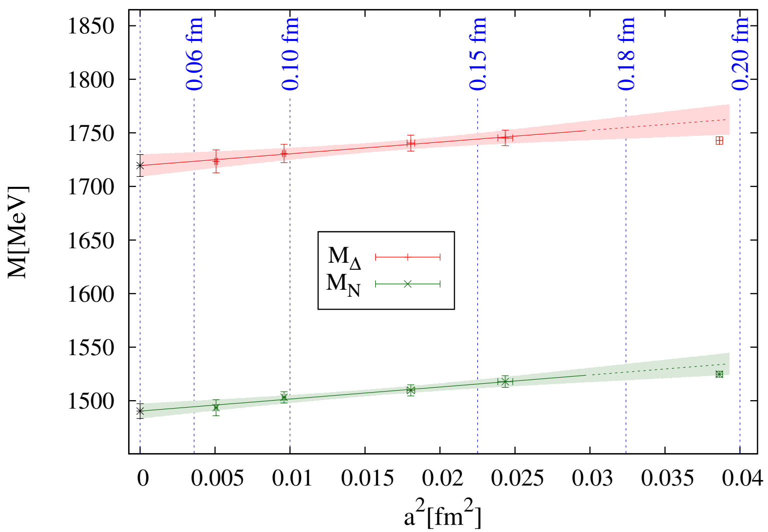
$\Rightarrow$ scaling study: $N_f = 3$ w/ 2 HEX action, 4 lattice spacings ($a \simeq 0.06 \div 0.15\,\mathrm{fm}$), $M_\pi L > 4$ fixed and

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

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



BMW '10



BMW '08

- 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 $a \sim 0.15\,\mathrm{fm}$

Does our smearing enhance discretization errors?

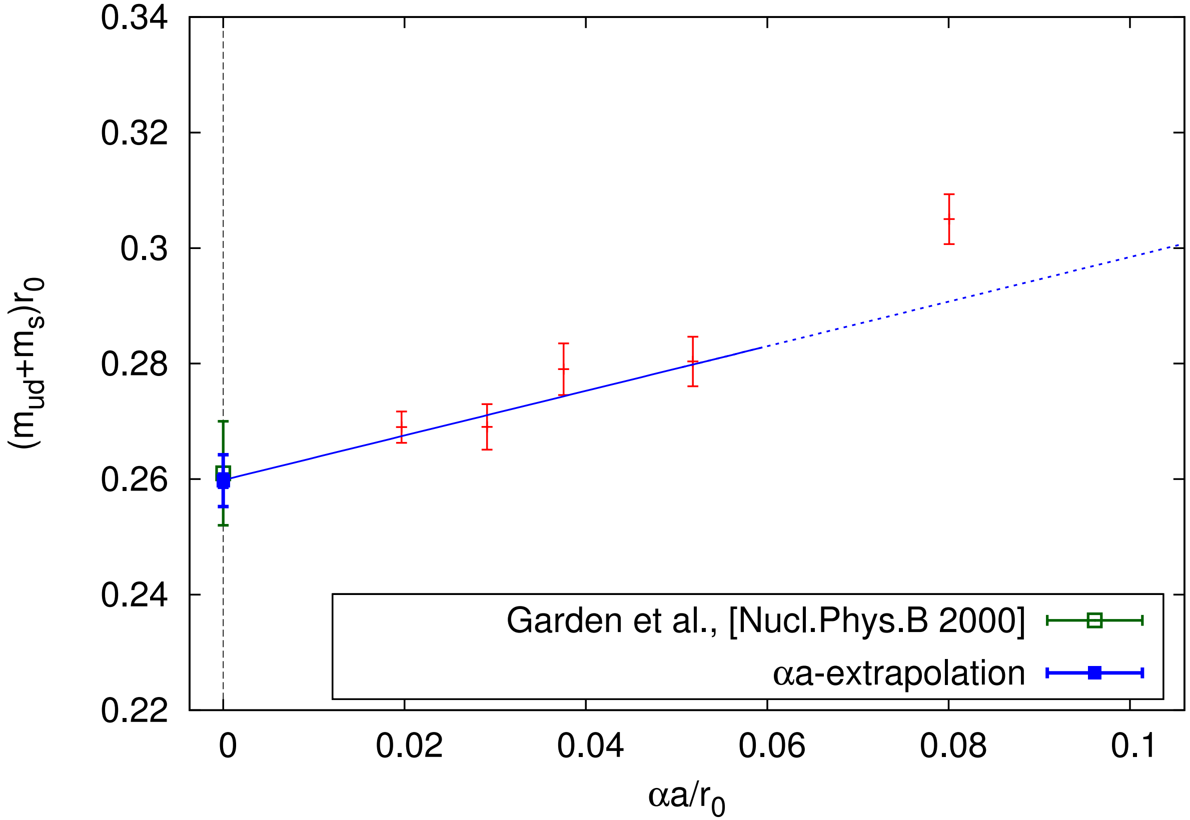
Perhaps 2 HEX works for spectral quantities but not for short distance dominated quantities
$\Rightarrow$ repeat ALPHA's 2000 *quenched* milestone determination of $r_0(m_s + m_{ud})^{\overline{\rm MS}}(2\,{\rm GeV})$

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 $\mu = 4\,{\rm GeV}$ (see below)
- Interpolate in $r_0 M_{PS}$ to $r_0 M_K^{\rm phys}$
- $m^{\rm RI}(4\,{\rm GeV}) \longrightarrow m^{\overline{\rm MS}}(2\,{\rm GeV})$ perturbatively

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

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



With full systematic analysis

$$r_0(m_s + m_{ud})^{\overline{\text{MS}}}(2\,\text{GeV}) = 0.262(4)(3)$$

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

$N_f = 2 + 1$ simulation parameters

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

- $5\ a \simeq 0.054 \div 0.116\,\mathrm{fm}$
- $M_\pi^{min} \simeq 135, 130, 120, 180, 220\,\mathrm{MeV}$
- L up to 6 fm and such that $\delta_{\rm FV} \leq 0.5\%$ on M_π for all runs
- $10 + 3$ different values of m_s around $m_s^{\rm phys}$
- Determine lattice spacing using M_Ω

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

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

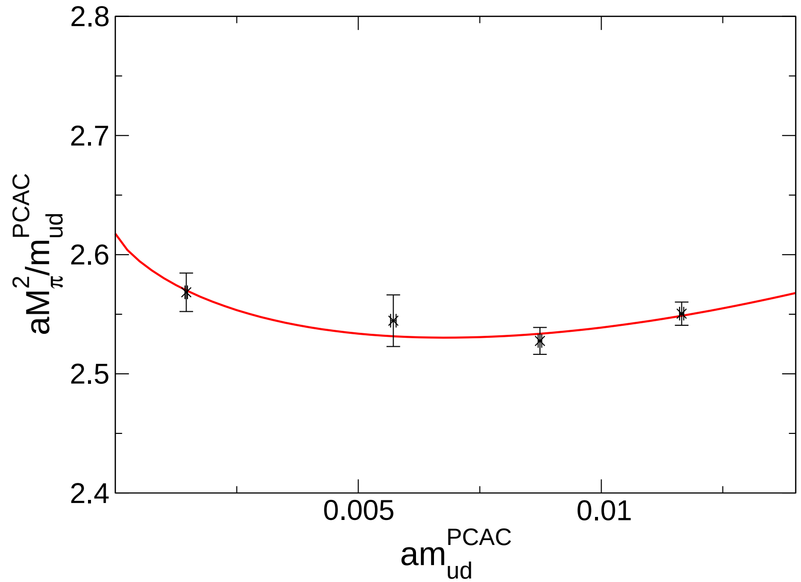
Do we see chiral logs?

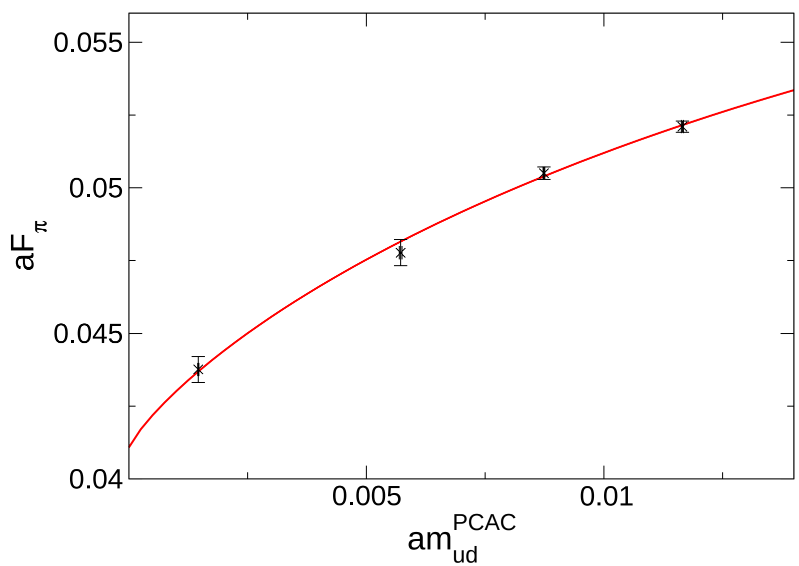
Simultaneous fit of M_π^2 and F_π vs m_{ud} to NLO $SU(2)$ χPT expressions (Gasser et al, '84)

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

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/

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

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

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

and subtracted bare masses

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

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

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

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

Benefits:

- Only Z_S (non-singlet) is required and difficult RI/MOM Z_P is circumvented
- No need to determine m^{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 $S(p) \to \bar{S}(p) = S(p) - \mathrm{Tr}_D[S(p)]/4$ (Becirevic et al '00)

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

For controlled errors, require:

(a) $\mu \ll 2\pi/a$ for $a \to 0$ 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 $\mu_{\mathrm{ren}} \sim 2\,\mathrm{GeV}$ as common renormalization point for all β
- Can take $a \to 0$

  $\Rightarrow$ continuum $m^{\mathrm{RI}}(\mu_{\mathrm{ren}})$ determined fully nonperturbatively ...
- ...but not very useful for phenomenology since RI/MOM perturbative error still significant at such μ_{ren}

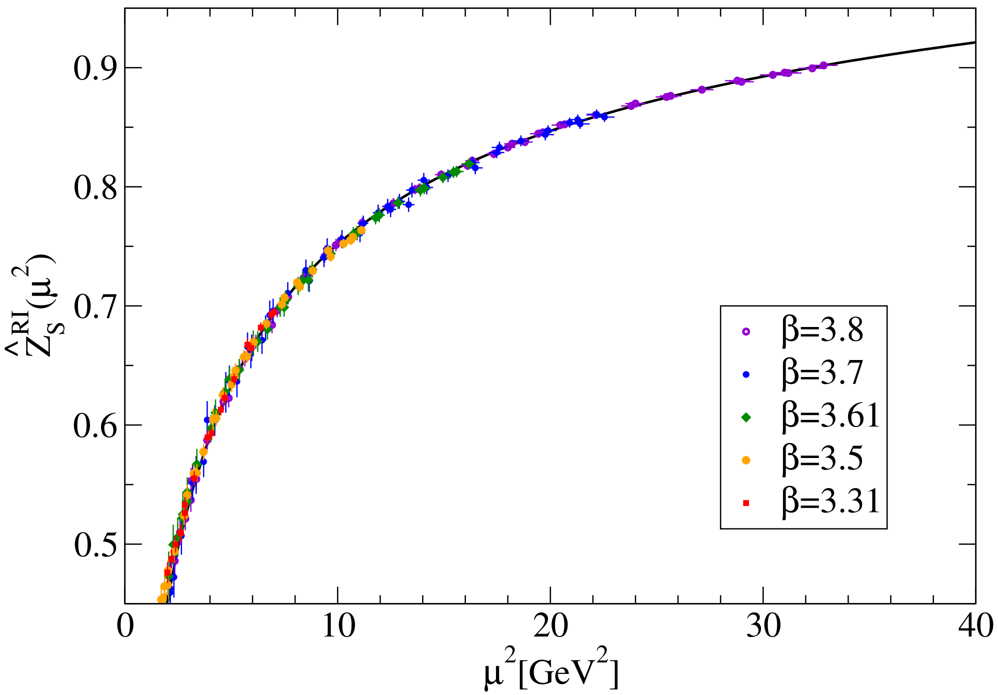
Ad (b): nonperturbative continuum running to 4 GeV

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

For $\mu : \mu_{\rm ren} \to 4\,\mathrm{GeV}$, always have at least 3 a w/ $\mu \lesssim \pi/2a$

$\Rightarrow$ can determine nonperturbative running in continuum limit

$$R^{\rm RI}(\mu_{\rm ren}, 4\,\mathrm{GeV}) = \lim_{a\to 0} \frac{Z_S^{\rm RI}(4\,\mathrm{GeV}, a)}{Z_S^{\rm RI}(\mu_{\rm ren}, a)}$$



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

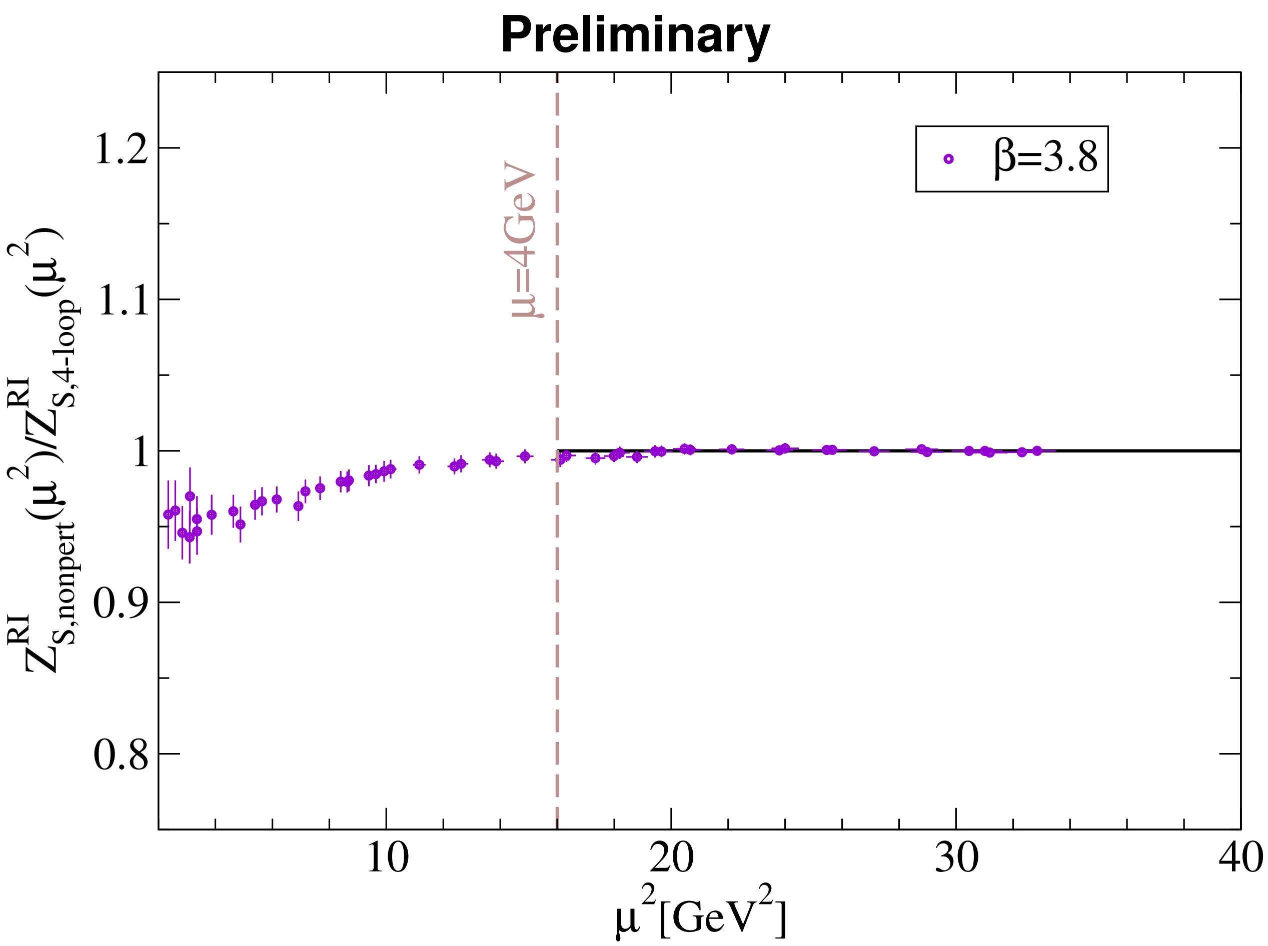
Preliminary

Running is very similar at all 4 β

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

Ad (b): running above 4 GeV

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

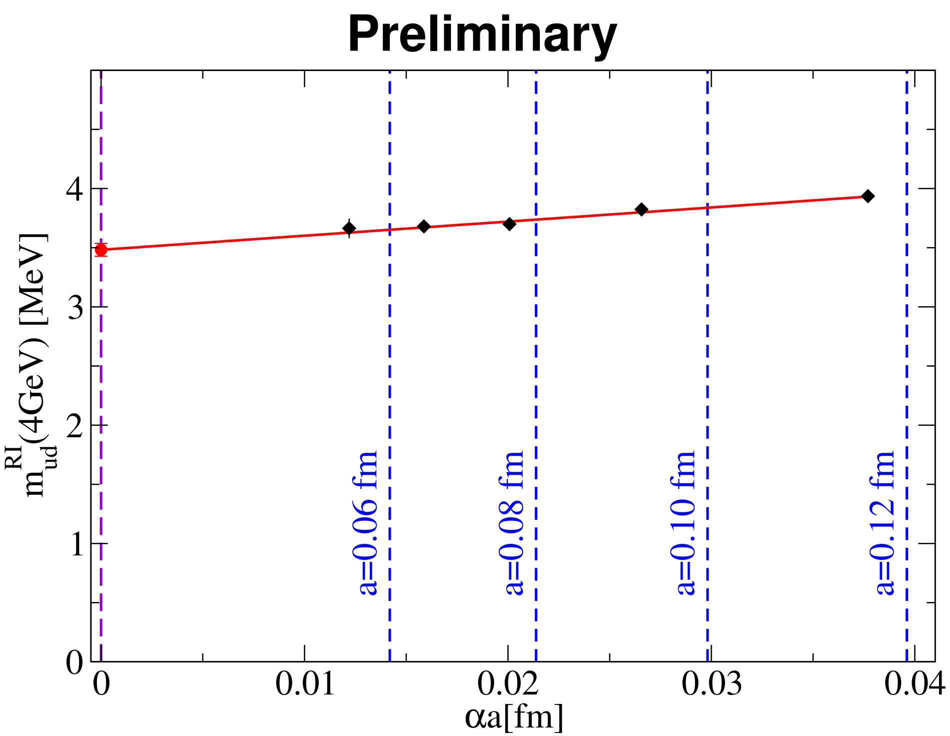


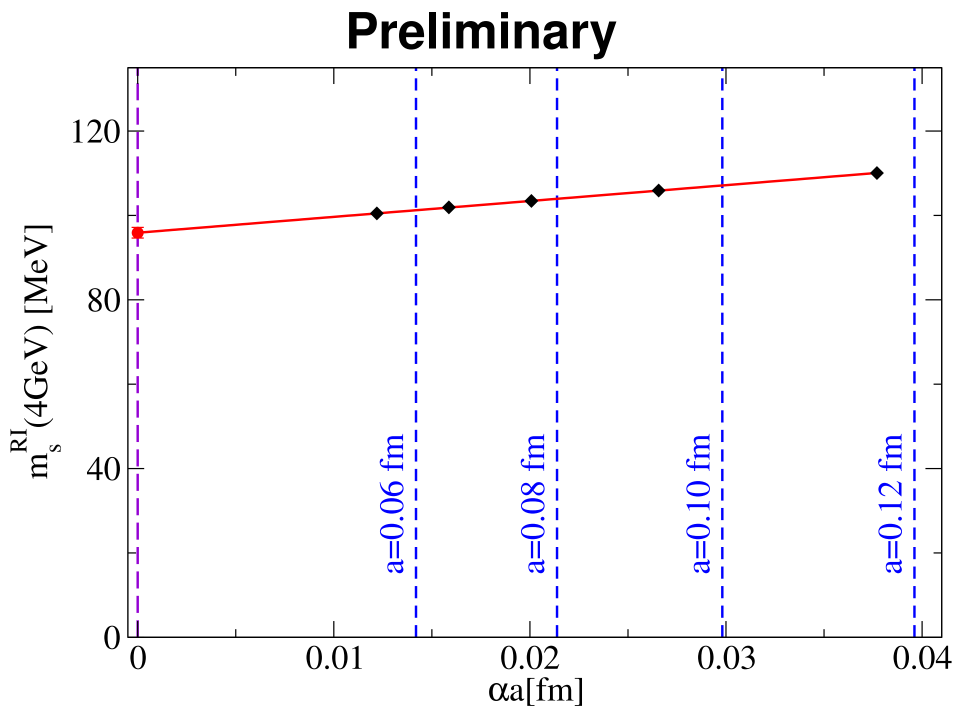
Continuum extrapolation of renormalized masses

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 $M_\pi < 340, 380\,\mathrm{MeV}$

Example of continuum extrapolations (only statistical errors on data)





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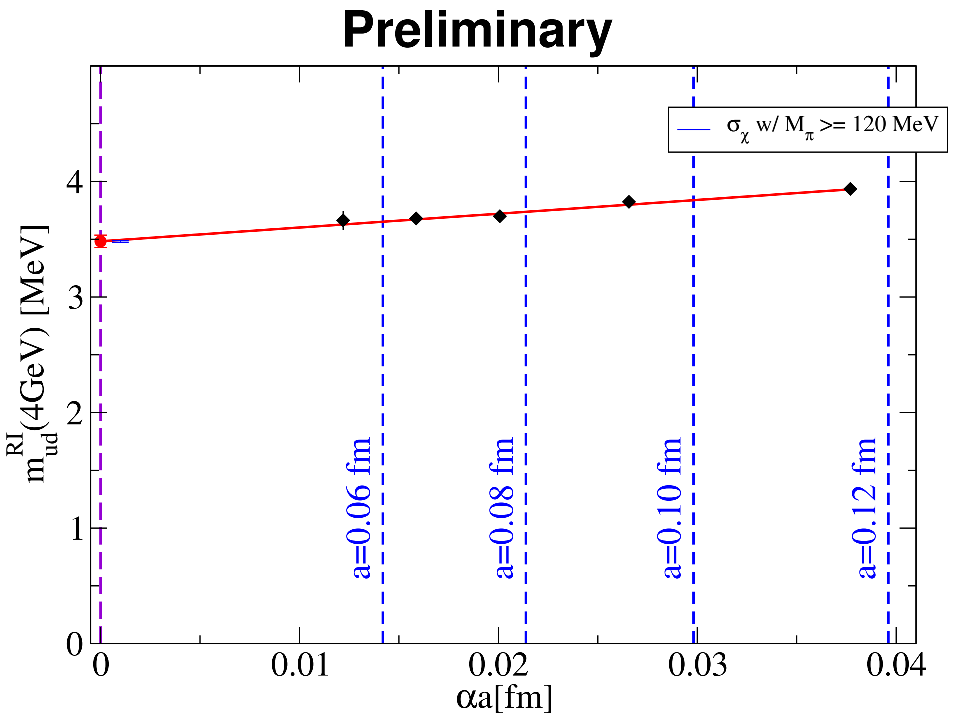
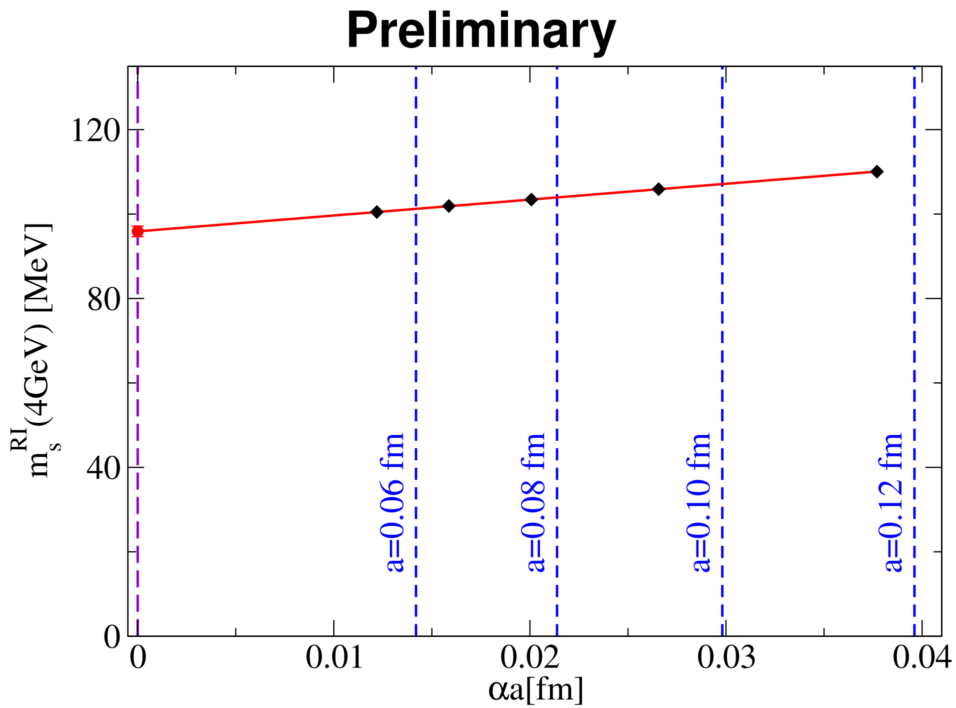
... and syst. error due to chiral interp.





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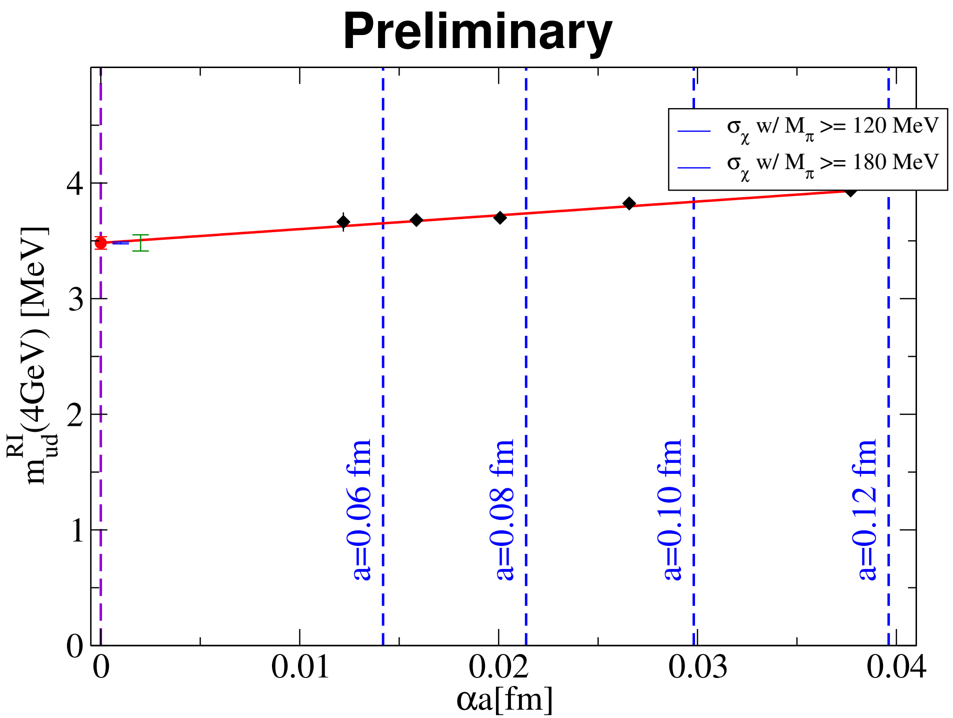
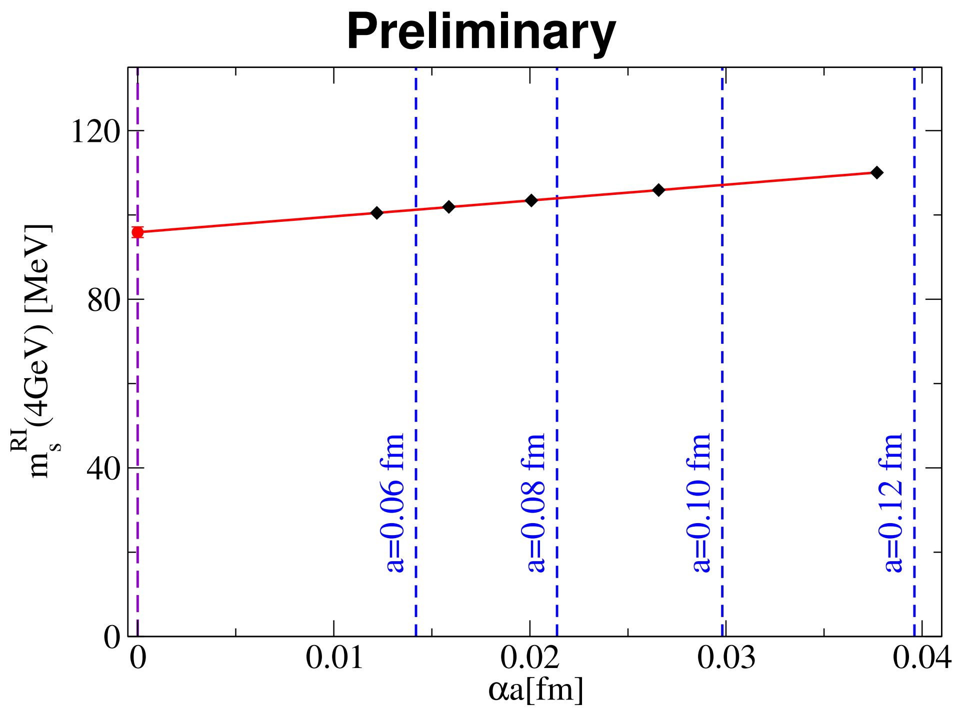
Example of continuum extrapolations (only statistical errors on data)

... and syst. error due to chiral extrap. if $M_\pi \geq M_\pi^{\mathrm{val}}|_{\mathrm{MILC}}^{\mathrm{min}} \simeq 180\,\mathrm{MeV}$





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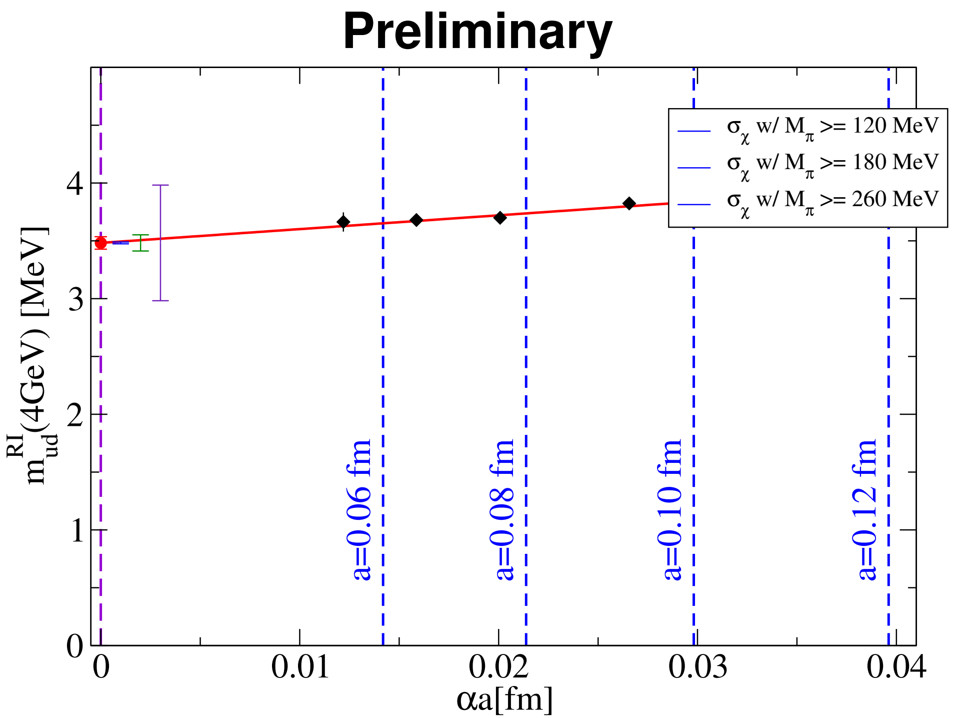
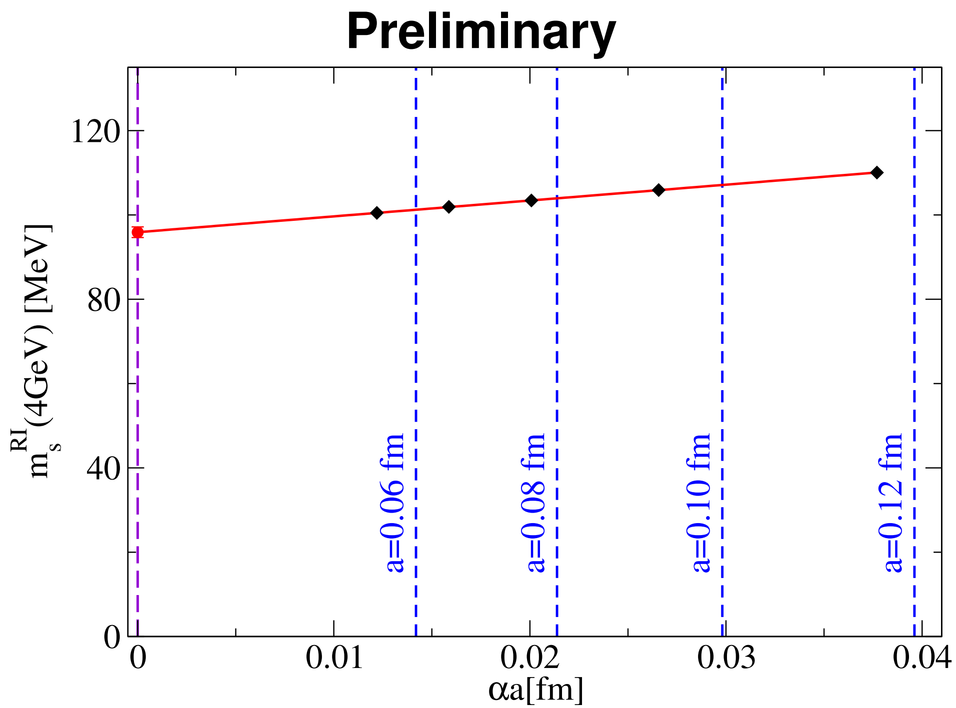
- $SU(2)$ χPT
- or low-order polynomial anszätze
- w/ cuts on pion mass $M_\pi < 340, 380\,\mathrm{MeV}$

Example of continuum extrapolations (only statistical errors on data)

... and syst. error due to chiral extrap. if $M_\pi \geq M_\pi^{\mathrm{RMS}}|^{\mathrm{min}}_{\mathrm{MILC}} \simeq 260\,\mathrm{MeV}$ (very small range)





Conclusions

- Ab initio calculation of light hadrons masses
  $\rightarrow$ excellent agreement w/ experiment
  $\Rightarrow$ vindication of (lattice) QCD in nonperturbative domain
- F_K/F_π in same approach
  $\rightarrow$ very competitive determination of $|V_{us}|$
  $\rightarrow$ stringent tests of the SM and constraints on NP
- $N_f = 2+1$ simulations have been performed all the way down to $m_{ud}^{\rm phys}$ and below w/ $m_s \simeq m_s^{\rm phys}$:
  - 5 $a \simeq 0.054 \div 0.116\,\mathrm{fm}$
  - $M_\pi^{min} \simeq 135, 130, 120, 180, 220\,\mathrm{MeV}$
  - L up to 6 fm and such that $\delta_{\rm FV} \leq 0.5\%$ on M_π for all runs

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

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

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

- Currently finalizing analysis of light quark masses

Conclusions

- Systematic error will be estimated following an extended frequentist approach (Dürr et al, Science '08)

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

$\Rightarrow$ will significantly improve knowledge of m_{ud} and m_s whose errors are, at present, 12% [FLAG] $\div$ 30% [PDG]

- HPQCD published results on m_{ud} w/ similar uncertainties, but these are obtained by fixing $N_f = 2 + 1$ QCD parameters w/:
  - r_1 for the scale – their r_0 is 3.5 σ away from PACS-CS '09
  - m_c for the scale (?) and for renormalization – their m_c has an error 13 times smaller than PDG!
  - $M_{\bar{s}s}$ for m_s – but m_s is needed to determine $M_{\bar{s}s}$!?
  - MILC m_s/m_{ud} for m_{ud} – not their m_s/m_{ud}!?

Conclusions

- In addtion, these results 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

  $\Rightarrow \delta_\chi m_{ud} \sim 0.1\% \longrightarrow \delta_\chi m_{ud} \sim 15\%$
- Imposing the cut $M_\pi \geq 180\,\mathrm{MeV}$ (lightest MILC valence pion) on our results

  $\Rightarrow \delta_\chi m_{ud} \sim 0.1\% \longrightarrow \delta_\chi m_{ud} \sim 2\%$

$\Rightarrow$ smaller error requires assumptions on mass dependence of results which go beyond (partially quenched) NLO $SU(2)$ χPT

- 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

Our "particle accelerators"

IBM Blue Gene/P (Babel), GENCI-IDRIS Paris
139 Tflop/s peak

IBM Blue Gene/P (JUGENE), FZ Jülich
1. Pflop/s peak

BULL cluster (1024 Nehalem 8 core nodes), GENCI-CCRT Bruyère-le-Châtel
100 Tflop/s peak

And computer clusters at Uni. Wuppertal and CPT Marseille