Heavy[†] Flavor Physics on the Lattice

[†]*and some light*

C. Bernard

Washington University,

St. Louis, MO USA

Outline

- “Grading” Simulations and Lattice Systematics
- Staggered quark issues
- “Gold Plated Quantities” for lattice calculations
- MILC ensembles and state of the art:
  - f_π, f_K calculations as model for heavy-light calculations
  - Current heavy-light status
- Future ensembles
- Expected future errors in heavy-light quantities
- Lattice Data Group?

Grading Simulations

- Lattice QCD is supposed to be QCD from first principles, but of course this cannot be done exactly $\Rightarrow$ systematic (and statistical) errors.
- Any simulation worth its salt (or cycles) should be estimating or bounding errors from all sources.
- But given limitations of algorithms, analysis techniques, and computer time, the error estimates may be less or more reliable.
- I want to grade simulations (e.g. A, B, C, D, F) based on the reliability of the error estimates, so that we can know how seriously to take the final results.

Grading Simulations

- Grade is **NOT** a judgment of how interesting, innovative, or important the simulation is — just a way to say how well it was possible to estimate errors.
- Grade is necessarily somewhat (you might say very!) subjective.
- But still a crucial exercise, if we are to rely on lattice results e.g. for CKM determinations.

Quenching

- In the past, most lattice calculations left out the effects of sea (“dynamical”) quarks.
- Reduces computer time by large factor: $\sim$100–1000 or more.
- But an uncontrolled approx: errors typically 10%–20%.
- “Quenched QCD” is a (reasonably good) model; it’s **NOT** QCD
- It’s time to stop doing quenched lattice calculations (except for exploratory studies). Grades of quenched calculations:
  - F: no way to estimate quenching effect
  - D: some basis for estimate of quenching effect
  - C: direct estimate of quenching effect, perhaps by [small] simulation with [some] dynamical quarks for comparison.

Partial Quenching

- “Partial quenching” is a generic term used to describe simulations where the valence and sea quark masses are different [C.B. & Golterman].
- MAY be intermediate between quenched QCD and the real world, e.g. 2 sea quark flavors (same as taking $m_s^{\rm sea} = \infty$).
  - In this case it’s not as bad as complete quenching, but still a pejorative term. (Best grade = C).
  - This $N_f = 2$ case is sometimes called “unquenched” or worse, “full QCD.” Such usage should be banned!
- BUT if 3 (light) sea quark flavors, partially quenched QCD contains real “full QCD” ($m^{\rm valence} = m^{\rm sea}$) as special case [Sharpe & Shoresh].
  - Now it’s good, even better than the real world!
  - Separate valence and sea quark mass dependences.
  - Simulations I will discuss have 3 (light) sea quarks; are either partially quenched QCD or full QCD.

Systematic Errors

- In simulation, lattice spacing a, linear lattice dimension L, and light quark mass m_l are always compromises.
- Computer time
    - $\propto a^{-7}$ at fixed L and m_l
    - $\propto L^4$ at fixed a and m_l
    - $\propto m_l^{-2.5}$ at fixed a and L:

Systematic Errors

- Given constraints, need to:
  - Extrapolate $a \to 0$ $\Rightarrow$ “continuum extrapolation” error, or at least compare various a values $\Rightarrow$ “discretization error”
  - Extrapolate down in m_l to physical u, d quark mass(es) $\Rightarrow$ “chiral extrapolation error”
  - Extrapolate $L \to \infty$ $\Rightarrow$ “finite volume error.”
    - For simple quantities, may be possible to work with a single L value large enough that error is well-understood and small enough.
    - Don’t have this option today for other two errors.

Systematic Errors

- Continuum extrapolation/discretization errors are tricky:
  - For the fastest version of light quarks (“staggered” quarks), leading error is $\mathcal{O}(a^2)$ but has a large coefficient and complicated effects (“taste violations”).
  - For heavy quarks, typically $am_Q \sim 1$, and special methods are needed to get extract continuum physics:
    - Fermilab approach [El-Khadra, Kronfeld, Mackenzie]
    - NRQCD [Lepage and Thacker]
    - For charm physics, extrapolation up from smaller am_Q
  - These techniques are viable, but require comparison of different a values to be convincing that discretization errors are under control.
    - To get an A, simulation needs at least 3 different values of lattice spacing (and not too coarse).
    - With 2 values of spacing, maximum grade = B.
    - With 1 value, maximum grade = C.

Systematic Errors

- Chiral perturbation theory helps to reduce systematic errors:
  - gives functional form of mass dependence for chiral extrapolation
  - gives analytic expression for finite volume dependence
  - can incorporate effects of finite a for light quarks, e.g. “staggered chiral perturbation theory” (SχPT) $\Rightarrow$ help to control all extrapolations together
- Essentially all interesting quantities with light (u, d) quarks have significant curvature $\sim m_\pi^2 \ln(m_\pi^2/\Lambda_\chi^2)$ $\Rightarrow$ must get to small quark mass (probably $m_{u,d} \sim m_s/4$ to $m_s/8$) to control such chiral logs in extrapolation.
- If only have large mass ($m_{u,d} \gtrsim m_s/2$), will be stuck with large (perhaps 10%–20%) and unreliable error estimates [Kronfeld & Ryan].
  - Best grade = D, unless quantity insensitive to chiral logs.

Systematic Errors

- CKM physics $\Rightarrow$ interested in matrix element of a (typically vector or axial vector) weak current or operator
- Usually, renormalization is needed: lattice and continuum versions of the current must be related by perturbation theory (and/or corresponding non-perturbative methods).
- For light meson decays ($\pi \to \mu\nu$, $K \to \mu\nu$, $K \to \pi\ell\nu$) we may be lucky:
  - can often use currents that obey PCAC or CVC on the lattice
  - lattice & continuum currents are the same: no perturbation theory needed
- But for heavy flavor physics ($B(D) \to \ell\nu$, $B(D) \to \pi\ell\nu$, B-$\bar{B}$ mixing, etc) there will be a systematic error from perturbation theory.

Systematic Errors

- One-loop calculations have unacceptably large errors ($\sim$10%).
- Luckily, non-perturbative method developed by Fermilab lattice group [Hashimoto et al.] gets most of renormalization factor, leaving much smaller term to be calculated by perturbation theory $\Rightarrow$ smaller errors.
- Appears to work well even when heavy & light quarks have different lattice actions: Reduces error to $<1\%$ in recent $D \rightarrow \pi(K)\ell\nu$ calculation [Aubin et al. (Fermilab Lattice, MILC, HPQCD), PRD 94 (2005) 011601].
- Probably will be checked (and reduced still further) by two-loop calculations using “automated perturbation theory,” [Trottier, Lepage, Nobes & collabs., based on work by Lüscher & Weisz].
- Many interesting quantities, e.g. ratios like f_{B_s}/f_B, are independent or nearly independent of perturbation theory.

Including Sea Quarks in Simulations

- To date, realistic simulations have only been done with staggered quarks [Kogut & Susskind].
  - very fast
  - have residual chiral symmetry that protects from “exceptional configurations” $\Rightarrow$ can go to low quark mass
- Domain wall quarks [Kaplan; Shamir; Furman & Shamir]: perhaps 10 to 20 times slower; some realistic simulations will are likely to come on line in the next two years. (Domain wall quarks are approximation to overlap quarks [Narayanan & Neuberger], which have exact lattice chiral symmetry but are even more expensive and unlikely to be used for dynamical simulations soon.)
- Twisted mass quarks [Frezzotti, Grassi, Sint & Weisz]: intermediate in speed between staggered and domain wall. May ultimately be very useful, but are relatively new and probably not ready for production running.

Staggered Baggage

Staggered quarks have an incomplete reduction of lattice doubling symmetry

- Each staggered lattice field (each staggered flavor) $\Rightarrow$ 4 equivalent particles in continuum.
- The quantum number of this unphysical multiplication of d.o.f. is called “taste.”
- Taste symmetry, while probably exact in the continuum, is violated on the lattice at $\mathcal{O}(\alpha^2 a^2)$ (for improved staggered).
- Although formally non-leading (leading discretization errors are $\mathcal{O}(\alpha a^2)$), taste violations are numerically important.
- Leads to both practical and theoretical issues.

Staggered Baggage

- Practical issue: taste violations must be taken into account in χPT used for extrapolation in light quark mass: SχPT [Lee & Sharpe; Aubin & C.B.; Sharpe & Van de Water]
- Theoretical issue: need to eliminate taste degree of freedom for sea quarks in simulations
  - Reduce tastes to 1 per flavor by taking $\sqrt[4]{\mathrm{Det}}$
  - At finite lattice spacing this is nonlocal operation.
    - Could it introduce nonuniversal behavior???
    - Might the $a \to 0$ limit of staggered theory with $\sqrt[4]{\mathrm{Det}}$ not be QCD???

Staggered Baggage

- What is known:
  - $\sqrt[4]{\mathrm{Det}}$ correct to all orders in perturbation theory, if normal staggered quarks w/o $\sqrt[4]{\mathrm{Det}}$ behave as expected.
  - Normal staggered gives correct anomaly for 4 tastes [Sharatchandra, Thun, Weisz]; taking $\sqrt[4]{\mathrm{Det}}$ then adjusts triangle graph appropriately for 1 taste.
  - Non-perturbative evidence against disaster is growing:
    - Dürr and Hoelbling, PRD 69 (2004) 034503 & hep-lat/0411022; Dürr, Hoelbling and Wenger, PRD 70 (2004) 094502 & hep-lat/0409108
    - Follana, Hart & Davies, PRL 93 (2004) 241601
    - Maresca and Peardon, hep-lat/0411029
    - Adams, hep-lat/0411030
    - Shamir, hep-lat/0412014: Proof for free theory; gives a renormalization group framework to think about & test interacting theory. MILC is now doing some of these tests.

Staggered Baggage

- A year ago, I would have subtracted one full grade (e.g. B → C) because of uncertainties about staggered.
- Now because of above investigations + agreement with experiment of known numerical results, including details of SχPT, I subtract only one fractional grade (e.g. B → B-).
- After more tests (in progress), we may be able to eliminate penalty completely.

Gold-plated Quantities

So what quantities can the lattice compute well (few %) in the next ~ 5 *years?*

- At most one hadron in initial and final state
  - large enough volume, small enough a are then feasible for full theory.
- Stable (or very narrow) hadrons, not near thresholds
  - No ρ or K^*, sorry!
  - Unstable particles require very large volumes (and untested techniques) to treat decay products correctly
  - Decays like $B \to \rho$ will be calculated, but errors will not be very well controlled ($\sim 10\%$?) — model dependence in answers and error estimates.
  - $B \to D^* \ell \nu$ probably ok

Gold-plated Quantities

So what quantities can the lattice compute well (few %) in the next ~ 5 *years?*

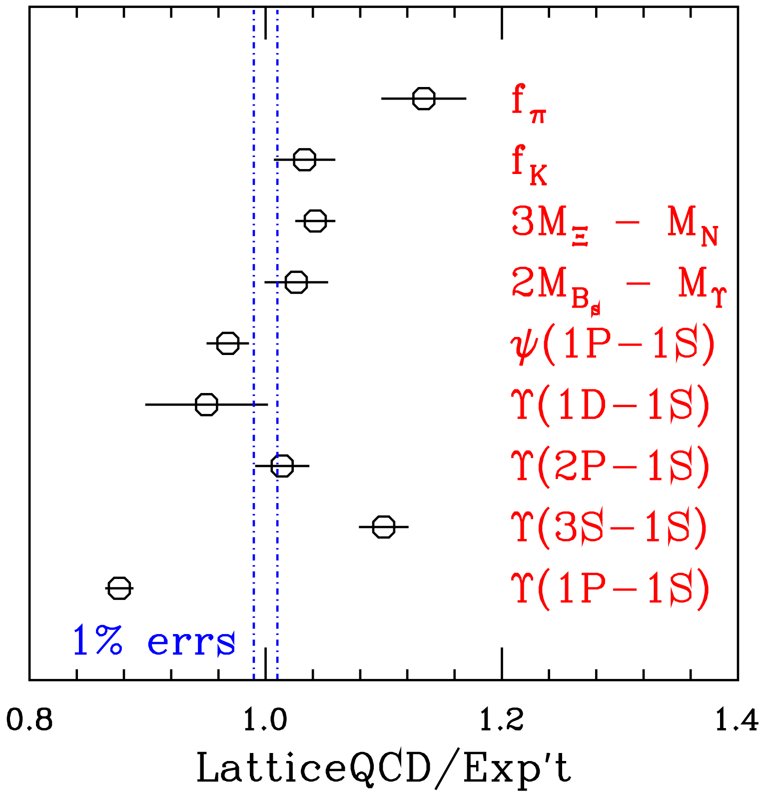
- The η also probably excluded. [Need to include η-η' mixing $\Rightarrow$ disconnected graphs $\Rightarrow$ difficult]
- No high momenta (need $|\vec{p}|a \ll 1$).
  - probably limited to $|\vec{p}| \lesssim 1\mathrm{GeV}$
  - $\Rightarrow q^2 \gtrsim 16\ \mathrm{GeV}^2$ for $B \to \pi$ semileptonic form factors.
- Chiral extrapolation must be under good control; could limit $\vec{p}$ still further. Worst case $\sim 500\ \mathrm{MeV}$? (thanks to L. Lellouch for discussion)
- We call such quantities "gold-plated" = "no excuses"

MILC Configurations

- Since 1999, MILC has been generating improved staggered configurations w/ 3 sea-quark flavors (u, d, s).
- Generically call this the MILC0 set:
  - "coarse" runs at $a \approx 0.125$ fm, $L \approx 2.5$ fm, $m_s \approx 1.2 m_s^{\mathrm{phys}}$
    - Lowest $m_{u,d} \sim 10\,\mathrm{MeV}$ ($m_\pi \approx 260\,MeV$).
    - Call the coarse subset by itself MILC-0.5
  - "fine" runs at $a \approx 0.09$ fm, $L \approx 2.5$, $m_s \approx 1.1 m_s^{\mathrm{phys}}$
    - Lowest $m_{u,d} \sim 15\,\mathrm{MeV}$ ($m_\pi \approx 320\,MeV$).
- Supplemented by additional runs to make MILC$+0.5$
  - Coarse set with $m_s \approx 0.7 m_s^{\mathrm{phys}}$ (for m_s dependence).
  - Fine set with $m_{u,d} \sim 10\,\mathrm{MeV}$ ($m_\pi \approx 260\,MeV$)
    - in progress; part of MILC1.
- MILC0 configurations publicly available: `http://qcd.nersc.gov/`

Results with MILC0 set

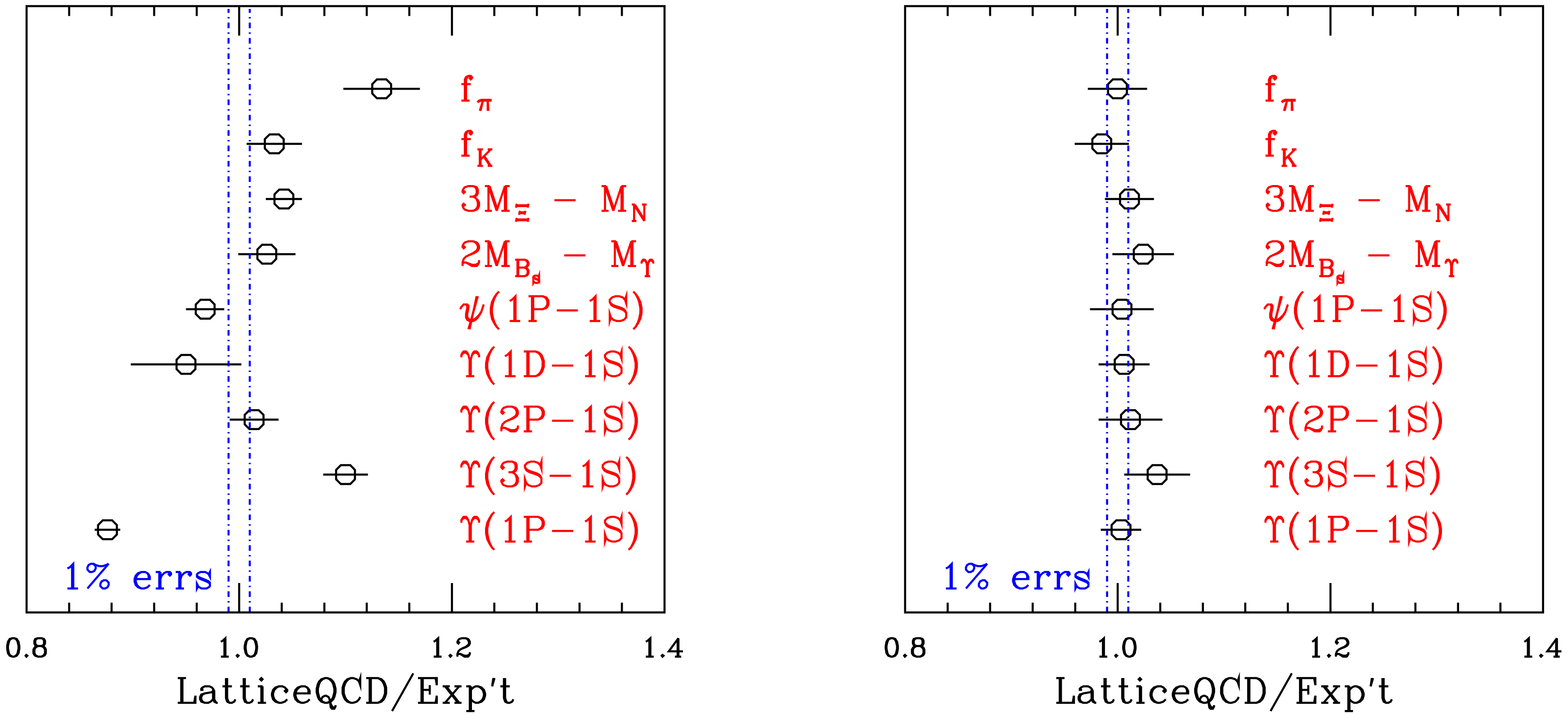
Davies, et, (Fermilab, HPQCD, MILC, UKQCD), PRL 92 (2004) 022001 (majority of results are B's, some are C's):



Quenched Approximation

Results with MILC0 set

Davies, et, (Fermilab, HPQCD, MILC, UKQCD), PRL 92 (2004) 022001 (majority of results are B's, some are C's):



Quenched Approximation

Full QCD ($n_F = 3$)

[scale from Υ 2S-1S; $m_{u,d}$, m_s, m_c, m_b from m_π, m_K, m_{D_s}, m_Υ]

Current MILC calculation of f_π, f_K

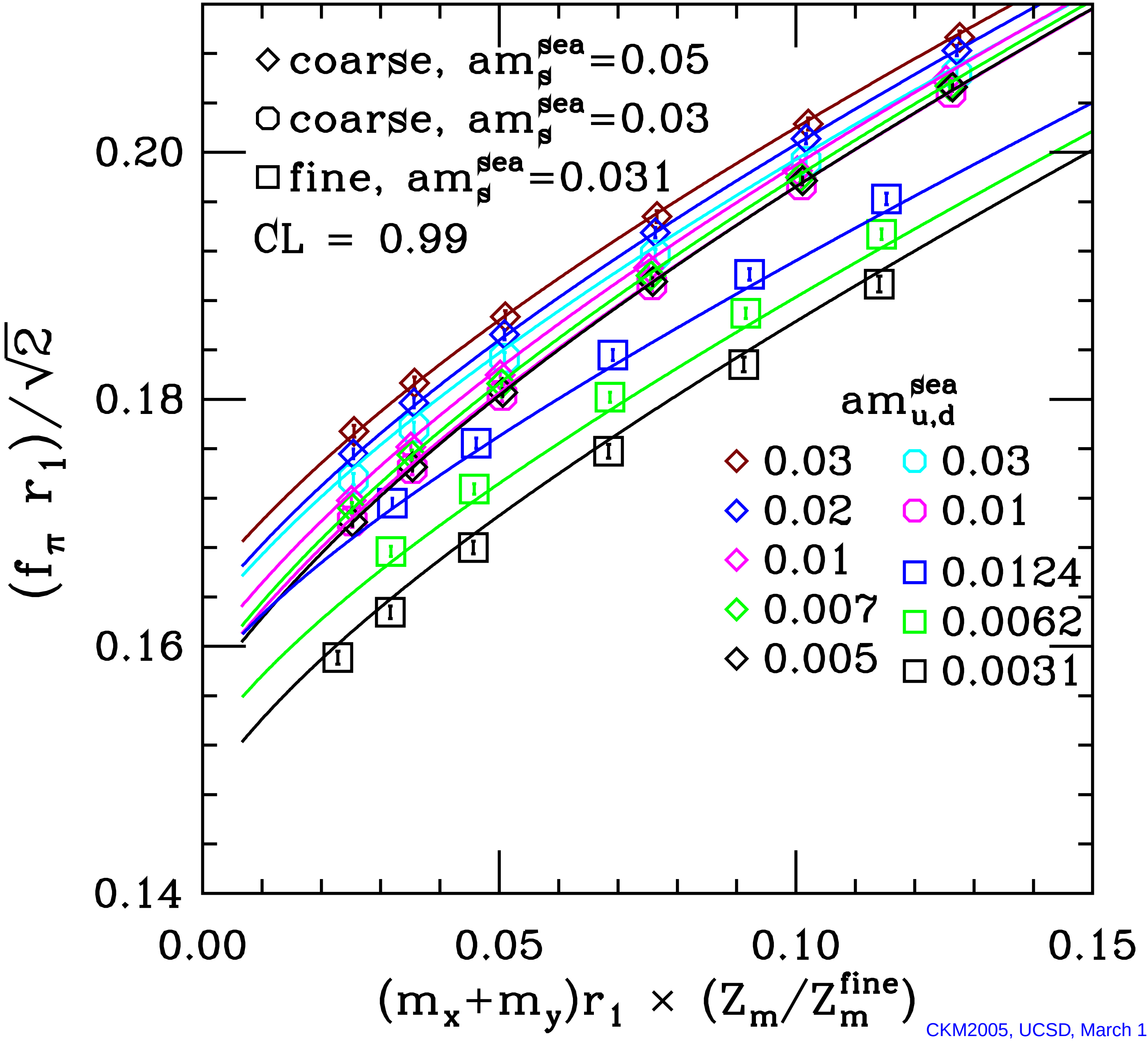
- Furthest along: full MILC0 analysis is published; preliminary MILC$+0.5$
- Can serve as model for computations in (near) future of heavy-light leptonic and semileptonic decay constants.
- Input to heavy-light error estimates to follow.

Current MILC calculation of f_π, f_K

Preliminary

MILC$+0.5$

- Fit partially quenched data to SχPT.

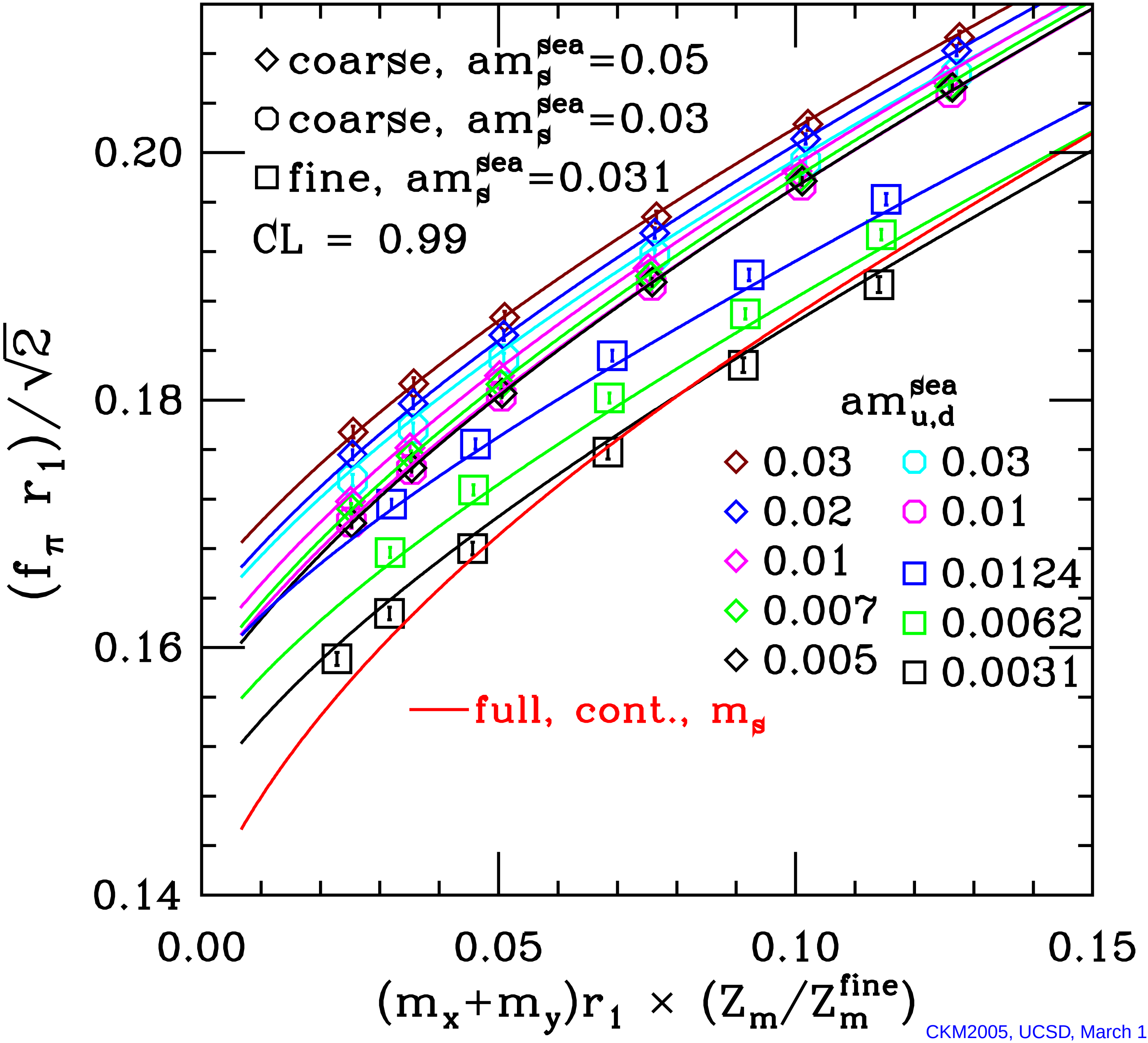


Current MILC calculation of f_π, f_K

Preliminary

MILC$+0.5$

- Extrap fit params to continuum
- Set $m_{sea} = m_{val}$ and plot as function of m_{val}

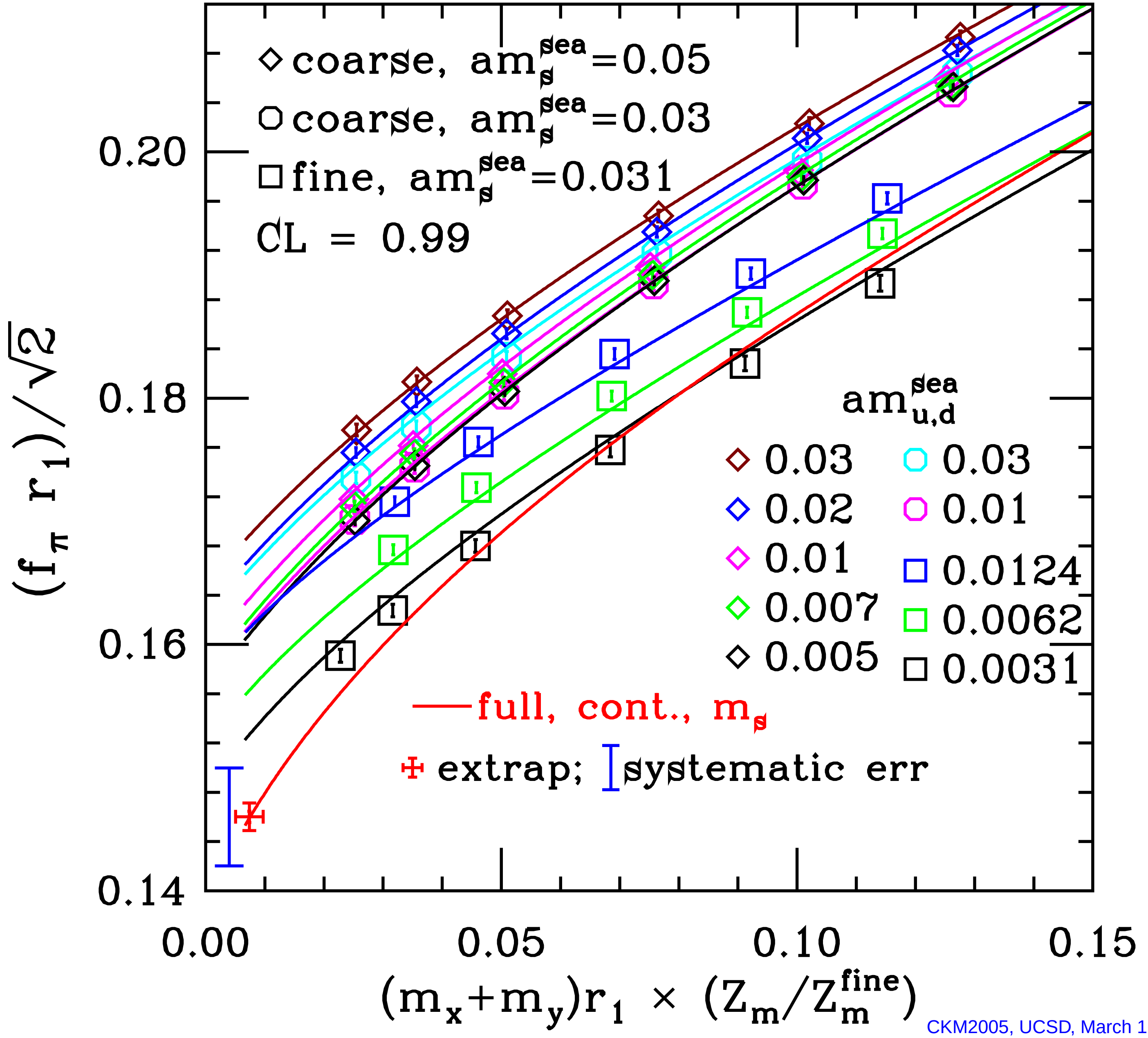


Current MILC calculation of f_π, f_K

Preliminary

MILC+0.5

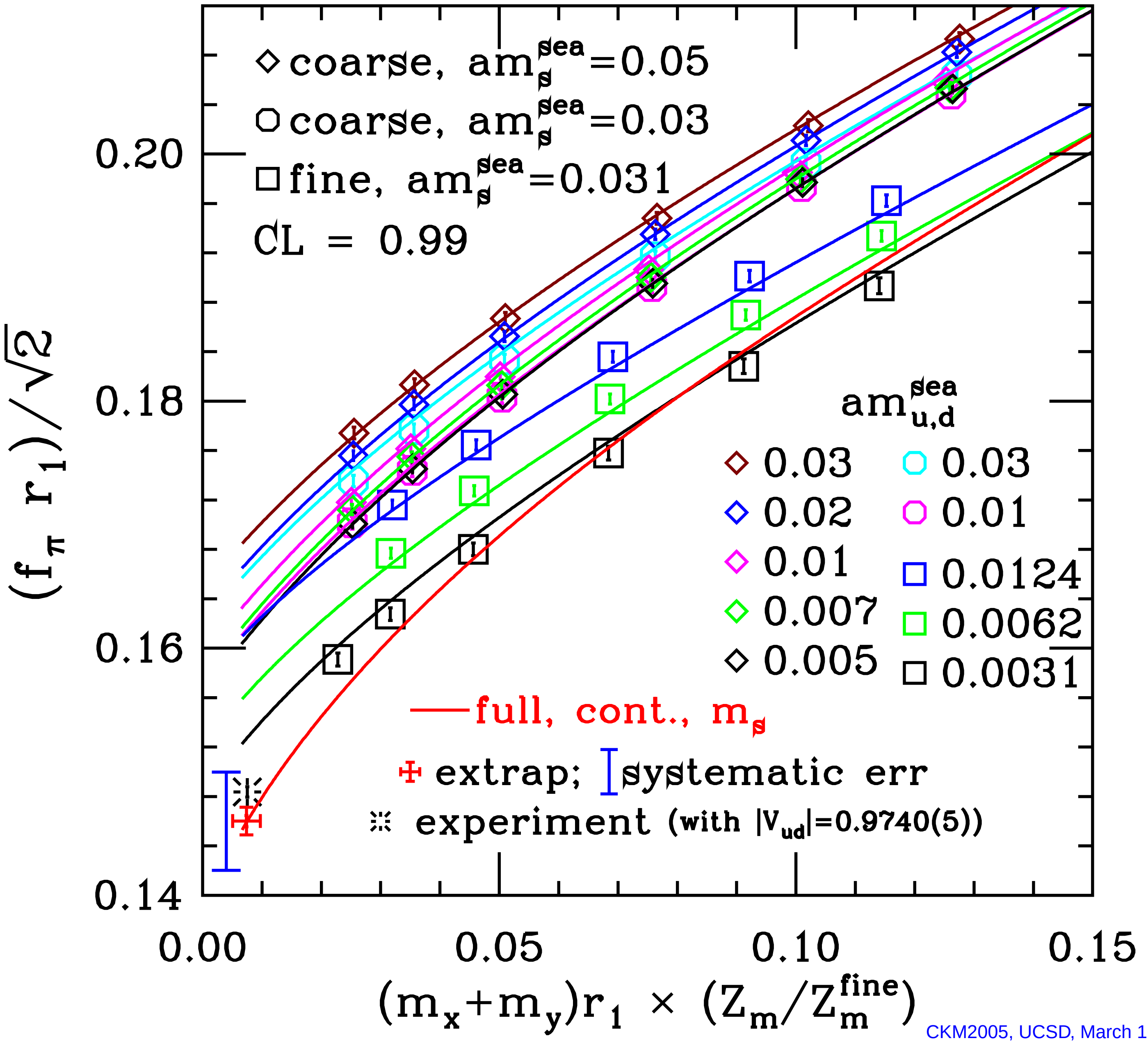
- Extrap to $m_{val} = m_{u,d}^{\mathrm{phys}}$ (determined from m_π).



Current MILC calculation of f_π, f_K

Preliminary
MILC+0.5

- Comparison with expt.



Light Flavor Results

From MILC0 [MILC (Aubin et al.), PRD 70 (2004) 114501]:

$$\begin{aligned} f_\pi &= 129.5 \pm 0.9 \pm 3.5 \text{ MeV} \\ f_K &= 156.6 \pm 1.0 \pm 3.6 \text{ MeV} \\ f_K/f_\pi &= 1.210(4)(13) \;\Rightarrow |V_{us}| = 0.2219(26) \end{aligned}$$

[using Marciano, PRL 93 (2004) 231803].
Gets a B (two lattice spacings) → B- (staggered $\sqrt[4]{\text{Det}}$ penalty).

Preliminary results from MILC+0.5:

$$f_K/f_\pi = 1.204(3)(10??) \;\Rightarrow |V_{us}| = 0.2231(20??)$$

This calculation, when finished, may deserve a B+ → B.

Heavy Flavor Results from MILC -0.5

- Wingate et al. PRL 92 ('04) 022001:

$$\begin{aligned} f_{B_s} &= 260(7)(28)\ \mathrm{MeV} \\ f_{D_s} &= 290(20)(41)\ \mathrm{MeV} \end{aligned}$$

- Fermilab, MILC, HPQCD (Simone et al.), hep-lat/0410030 (preliminary):

$$\begin{aligned} f_{D_s} &= 263(^{+5}_{-9})(24)\ \mathrm{MeV} \\ f_D &= 225(^{+11}_{-11})(21)\ \mathrm{MeV} \\ \frac{f_{D_s}\sqrt{m_{D_s}}}{f_D\sqrt{m_D}} &= 1.20(6)(6) \end{aligned}$$

- Gray et al. hep-lat/0409040 (preliminary):

$$f_{B_s}\sqrt{\hat{B}_{B_s}} = 244(20)(35)\ \mathrm{MeV}$$

Heavy Flavor Results from MILC-0.5

- Fermilab, MILC, HPQCD (Aubin et al.), PRL 94 ('05) 011601:

$$D \to \pi \ell \nu : \qquad |V_{cd}| = 0.239(10)(24)(20)$$

$$D \to K \ell \nu : \qquad |V_{cs}| = 0.969(39)(94)(24)$$

(errors are statistical, lattice systematic, and experimental)

- Shigemitsu et al., hep-lat/0409040 (preliminary):

$$B \to \pi \ell \nu : \qquad |V_{ub}| = 3.52(44)(73) \times 10^{-3}$$

(errors are lattice systematic & statistical, and experimental)

- Fermilab, MILC, HPQCD (Okamoto et al.,) hep-lat/0409116 (preliminary):

$$B \to \pi \ell \nu : \qquad |V_{ub}| = 3.0(4)(6) \times 10^{-3}$$

$$B \to D \ell \nu : \qquad |V_{cb}| = 3.8(1)(6) \times 10^{-2}$$

(errors are lattice systematic & statistical, and experimental)

Heavy Flavor Results from MILC-0.5

- All of the above heavy-flavor results get a C (only one lattice spacing in MILC-0.5) $\rightarrow$ C- (staggered $\sqrt[4]{\mathrm{Det}}$ penalty).
- All errors are estimated as well as possible within limits of simulations.
  - At the C- level, though, it is quite possible that some errors are off by a factor of 2 (or more?)
- But extension of analysis to full MILC0 set (and additional lattice spacings) is in progress. Most should upgrade to B range in less than a year.
- An existing B- (including staggered penalty) computation is HPQCD, Fermilab, UKQCD (Allison et al.), hep-lat/0411027:

$$m_{B_c} = 6304(12)\left({}^{+18}_{-\ 0}\right)\ \mathrm{MeV}$$

  - This is a lattice QCD prediction, and as a B-, it should be taken pretty seriously.
  - m_{B_c} expected to be measured in Run 2 of the Tevatron with a comparably sized error.

Future Lattice Precision

Next steps will require new dynamical configurations (lighter quark mass, smaller lattice spacing):

- MILC1
  - Halve a^2 OR $m_{u,d}$
  - ~ 6 Teraflop-years
  - Columbia QCDOC machines, now coming on line
  - Effort to be shared by DOE SciDAC project QCDOC in US, and UKQCD collaboration QCDOC in UK
  - Sharing of output is still problematic!
  - ETA: ~ 1 year for lattice generation; probably additional 1-2 years to get heavy-flavor physics out.

Future Lattice Precision

- DWF0
  - A domain wall ensemble comparable to MILC0
  - Probably feasible on world's QCDOCs (but very demanding)
  - Safe from all staggered baggage
  - Precision might be comparable to MILC1 because no taste violations
  - My guess ETA for heavy-flavor physics: 3-5 years (including analysis time)

Future Lattice Precision

Further in the future:

- MILC2
    - Halve a^2 AND $m_{u,d}$ from MILC0
    - ~ 50-100 Teraflop-years
    - Would require next generation of machines
    - ETA: 5-7 years (including analysis time)
- DWF1: Dynamical domain wall fermions (or equivalent) at comparable mass and spacings to MILC1
    - Comparable precision to MILC2
    - “Next next” generation of machines?
    - ETA: 7-10 years (including analysis time)

Future Lattice Precision

- Error estimates to follow are based on DOE SciDAC planning document prepared by S. Sharpe, C.B., A. El-Khadra, P. Mackenzie, and R. Sugar.
- Updated (by CB) to reflect current status & lessons from heavy-light MILC-0.5 and light-light MILC$+0.5$ analysis.
- Have not assumed any improvement in algorithms/techniques — but in fact such improvements are likely over the 10 year considered.

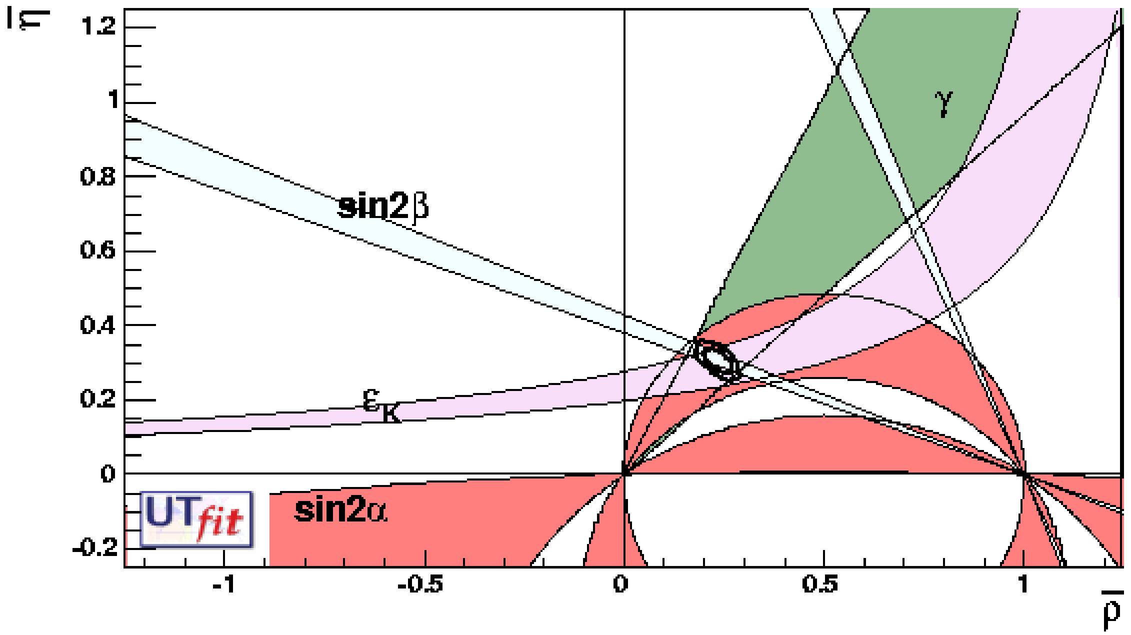
Lattice error estimates (%)

Quantity	**“now”** MILC-0.5	**0.5 – 2 yrs.** MILC0	**2 – 5 yrs.** MILC1/DWF0	**5 – 10 yrs.** MILC2/DWF1
f_{D_s}, f_{B_s}	10	7	5	3 – 4
f_D, f_B	11	7 – 8	5	4
$f_B\sqrt{B_B}$	17	8 – 13	4 – 5	3 – 4
ξ	–	4	3	1 – 2
$D \rightarrow \pi\ell\nu$ $D \rightarrow K\ell\nu$ $B \rightarrow \pi\ell\nu$ †	$\sim$11	8	6	4
$B \rightarrow D\ell\nu$ $B \rightarrow D^*\ell\nu$	$\sim$4	3	2	1
Expected grade	C	B	A	A

† restrict $q^2 \gtrsim 16\ (\mathrm{GeV})^2$ for $B \rightarrow \pi\ell\nu$

UTfit Collaboration: Unitarity Triangle in 2010

An important point is that the relative precisions on CP‑ violating quantities are on phase with CP‑ conserving quantities



Lattice Calculations play a central role

So 2010 should be the era of Lattice at <5%

	indirect	direct
sin(2b)	0.693 ± 0.029	0.695 ± 0.015
sin(2a)	‑ 0.512 ± 0.147	‑ 0.5 ± 0.2
g[°]	52.8 ± 4.2	54 ± 5

	indirect	direct
B_K	0.820 ± 0.072 (8.5%)	0.930 ± 0.046 (5%)
$f_{B_s}\sqrt{\hat{B}_{B_s}}$	278.6 ± 11.5 (4.1%)	276 ± 14.0 (5%)
ξ	1.186 ± 0.032 (2.7%)	1.200 ± 0.037 (3%)

(Thanks to V. Lubicz)

Lattice Data Group?

- Experimenters and phenomenologists would like there to be a LDG (Lattice Data Group), so that they can find THE lattice results with a “stamp of approval.”
- A reasonable request, but. . .
  - To my mind, a LDG only makes sense when we have several A (or at least B) simulations to compare or average.
    - Lower grade simulations just don’t have enough info to reliably think of errors as 1-σ, 2-σ, flat distribution, etc. Averaging them may give misleading results.
  - We’re not there yet, but should be within a year or two.
  - In the past I dragged my feet on this, but I now agree with those that think it’s time to plan for a LDG.
  - Of course, my grading criteria are certainly idiosyncratic and probably biased — the LDG will need to come up with its own criteria.