Lattice QCD on Blue Waters

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Presenter: Steven Gottlieb (Indiana)
(USQCD)

NCSA Blue Waters Symposium for
Petascale Science and Beyond
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Collaborators

- ✦ *Ziyuan Bai, Norman Christ [Co-PI], Chris Kelly (Columbia)*
- ✦ *Alexei Bazavov (Indiana→MSU)*
- ✦ *Peter Boyle (Edinburgh)*
- ✦ *Kate Clark, Mathias Wagner (NVIDIA)*
- ✦ *Carleton DeTar (Utah)*
- ✦ *Chulwoo Jung (BNL)*
- ✦ *Robert Sugar [Co-PI] (UCSB)*
- ✦ *Doug Toussaint (Arizona)*

Key Challenges

- ✦ *Calculations of QCD must support large experimental programs in high energy and nuclear physics*
- ✦ *QCD is a strongly coupled, nonlinear quantum field theory*
- ✦ *Lattice QCD is a first principles calculational tool that requires large scale computer power*
- ✦ *Using the highly improved staggered quark (HISQ) action, we study fundamental parameters of the standard model of elementary particle physics*
    - *quark masses, CKM mixing matrix elements*
- ✦ *We also use the Domain Wall quark action to study kaon physics which requires a chiral action*
    - *Direct CP violation $K \to \pi\,\pi$ decay*
    - *K_L - K_S mass difference*

Why Blue Waters?

- ✦ *Lattice field theory calculations proceed in two stages:*
  - *Generate gauge configurations, i.e., snapshots of quantum fields*
  - *Compute physical observables on the stored configurations*
- ✦ *First stage is done in a few streams*
- ✦ *When computing observables on stored configurations, many jobs may be run in parallel given sufficient capacity*
- ✦ *We can use Blue Waters' GPUs for some production running in our projects, e.g.,*
  - *Decay constant calculations*
- ✦ *We need large partitions to generate configurations*
- ✦ *We can run multiple parallel jobs for 2nd stage, if sufficient capacity*

Why Blue Waters ...

- ✦ *It is very expensive to use up and down quark masses as light as in Nature, i.e., the physical value*
  - *This has required using heavier quarks and extrapolating to the physical masses using chiral perturbation theory*
- ✦ *For the first time, Blue Waters is allowing us to create gauge configurations with small lattice spacing and quarks masses at the physical value*
- ✦ *This allows us to produce results with unprecedented precision*
- ✦ *The configurations created on Blue Waters will be used for multiple physics analyses spanning several years*

Blue Waters Team Contribution

- *We want to express special thanks to* ***Greg Bauer****,* ***Craig Steffen****, and* ***David King***
- *Blue Waters has been very busy and they were instrumental in helping us with a dedicated queue*

Shared Data

- ✦ *Configurations are made available through USQCD and in response to requests.*
- ✦ *Other groups use these configurations for additional physics projects.*
  - *Fermilab Lattice/MILC will be using them for several years to investigate a variety of weak decays of heavy-light mesons*
  - *A number of other groups also use MILC configurations for a wide variety of projects*
- ✦ *Some of the quark propagators are saved for other physics projects.*

Why It Matters

- ✦ *The standard model (SM) of elementary particle physics contains three of the four known forces:*
  - *strong, weak, and electromagnetic*
  - *gravity is not included*
- ✦ *Standard model explains a wealth of experimental data*
- ✦ *However, there are many parameters that can only be determined with experimental input, e.g., quark masses, strong coupling α_s*
- ✦ *There are theoretical reasons that argue that the standard model is incomplete*
- ✦ *There are a number of experiments whose results differ from SM value by more than two standard deviations*
- ✦ *Many of the most interesting aspects of the strong force require better calculations of a strongly coupled theory*

Calculating QCD

- ✦ *We need lattice QCD to carry out first principles calculations of many effects of the strong force*
- ✦ *This requires large scale numerical calculation*
- ✦ *The CKM matrix describes how quarks mix under weak interactions*
  - *Kobayashi and Maskawa received the 2008 Nobel Prize*
  - *our calculations are necessary to determine elements of matrix*
  - *If different decays give different results for the same matrix element, that requires new physical interactions (prize worthy!)*
- ✦ *A number of high energy and nuclear physics experiments can only properly be interpreted when QCD is taken into account.*

Kobayashi & Maskawa

- *Won 2008 Nobel prize for realization that with three (or more) generations can have CP violation, which might explain baryon asymmetry of Universe.*

KEK photo from nobelprize.org

CKM Matrix

✦ *Some relevant processes listed under each element*

$$\begin{pmatrix} \mathbf{V_{ud}} & \mathbf{V_{us}} & \mathbf{V_{ub}} \\ \pi \to l\nu & K \to \pi l\nu & B \to \pi l\nu \\ & K \to l\nu & \\ \mathbf{V_{cd}} & \mathbf{V_{cs}} & \mathbf{V_{cb}} \\ D \to \pi l\nu & D \to K l\nu & B \to D^{(*)} l\nu \\ D \to l\nu & D_s \to l\nu & \\ \mathbf{V_{td}} & \mathbf{V_{ts}} & \mathbf{V_{tb}} \\ \langle B_d | \overline{B}_d \rangle & \langle B_s | \overline{B}_s \rangle & \end{pmatrix}$$

First Row: Light Quarks

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- *Processes involving only light quarks test first row unitarity*

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✦ *Processes involving only light quarks test first row unitarity*

leptonic

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leptonic

semileptonic

Decay Constants

- *Leptonic decay rate (or branching fraction) of a meson is determined by a CKM matrix element, a decay constant, and other known quantities.*
- *Our job is to calculate the decay constant, so we can determine the CKM matrix element from the decay rate*

$$\mathcal{B}(D_{(s)} \to \ell\nu_\ell) = \frac{G_F^2 |V_{cq}|^2 \tau_{D_{(s)}}}{8\pi} f_{D_{(s)}}^2 m_\ell^2 m_{D_{(s)}} \left(1 - \frac{m_\ell^2}{m_{D_{(s)}}^2}\right)^2$$

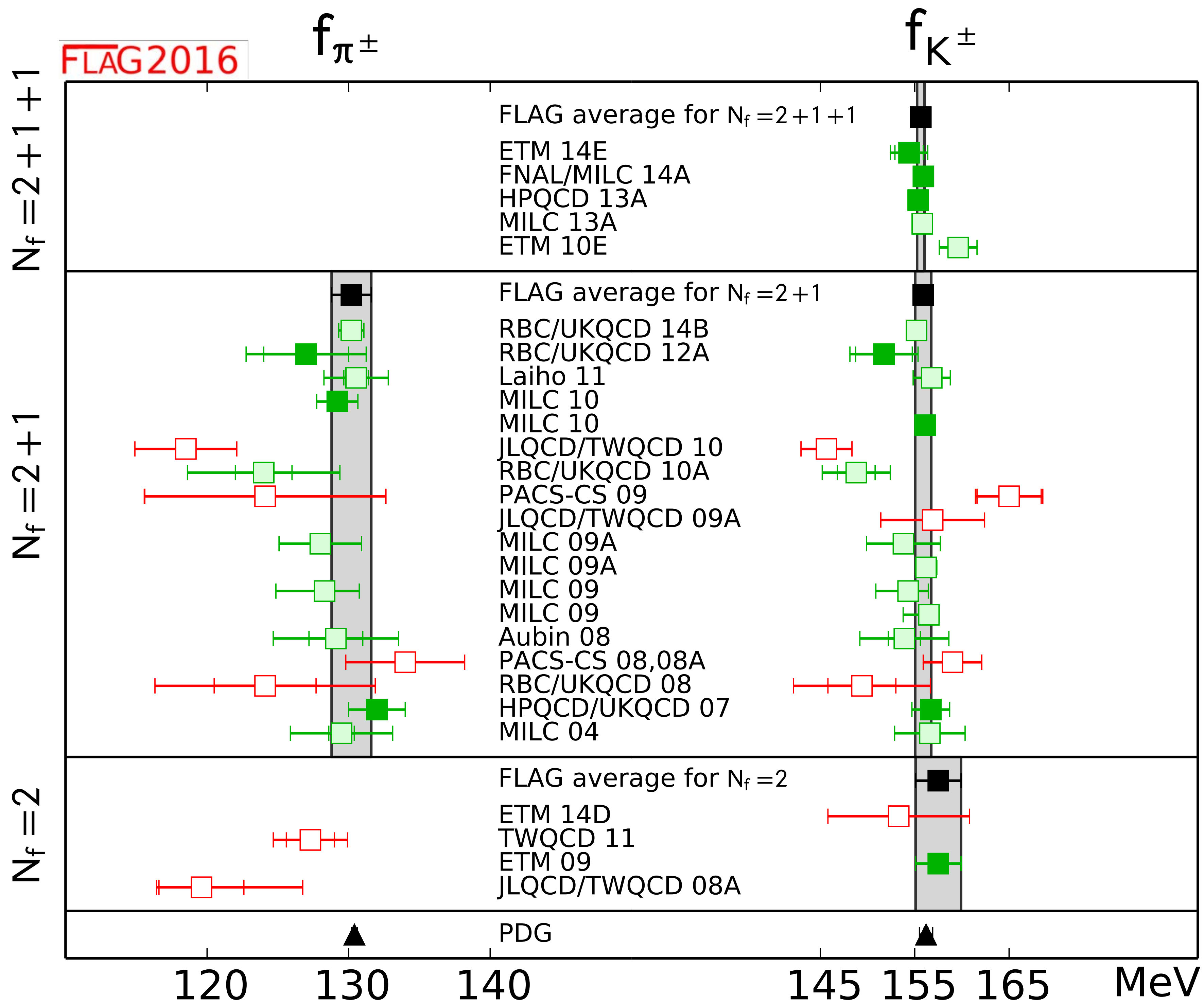
- *Formula is for a charm meson, in which case, q can be d, or s*
- *For π and K mesons, c is replaced by u for the up quark*
- *For B meson, c is replaced by b, and q can be u.*
- *B_s is a special case, but the decay constant can still be defined and calculated using lattice QCD*

FLAG Introduction

- *Flavor Lattice Averaging Group publishes reviews of results in lattice QCD, so a convenient source of state-of-the art comparisons*
- *I am a member of the heavy-quark semileptonic decay group, so I am happy to show results from latest FLAG review*
- *FLAG color coding:*
  - *solid green: included in average*
  - *open green: good calculation, but superseded*
  - *open red: errors are not well controlled, not in average*
  - *black (and vertical gray band): FLAG average*
- *FLAG has separate averages for different numbers of dynamical quarks: 2 (degenerate up & down), 2+1 (also strange), 2+1+1(also charm)*

f_π and f_K

- *Light decay constants as summarized by FLAG (Aoki, S., Aoki, Y., Bečirević, D. et al. Eur. Phys. J. C (2017) 77: 112. doi:10.1140/epjc/s10052-016-4509-7)*
- *Some calcs. use f_π to set the scale so fewer results on left*
- *Ratio of decay constants is easy to calculate and used to test unitarity*

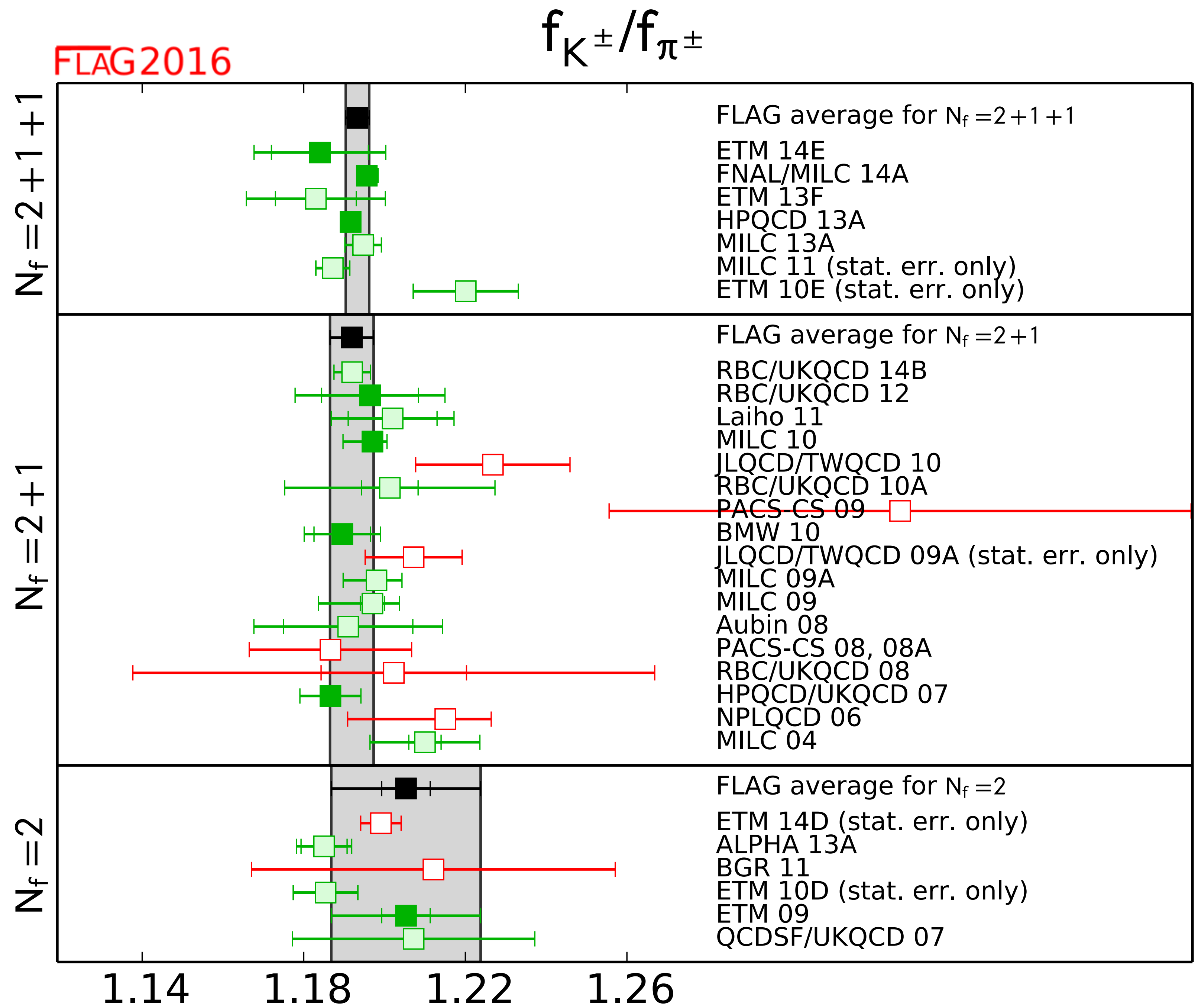


f_π/f_K

- *Light decay constant ratio summarized by FLAG*
- *FNAL/MILC 14A 1.1956(28) : 0.23% error*
- *From experimental measurement:*

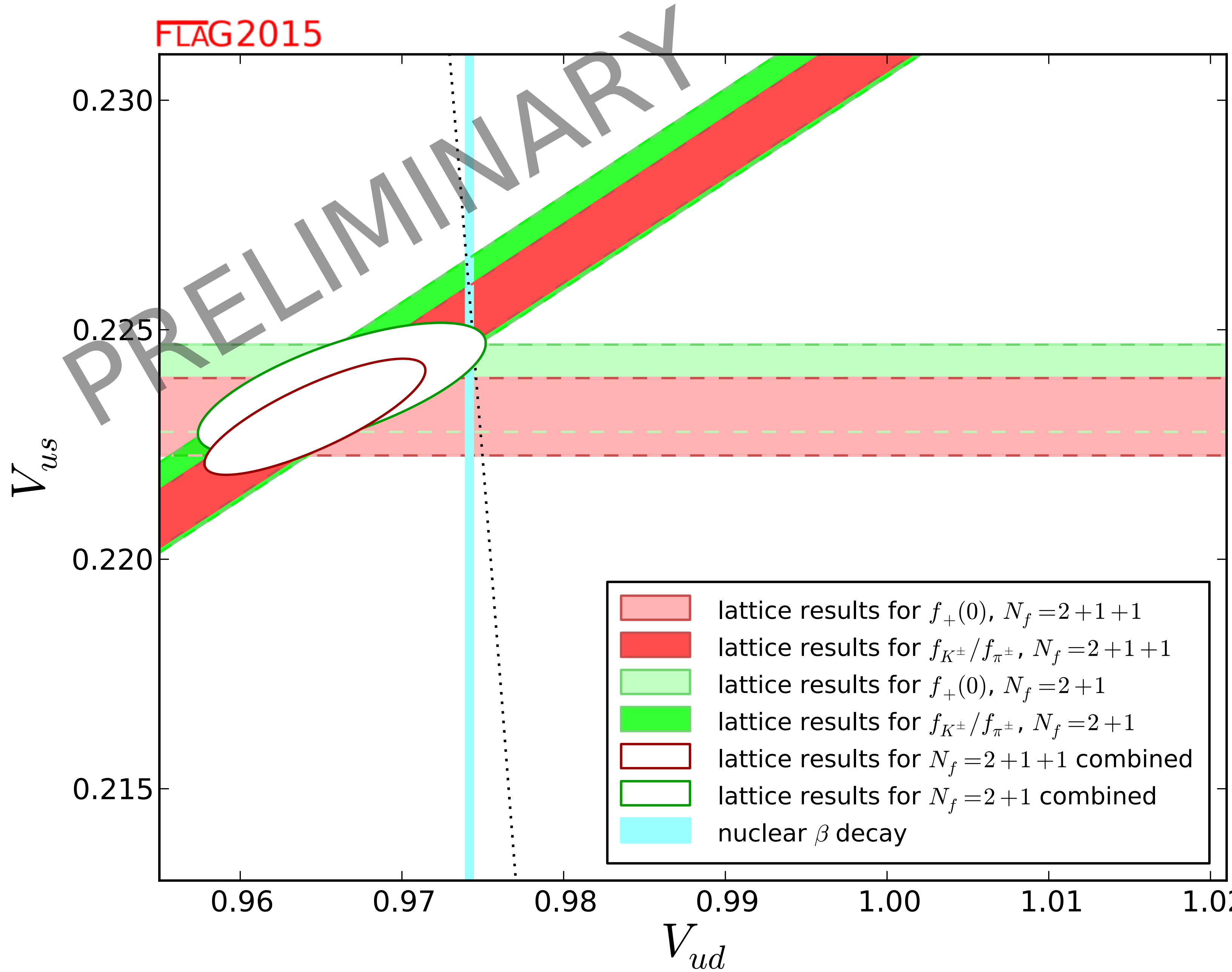
$$\left|\frac{V_{us}}{V_{ud}}\right| \frac{f_{K^\pm}}{f_{\pi^\pm}} = 0.2758(5)$$

- *0.18% error*
- *Will update this year*



First Row Unitarity (FLAG)

- *Preliminary FLAG3 results for 2+1 and 2+1+1 flavors*
- *Matrix elements not squared here*
- *Dotted line is unitarity*
- *2+1 flavors has larger error and consistent with unitarity*



Second Row: Charm Quark

leptonic

Second Row: Charm Quark

✦ *Processes involving charm quark test second row unitarity*

leptonic

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leptonic

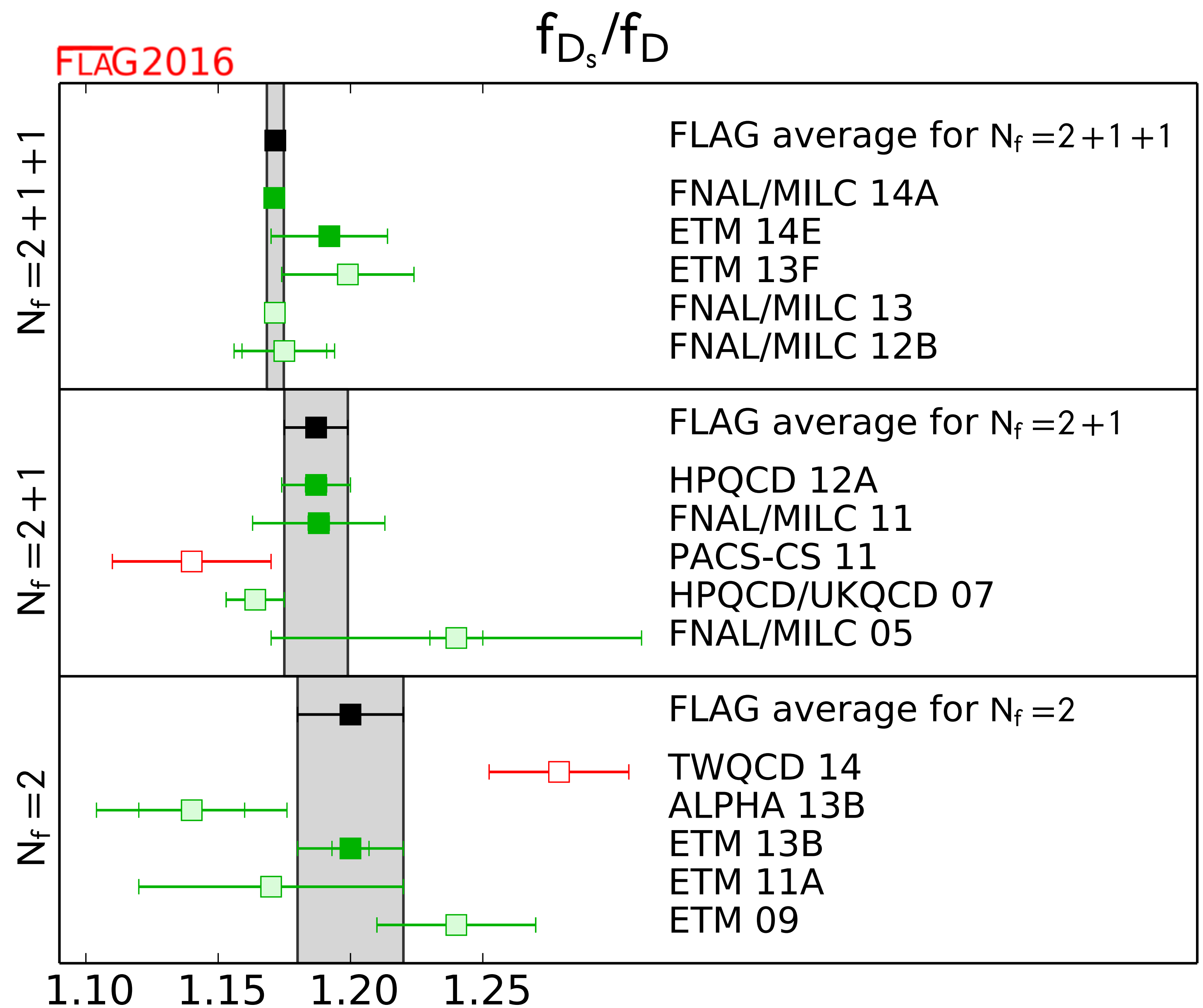
semileptonic

FLAG Charm Decay Constant Ratio

- *Note remarkable improvement over 12 years for FNAL/MILC*

$$f_{D_s}/f_{D^+} = 1.1712(10)(^{+29}_{-32})$$

- *FLAG 1.1716(32) for 2+1+1 flavors*
- *Our latest results from Blue Waters will reduce the error in last two digits from 32 to 11*



Extraction of V_{cd} & V_{cs}

- The experimental results for charm meson leptonic decays are summarized by the Heavy Flavor Averaging Group (HFAG):

$$f_D|V_{cd}| = 46.40(1.98)\mathrm{MeV}, \qquad f_{D_s}|V_{cs}| = 253.1(5.3)\mathrm{MeV}$$

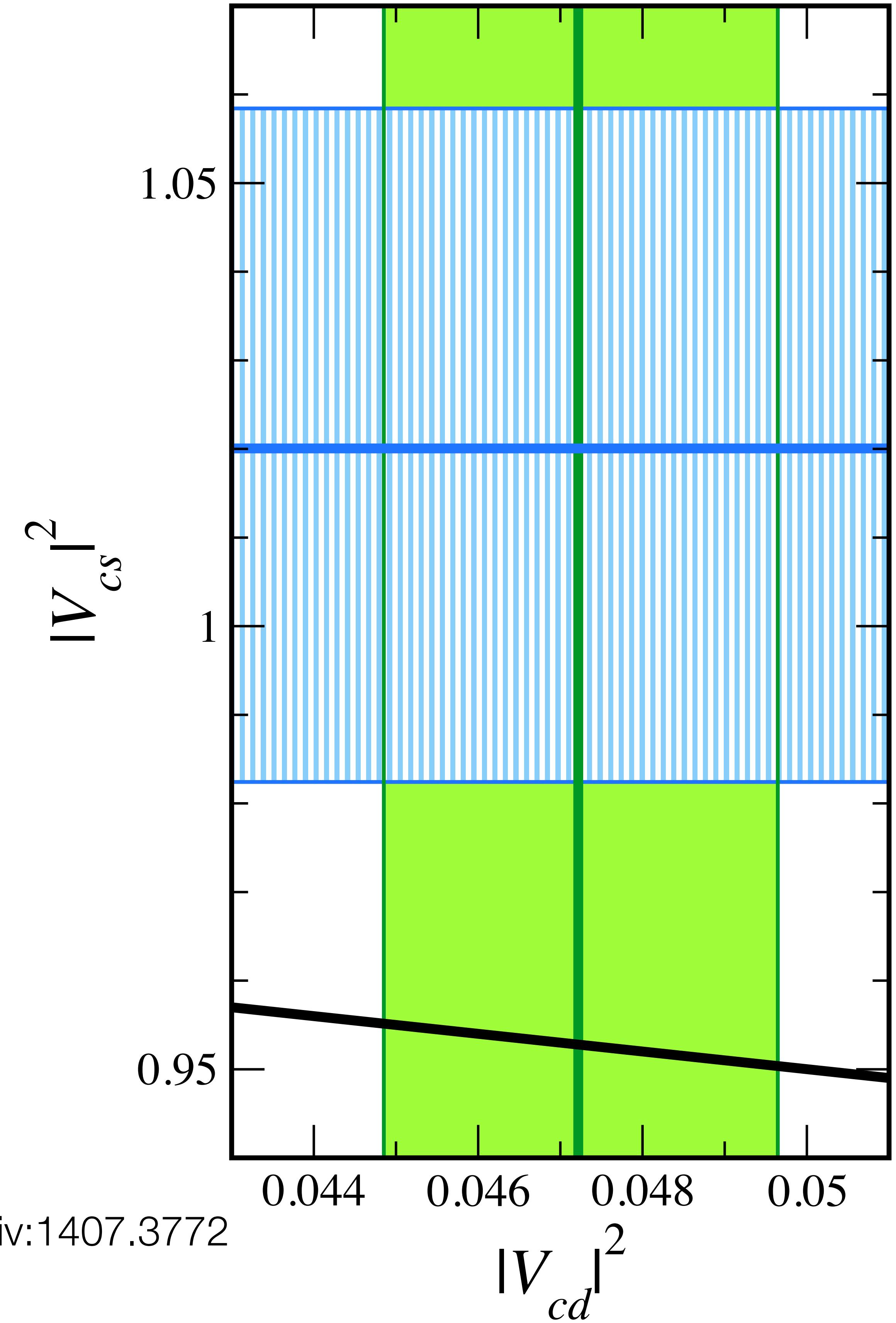
- Experimental error is 2.1-4.3%.
- Using decay constants from LQCD, we get CKM matrix elements:

$$|V_{cd}| = 0.217(1)(5)(1), \quad |V_{cs}| = 1.010(5)(18)(6)$$

- Errors are lattice, experiment, and structure dependent electromagnetic, respectively.

Second Row Unitarity

- Black line is unitarity
- Horizontal blue band is D_s leptonic decay
- Vertical green band is D^+ leptonic decay
- Note the ≈1.8 σ tension with unitarity
- Fajfer et al,. PRD91, (2015) 094009 bound new physics
- Fewer results for semileptonic D meson decays
- Expt. error dominant now.



FNAL/MILC, Phys.Rev. D90 (2014) 7, 074509 arXiv:1407.3772

Third Column: Bottom Quark

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- *Processes involving bottom quark are in third column and third row*

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$$
\begin{pmatrix}
\mathbf{V_{ud}} & \mathbf{V_{us}} & \mathbf{V_{ub}} \\
 & K \to \pi l \nu & B \to \pi l \nu \\
\pi \to l \nu & K \to l \nu & \boxed{B \to l \nu} \\
\mathbf{V_{cd}} & \mathbf{V_{cs}} & \mathbf{V_{cb}} \\
D \to \pi l \nu & D \to K l \nu & B \to D^{(*)} l \nu \\
D \to l \nu & D_s \to l \nu & \\
\mathbf{V_{td}} & \mathbf{V_{ts}} & \mathbf{V_{tb}} \\
\langle B_d | \bar{B}_d \rangle & \langle B_s | \bar{B}_s \rangle &
\end{pmatrix}
$$

leptonic

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semileptonic

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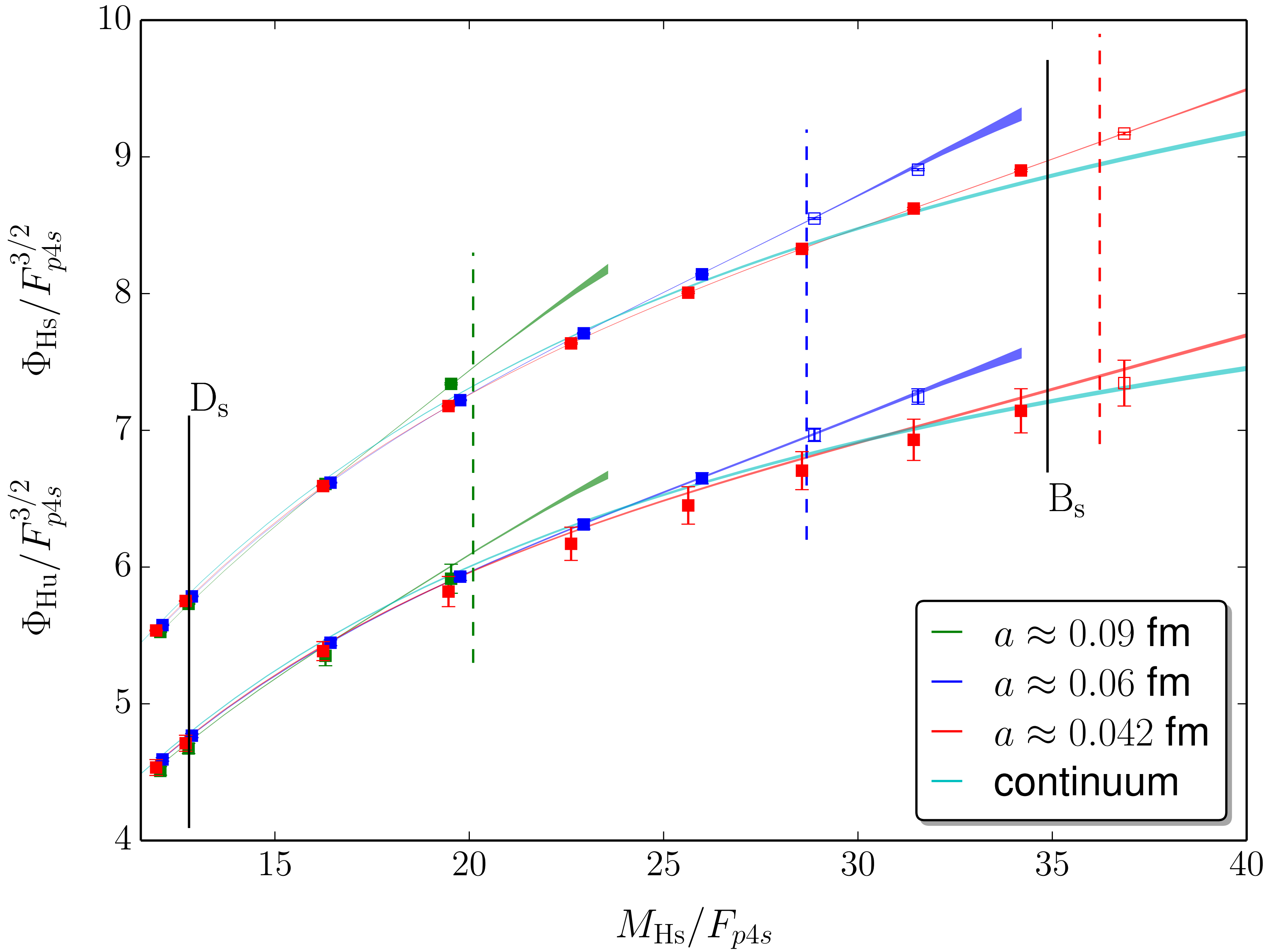
B meson decay constants

- *Improvement in D meson decay constants comes from using highly improved staggered quarks (HISQ) for the charm quark*
- *For heavy HISQ quarks, we want am_q <0.9, which is not difficult to attain for charm; however, $m_b/m_c \approx 4.6$*
- *For B mesons, $am_b \approx 0.84$ for $a \approx 0.042$ and >0.9 for all our coarser ensembles*
- *However, HPQCD has shown that it is practical increase mass of heavy quark as lattice spacing decreases to gain useful information from the coarser ensembles*
- *This analysis also results in charm and bottom quark masses*
- *Blue Waters has been instrumental in allowing us to go to smaller lattice spacing*
- *Results shown on next slide…*

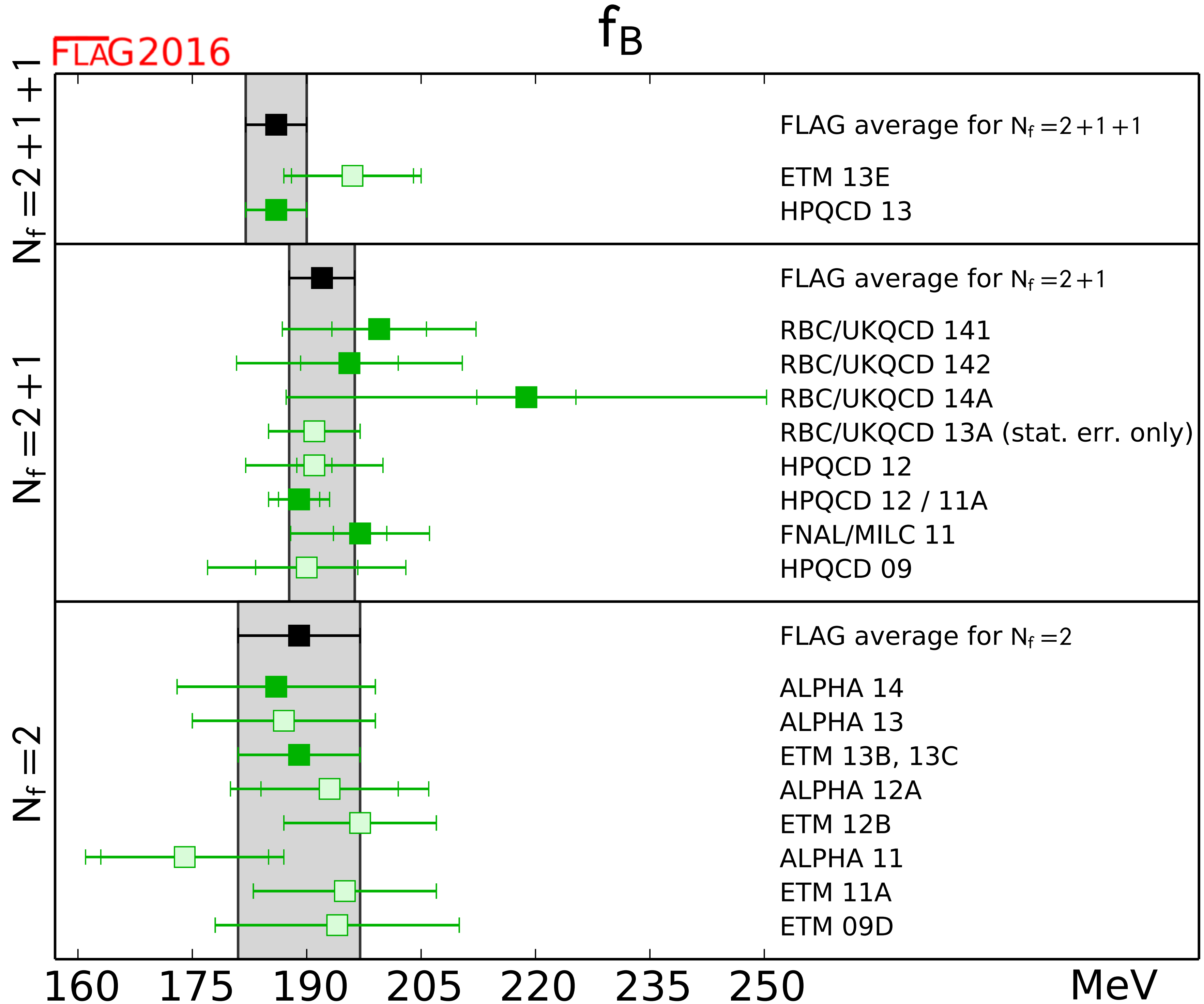
Heavy-light decay constants



- *x-axis: meson mass*
- *y-axis: proportional to decay constant*
- *Solid vertical lines at physical meson mass*
- *Three lattice spacings*
- *Dashed vertical lines at am_h= 0.9*
- *Note how coarser ensembles diverge further to the left*
- *Red data & curve new from Blue Waters*

New Level of Precision for f_B

- *Current FLAG average for N_f=2+1+1 is 186(4) MeV*
- *We plan to publish new result this summer with an error of 0.82 MeV, factor of five reduction in error.*
- *Errors for other heavy-light decay constants will be smaller.*



High Precision Required

- ✦ *Without high precision calculations of QCD, we cannot accurately determine CKM matrix elements from expensive (many hundreds of megadollars), high precision experiments*
- ✦ *New interactions outside the standard model are expected to be weak, so their effects are small*
- ✦ *Understanding QCD is important for a deeper understanding of the fundamental laws of physics*
- ✦ *Precision Higgs boson studies at Large Hadron Collider require higher precision values for quark masses and strong coupling constant*
- ✦ *Muon g-2 theory error dominated by QCD effects*

Accomplishments

- ✦ *Blue Waters has allowed us to produce the most realistic gauge configurations to date*
- ✦ *These are the most challenging calculations we have ever undertaken ($144^3 \times 288$, physical light quarks, $a=0.042$ fm; $64^3 \times 192$, $m_l/m_s=0.2$, $a=0.042$ fm; $96^3 \times 288$, $m_l/m_s=0.2$, $a=0.03$ fm)*
- ✦ *HISQ configurations have allowed us to make the most precise calculations of a number of meson decays*
  - *2 Physical Review Letters (PRL), 2 Physical Review D (PRD)*
  - *One PRL was designated an Editors' Suggestion*
- *multiple conference proceedings*

Conclusions

- *Blue Waters has accelerated our scientific achievements by a large factor*
- *We have generated gauge configurations that will be useful to the broad USQCD physics program and are also shared internationally*
- *We have also carried out important physics analyses directly on Blue Waters*
  - *Many additional quantities are studied with the Blue Waters configurations at other supercomputer centers and on USQCD computers. (Some of those results were shown.)*
- *However, much more work remains to provide the theoretical input required to interpret a large number of experiments*
  - *We will be using output from Blue Waters for several years to analyze additional processes with unprecedented precision*