Lattice QCD on Blue Waters

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Collaborators

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- ✦*Kate Clark, Mathias Wagner (NVIDIA)*
- ✦*Carleton DeTar (Utah)*
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- ✦*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* $K \rightarrow \pi\pi$ *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 has allowed 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*

Shared Data

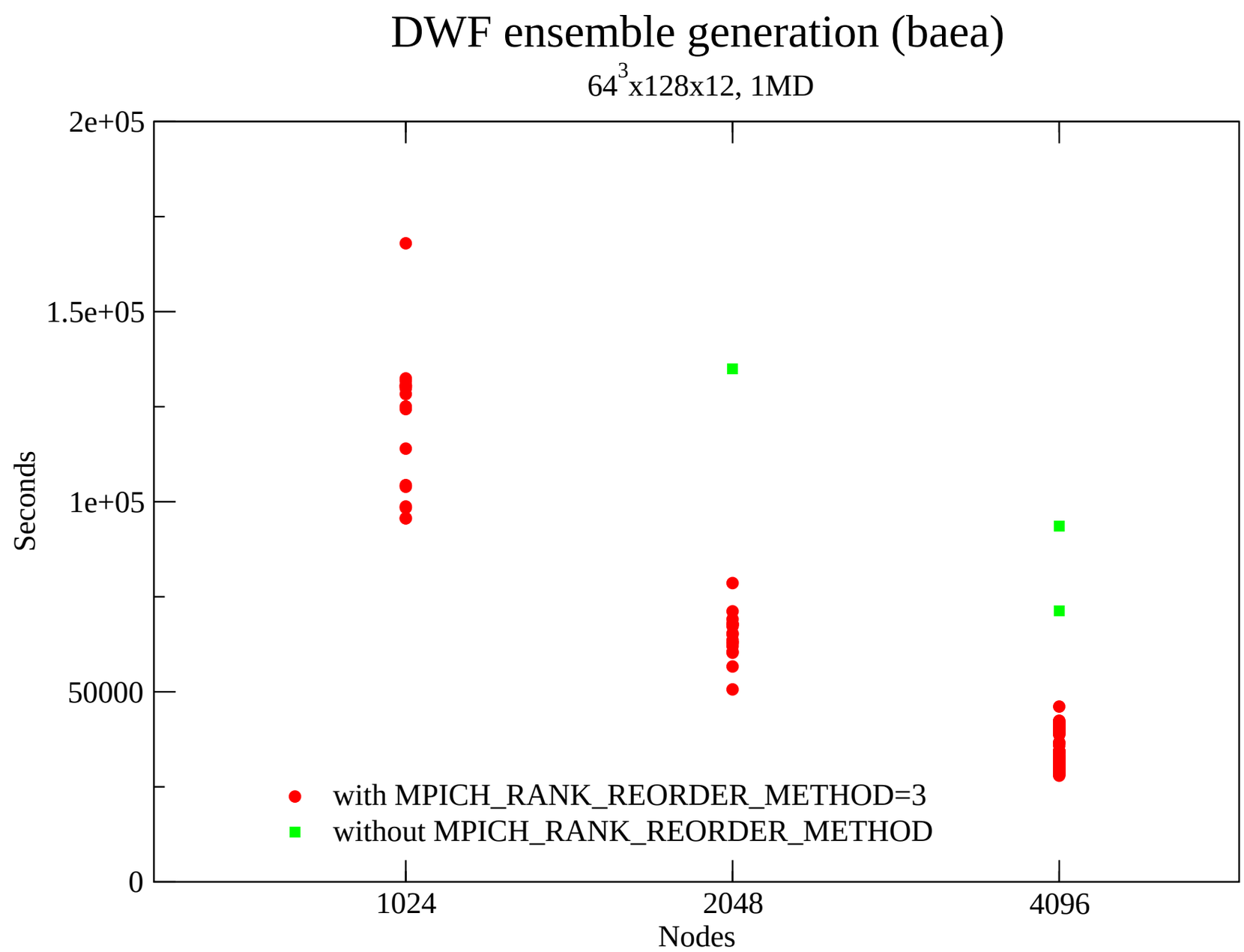
- *Configurations are made available through USQCD and in response to requests.*
- *Approximately 60 new archived physical mass 0.042 fm configurations generated on Blue Waters this year.*
- *Other groups use these configurations for additional physics projects.*
  - *Fermilab Lattice/MILC will be using 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.*

Shared Data II

- *Using a chiral action called domain wall fermions we use a $64^3 \times 128 \times 12$ five dimensional grid*
- *The spacing between grid points is roughly 0.08 fm.*
- *≈150 units of molecular dynamics evolution run on Blue Waters*
- *Configurations will be used for:*
  - *anomalous magnetic moment of muon*
  - *K_L - K_S mass difference*
  - *flavor physics, i.e., decays of heavy-light mesons*

Rank Reorder Improvements

- *grid order -C -Z -c 2,2,2,2 -g 16,16,16,16*
- *for running on 4096 nodes*
- *Green point for 1024 nodes would be off the graph. (Did not complete in 48 hours.)*



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*

Muon Anomalous Magnetic Moment

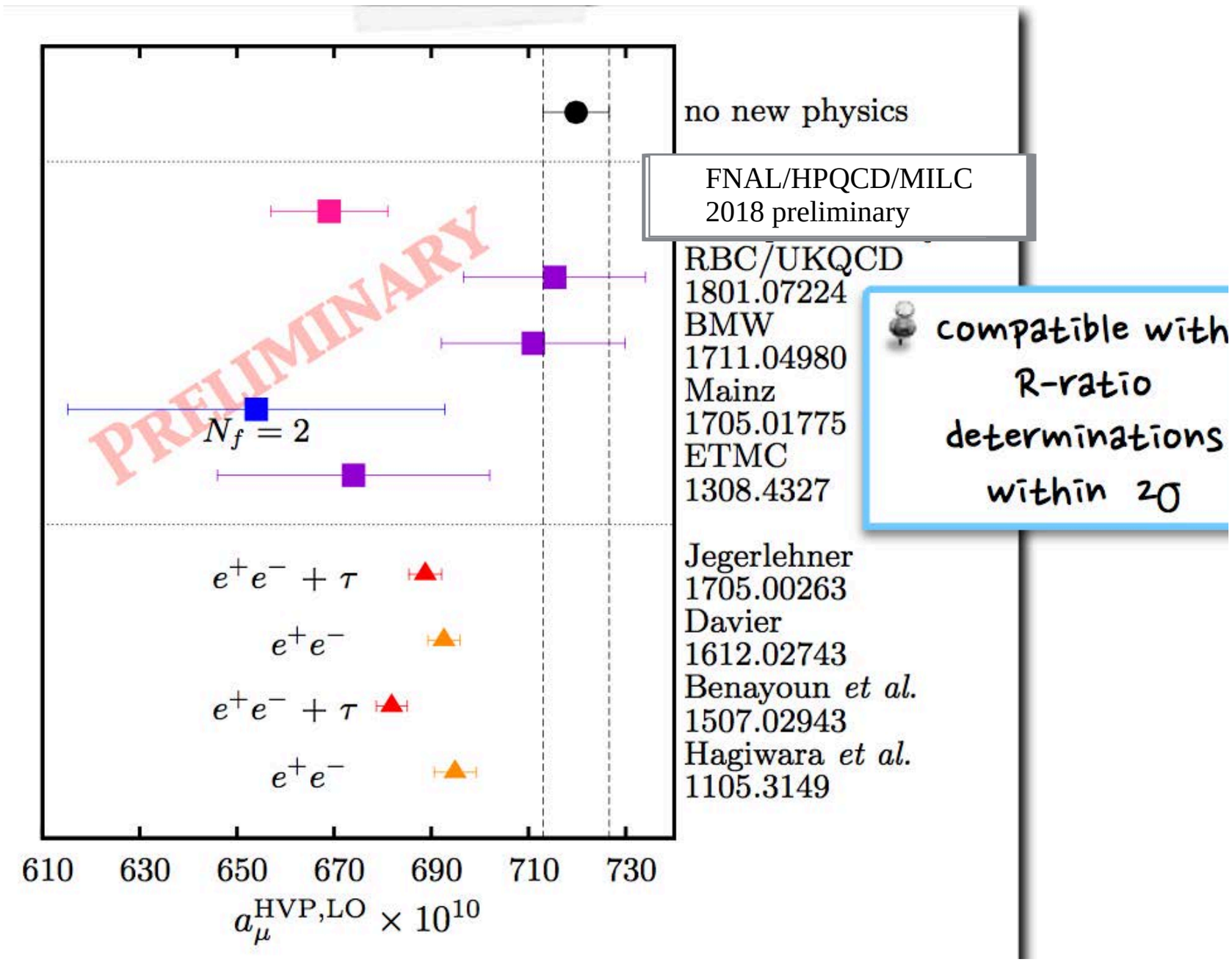
- *Often just denoted as g-2 this quantity could be very important for discovery of new physics*
- *One of the most precisely measured quantities in physics*
  - $a^{exp} = 116592080(63)\times10^{-11}$
  - $a^{thy} = 116591798(68)\times10^{-11}$
- *Currently more than 3 σ difference between theory and experiment*
- *Previous apparatus from BNL was moved to Fermilab and is currently running with a goal of reducing the experimental error by a factor of 4.*
- *We are using Blue Waters to reduce the theoretical error which is crucial for making good use of the improved experimental precision.*

Theory Summary

- ✦ *Magnetic moment gets contributions from several sources*
  - *QED (up to five-loop order)*
  - *Weak (two-loop order)*
  - *Hadronic Vacuum Polarization (HVP)*
  - *Light-by-light scattering (LbL)*
- ✦ *Latter two contributions depend on strong interaction and are difficult to calculate*
- ✦ *They dominate the theoretical error*
- ✦ *Next slide shows status of hadronic vacuum polarization*

Preliminary HVP

- *Black point in upper right is what HVP result with be with no new physics*
- *Below dotted line, R-ratio method involves experimental measurements*
- *Other colored points are from lattice QCD*
- *We will continue to reduce the error from lattice QCD*



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

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

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

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*

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

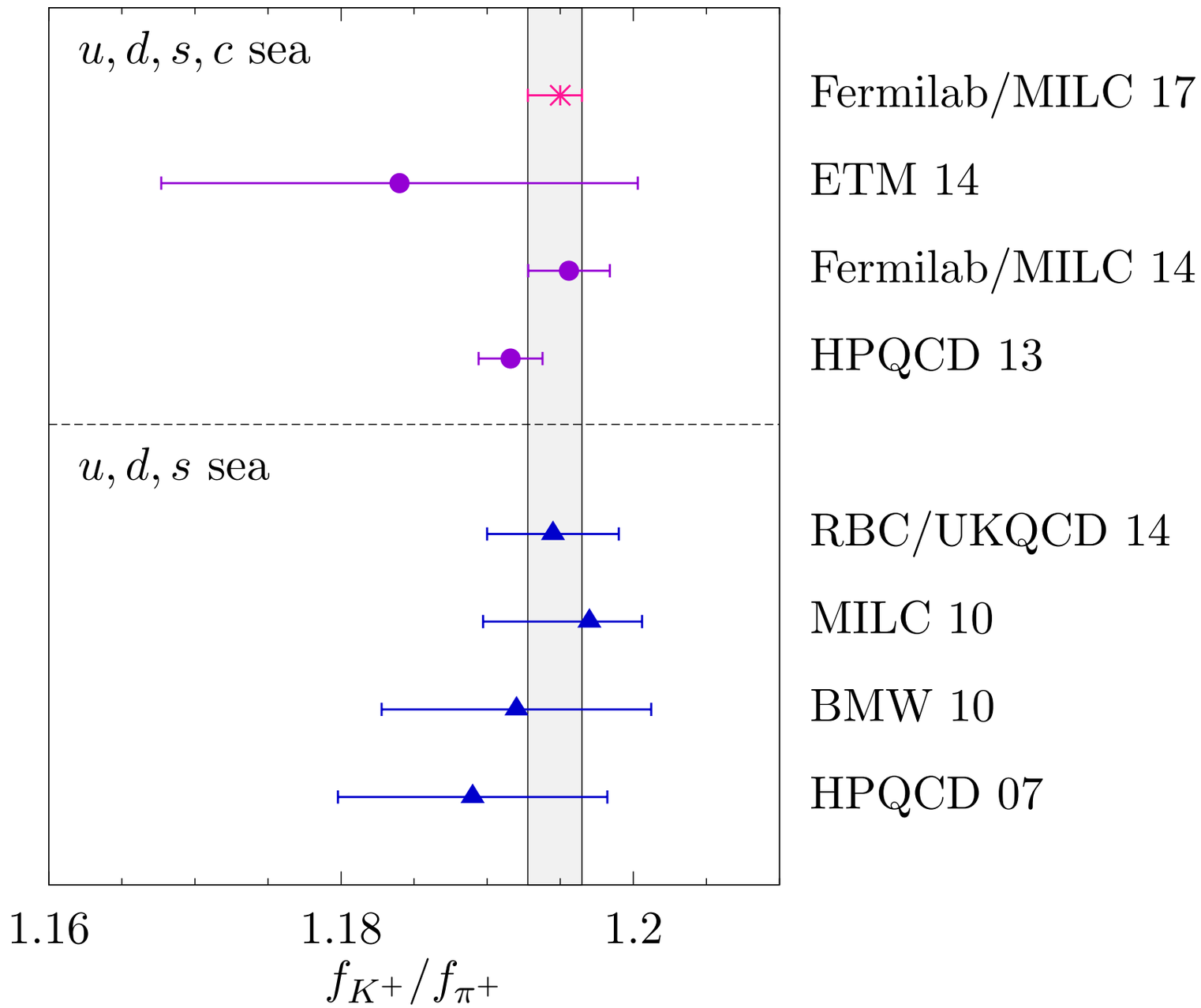
- *Formula is for a charm meson, in which case, q can be d, or s*
- *For π and K mesons, c is replaced by u for the up quark*
- *For B meson, c is replaced by b, and q can be u.*
- *B_s is a special case, but the decay constant can still be defined and calculated using lattice QCD*

f_π/f_K

- *Light decay constant ratio updated: 1712.09262*
- *FNAL/MILC 17 1.1950(+15-22) : 0.18% error (was 0.23%)*
- *From experimental measurement:*

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

- *0.18% error*



Second Row: Charm Quark

✦ *Processes involving charm quark test second row unitarity*

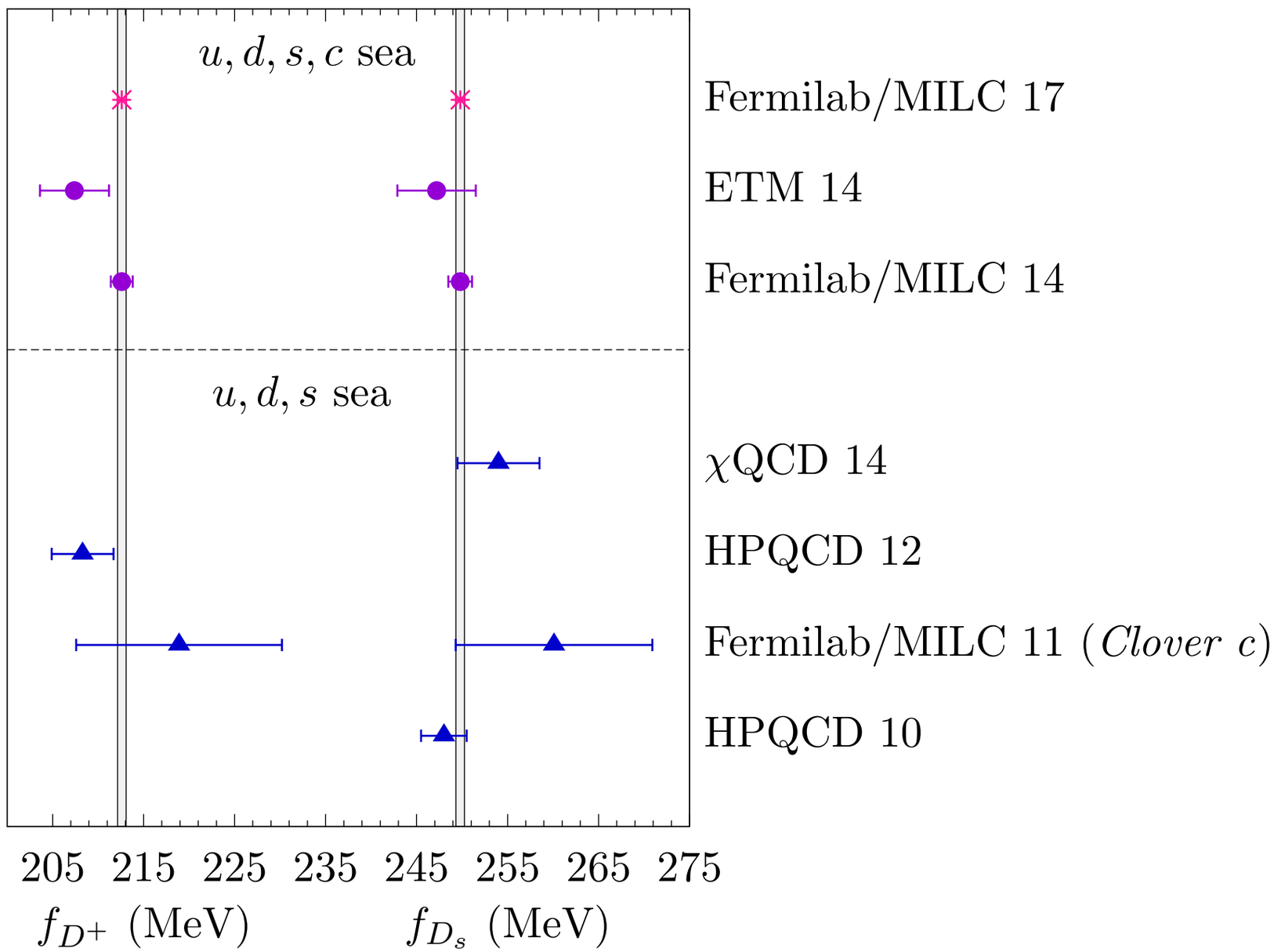
$$
\begin{pmatrix}
\mathbf{V_{ud}} & \mathbf{V_{us}} & \mathbf{V_{ub}} \\
 & K \to \pi l \nu & B \to \pi l \nu \\
\pi \to l \nu & K \to l \nu & B \to l \nu \\
\mathbf{V_{cd}} & \mathbf{V_{cs}} & \mathbf{V_{cb}} \\
D \to \pi l \nu & D \to K l \nu & B \to D^{(*)} l \nu \\
D \to l \nu & D_s \to l \nu &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

leptonic

semileptonic

Charm Decay Constants

- *Decay constants improved compared to three years ago*
- *Much improved compared to results with clover quarks*
- *Errors now <0.5 MeV, or 1/4%*



Third Column: Bottom Quark

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

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

semileptonic

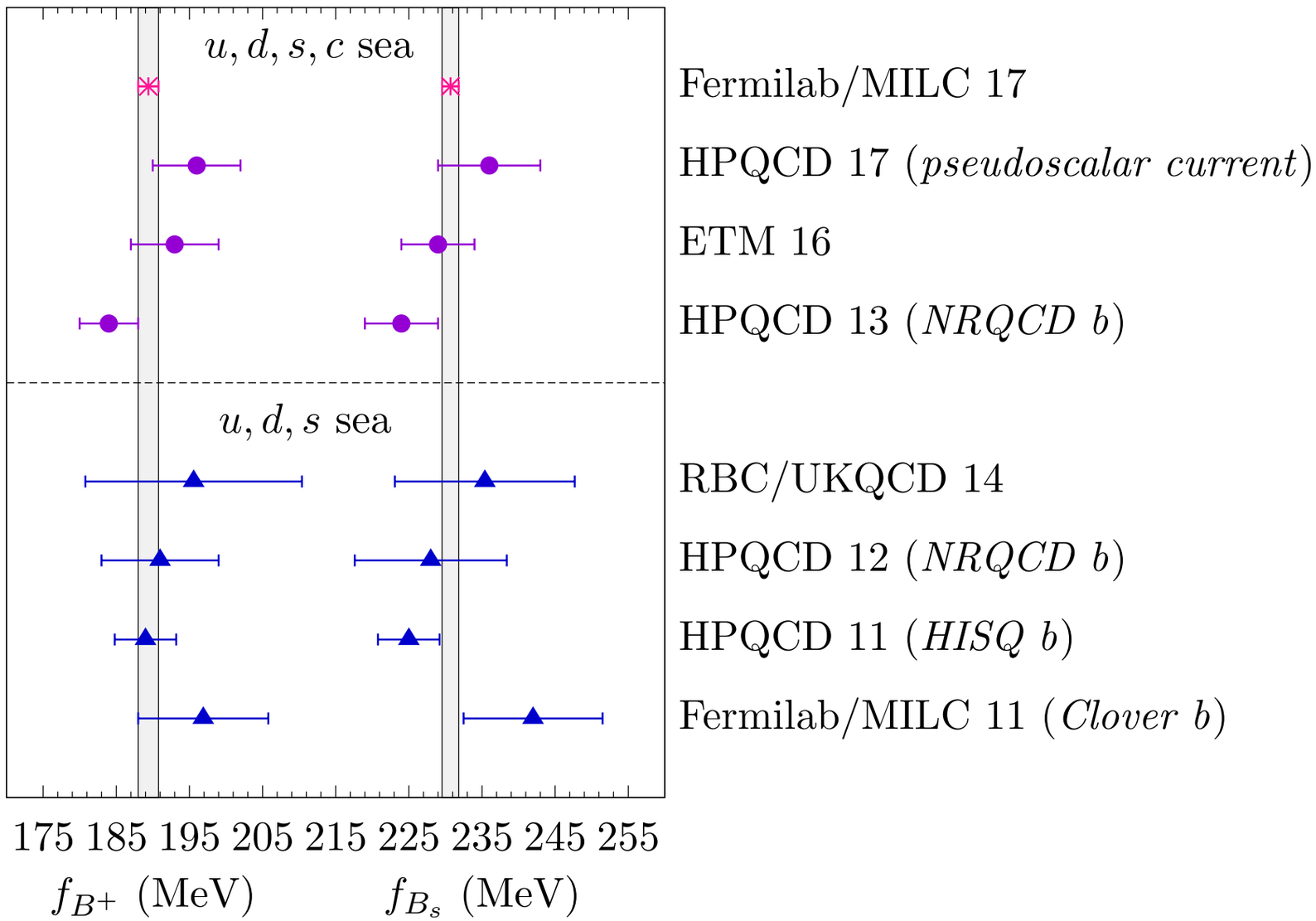
leptonic

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…*

New Level of Precision for $f_{B(s)}$

- *2016 FLAG average for u,d,s,c sea is 186(4) MeV*
- *Latest results have errors of 1.2-1.4 MeV, about a factor of three reduction in error.*



High Precision Required

- *Without high precision calculations of QCD, we cannot accurately determine CKM matrix elements from expensive (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*
  - *Two archival papers in last year in review, one on decay constants, other on quark masses*
- *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*