Lattice QCD on Blue Waters

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Collaborators

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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
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.
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.

$\approx 150$ 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.)

DWF ensemble generation (baea)

\[ 64^3 \times 128 \times 12, \text{1MD} \]

- with MPICH_RANK_REORDER_METHOD=3
- without MPICH_RANK_REORDER_METHOD

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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 $\alpha_s$

✧ 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
  - $a^{\text{exp}} = 116592080(63) \times 10^{-11}$
  - $a^{\text{thy}} = 116591798(68) \times 10^{-11}$
- Currently more than 3 $\sigma$ 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 will 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.
Won 2008 Nobel prize for realization that with three (or more) generations can have CP violation, which might explain baryon asymmetry of Universe.
Some relevant processes listed under each element

CKM Matrix

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

- Processes involving only light quarks test first row unitarity

\[
\begin{pmatrix}
V_{ud} & V_{us} & V_{ub} \\
\pi \rightarrow l\nu & K \rightarrow \pi l\nu & B \rightarrow \pi l\nu \\
V_{cd} & V_{cs} & V_{cb} \\
D \rightarrow \pi l\nu & D \rightarrow K l\nu & B \rightarrow D^{(*)} l\nu \\
D \rightarrow l\nu & D_s \rightarrow l\nu \\
V_{td} & V_{ts} & V_{tb} \\
\langle B_d | \bar{B}_d \rangle & \langle B_s | \bar{B}_s \rangle
\end{pmatrix}
\]
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.
Light decay constant ratio updated: 1712.09262

FNAL/MILC 17
1.1950(+15-22) : 0.18% error (was 0.23%)

From experimental measurement:
\[ \frac{V_{us}}{V_{ud}} \frac{f_K^\pm}{f_\pi^\pm} = 0.2758(5) \]

0.18% error
Processes involving charm quark test second row unitarity

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

\[ f_{D^+} \text{ (MeV)} \quad f_{D_s} \text{ (MeV)} \]

Fermilab/MILC 17
ETM 14
Fermilab/MILC 14
χQCD 14
HPQCD 12
Fermilab/MILC 11 (Clover c)
HPQCD 10

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Processes involving bottom quark are in third column and third row.

\[
\begin{pmatrix}
V_{ud} & V_{us} & V_{ub} \\
\pi \rightarrow l\nu & K \rightarrow \pi l\nu & B \rightarrow \pi l\nu \\
\pi \rightarrow l\nu & K \rightarrow l\nu & B \rightarrow l\nu \\
V_{cd} & V_{cs} & V_{cb} \\
D \rightarrow \pi l\nu & D \rightarrow K l\nu & B \rightarrow D(\ast) l\nu \\
D \rightarrow l\nu & D_s \rightarrow l\nu & \\
V_{td} & V_{ts} & V_{tb} \\
\langle B_d | \bar{B}_d \rangle & \langle B_s | \bar{B}_s \rangle
\end{pmatrix}
\]

- **semileptonic**
- **leptonic**
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\(^3\)×288, physical light quarks, a=0.042 fm; 64\(^3\)×192, m_l/m_s=0.2, a=0.042 fm; 96\(^3\)×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