Lattice QCD on Blue Waters

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Collaborators

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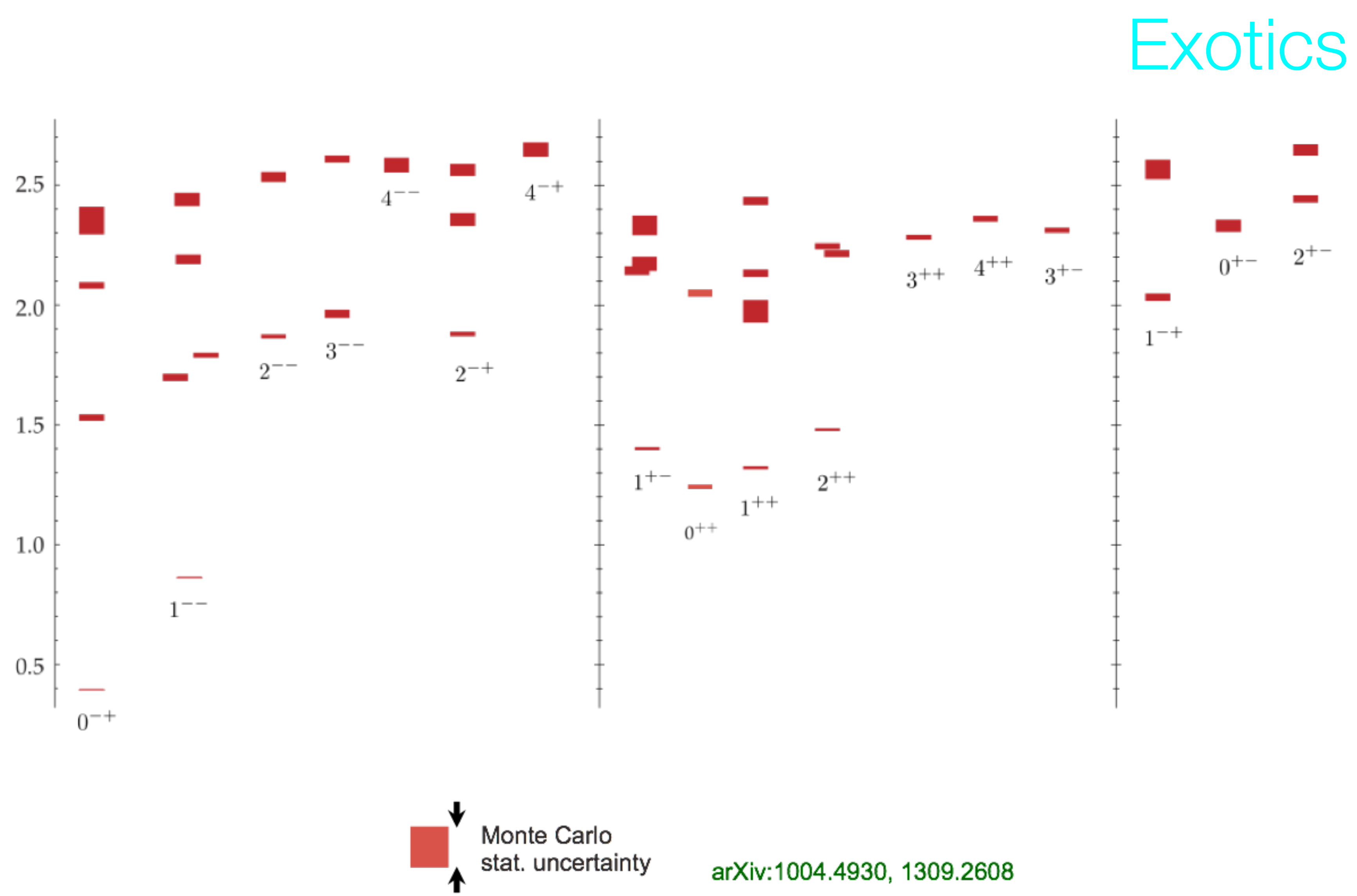
Key Challenges

- ✦ 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
- ✦ Using Wilson/Clover action, we study masses of excited and exotic states of QCD

Key Challenge II

- GlueX experiment will search for exotic states
- LQCD calculations suggests they exist
- Challenge: compute decay channels to guide search
- now working on $32^3 \times 256$ grid, with $m_\pi \sim 230$ MeV
- Moving to generate configurations at the physical pion mass



$24^3 \times 128$; $m_\pi \sim 390$ MeV

Why It Matters

- ✦ The standard model 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
- ✦ There are theoretical reasons that argue for the fact that the standard model is incomplete
- ✦ 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
- A central goal of nuclear physics is to predict new bound states of quarks, properties of glueballs and exotic states that are not predicted by quark model
- 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!)

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

Lattice QCD for Nuclear Physics

- ✦ Over $300 million has been spent to upgrade JLab to look for new QCD bound states
- ✦ Focus of GlueX experiment at Hall D and CLAS12 at Hall B
  - Experiments will start in 2015
- ✦ We want predictions prior to the experiment to maximize impact and synergy
- ✦ Lattice QCD input is needed to meet several key NSAC milestones
- ✦ Results are relevant to experiments such as COMPASS (CERN), BES III (Beijing), & others

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, order 1000 jobs may be run in parallel
- ✦ We can use Blue Waters' GPUs for the second stage in a number of our projects
  - Wilson Clover gauge generation runs well on GPUs
  - We are still optimizing some of the HISQ code to see how well we can do gauge generation on GPUs
- ✦ We need large partitions to generate configurations
- ✦ We can run many smaller parallel jobs for 2nd stage

Why Blue Waters II

- The Blue Waters file system is important for our work
- The combination of local disk and near line storage has been responsive and relatively easy to use
- Off site date movement with Globus Online has been relatively painless, e.g., over 500 TB moved to JLab

- We are concerned about long term storage as the recent demise of the NCSA mass storage system was very disruptive and caused months of pain as we had a 20+ year history there
- We are not trying to archive data on Blue Waters although the physics projects will continue for years

Why Blue Waters III

- 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
- We estimate that Blue Waters accelerates the progress of our nuclear physics calculation by approximately a factor of five, compared to other available resources

Accomplishments

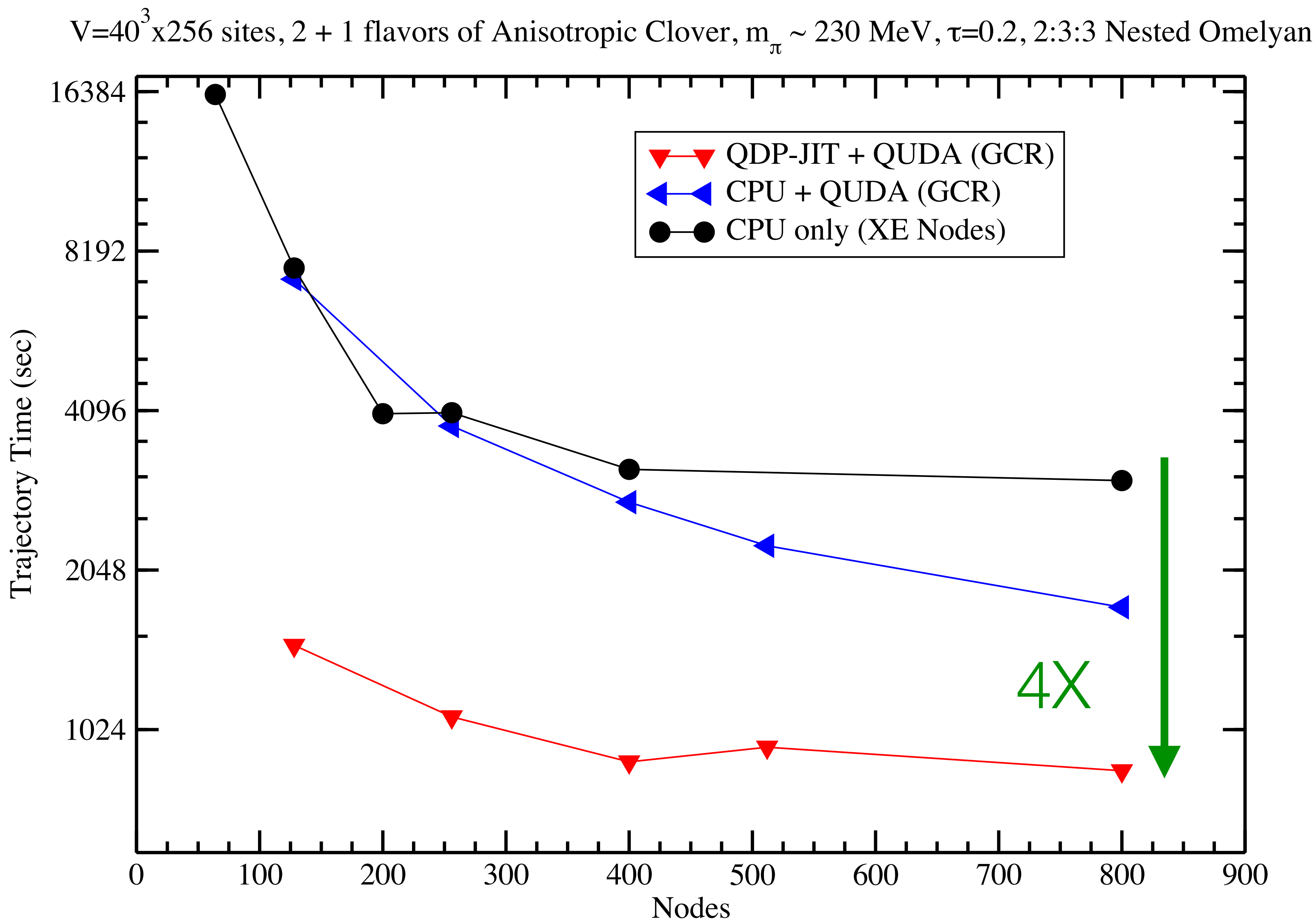
- ✦ Blue Waters has allowed us to produce the most realistic gauge configurations to date
- ✦ These are the most challenging calculations we have ever undertaken
- ✦ The HISQ configurations have allowed us to make the most precise calculations of a number of meson decays
  - Two papers have already appeared in *Physical Review Letters*
  - One was designated an *Editors' Suggestion*
- ✦ The Clover quark propagators produced on Blue Waters will play a major role in the spectrum calculations described before
  - 285 of 485 $32^3 \times 256$ configurations already completed

Accomplishments II

- Just-in-time compilation techniques have been developed to widen the range of code that can be ported efficiently to the GPUs
  - This work will appear in the proceedings of IPDPS '14
- Additional code development has been done (and will continue) on other parts of the code

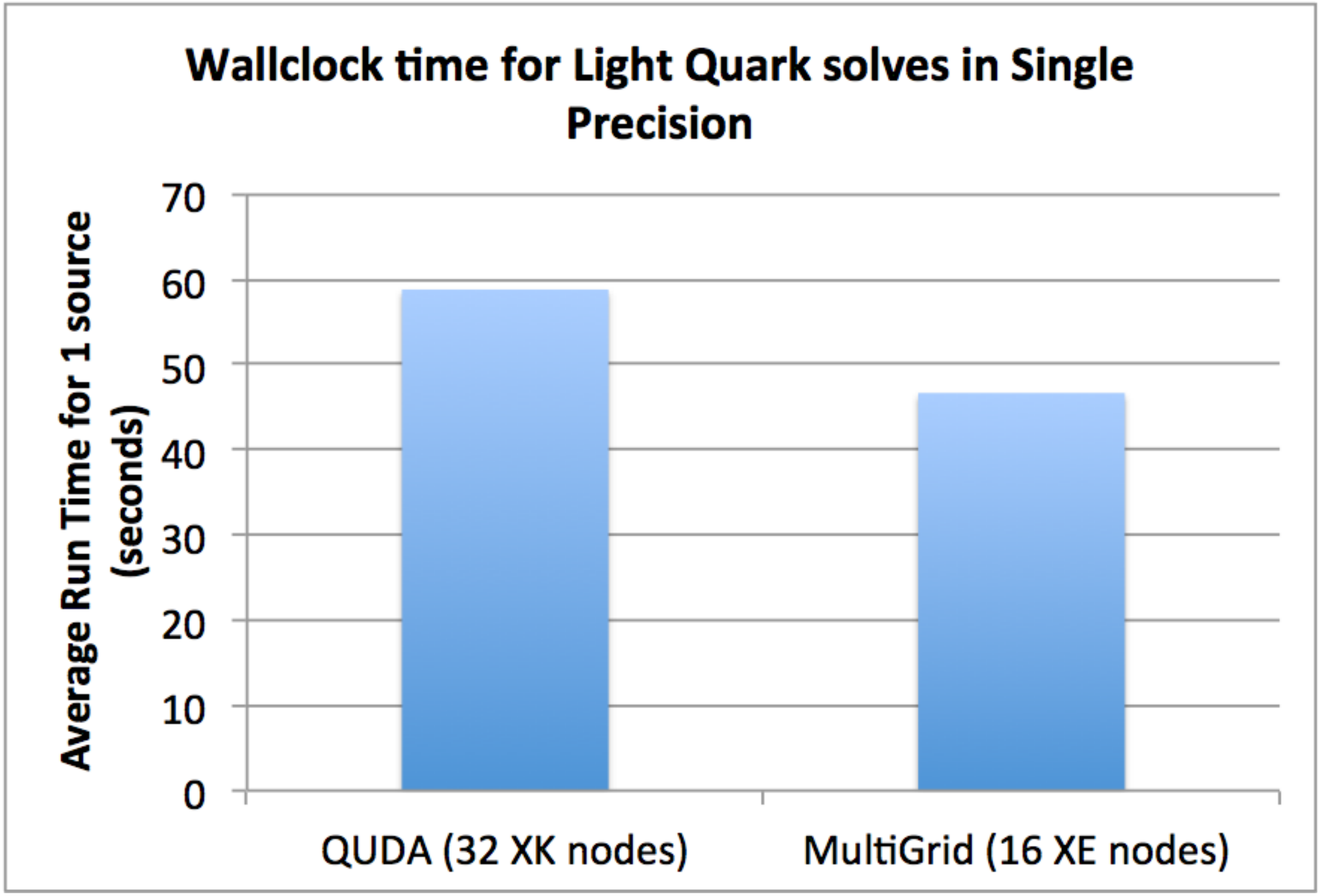
JIT Performance Improvement

- QDP-JIT (F. Winter) improves Chroma performance on GPUs
- QUDA used for linear solver
- Gauge generation speed 4 times better using XK GPUs than XE CPUs
- See IPDPS'14 proceedings



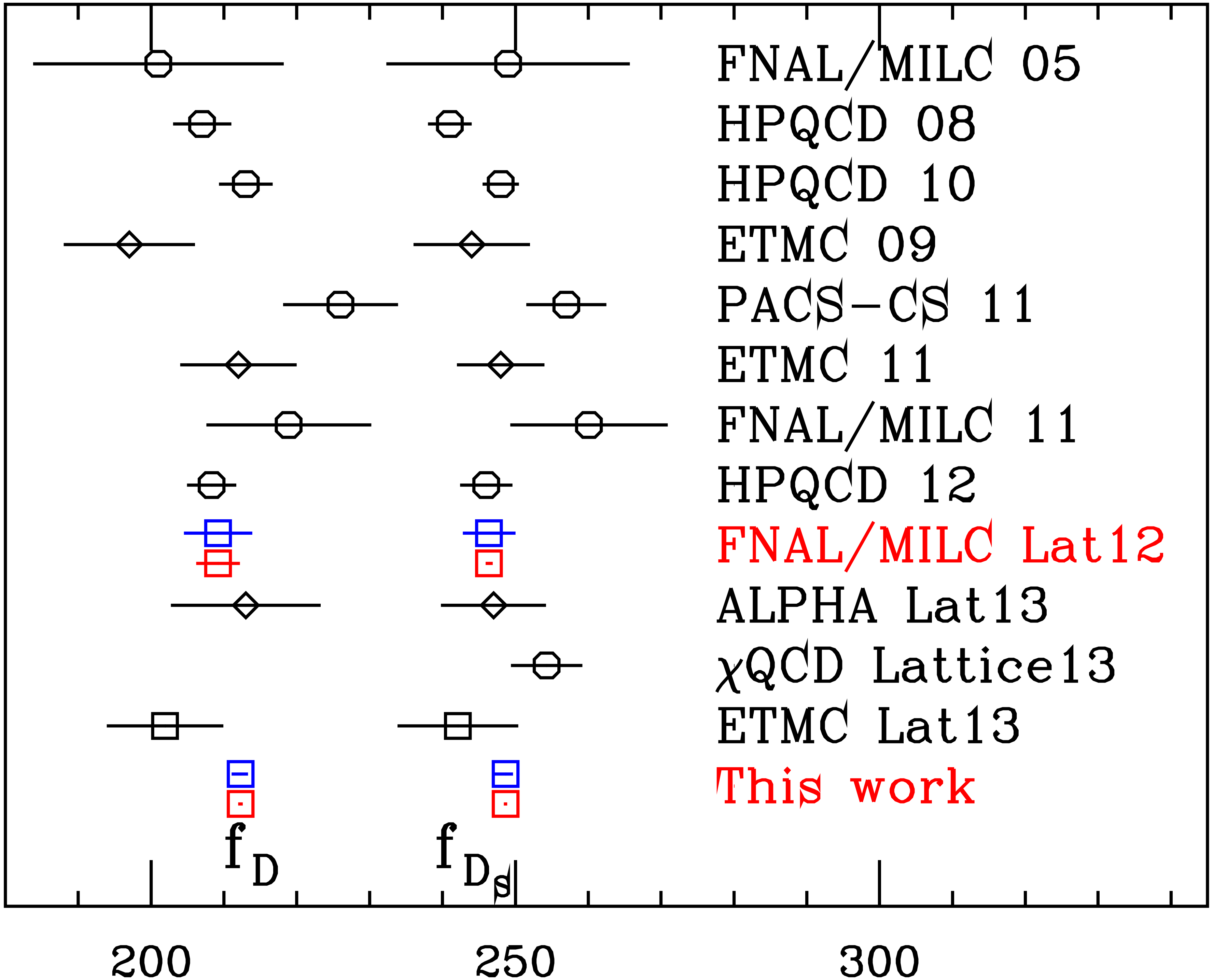
Multi-grid Solver

- Multi-grid solver (J. Osborn) integrated into Chroma (S. Cohen & B. Joo)
- 10× improvement over CPU solver for multiple right hand sides
- Allows better performance on XE nodes than BiCGStab on GPUs
- More stable than BiCGstab

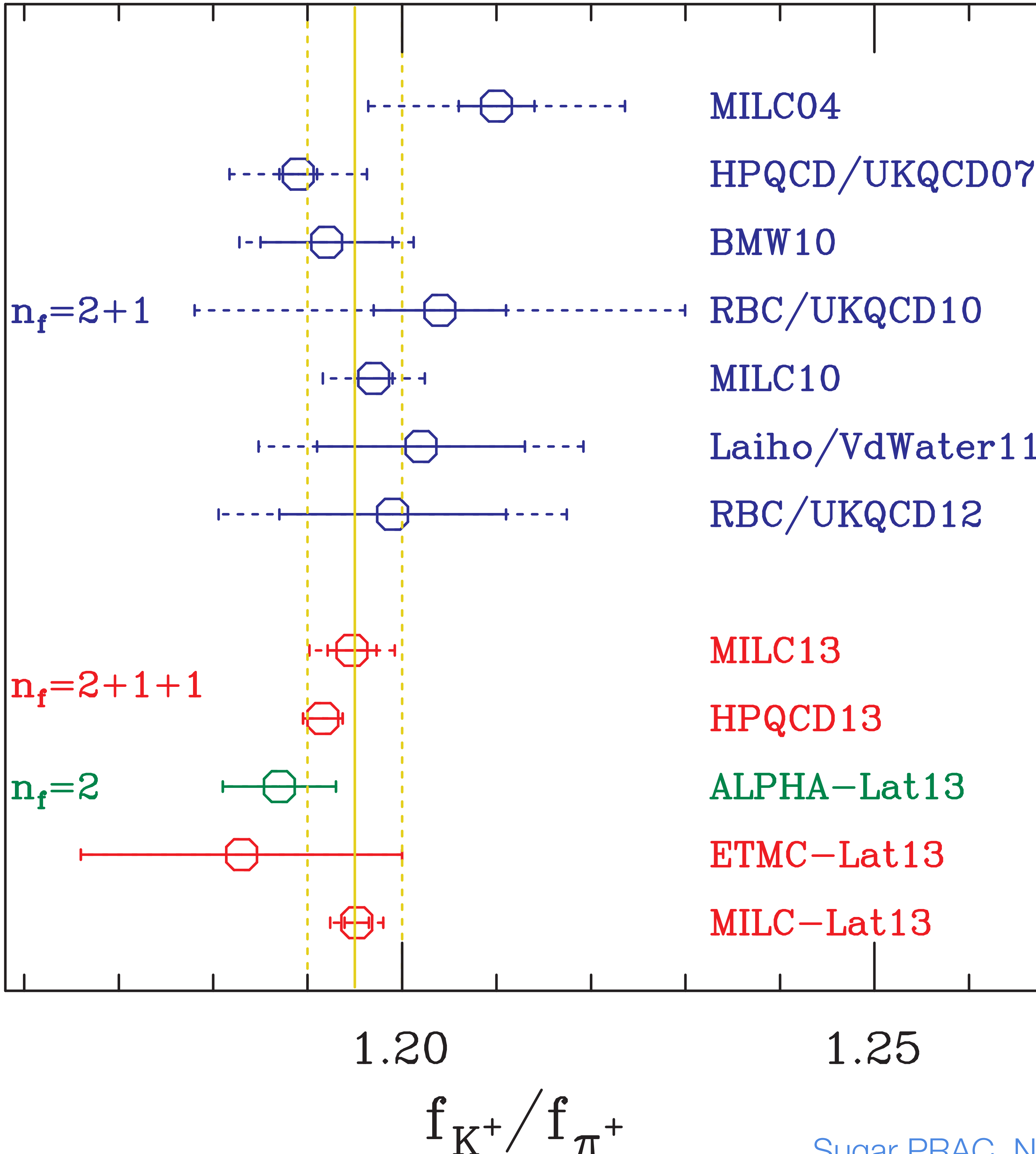


Charm Meson Decay Constants

- Note the progress over the past decade in improving precision
- Squares ($N_f=4$); octagons ($N_f=3$)
- This allows much better results for two CKM matrix elements
- Red points show statistical error only. Blue includes systematic errors



Light Meson Decay Constants



Decay Constants & Quark Masses

- Results from Lattice 13:

$$
\begin{aligned}
f_K/f_\pi &= 1.1957(\pm 27) && 0.23\% \\
f_D &= 212.3^{+1.0}_{-1.2}\text{MeV} && 0.6\% \\
f_{D_s} &= 248.7^{+1.0}_{-1.5}\text{MeV} && 0.6\% \\
f_D/f_{D_s} &= 1.171^{+3}_{-2} && 0.26\% \\
m_c/m_s &= 11.74(6) && 0.5\% \\
m_s/m_l &= 27.37(12) && 0.4\% \\
m_u/m_d &= 0.462(18) && 3.9\%
\end{aligned}
$$

- Last result is sensitive to electromagnetic corrections for which we are developing code