Lattice QCD on Blue Waters

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Collaborators

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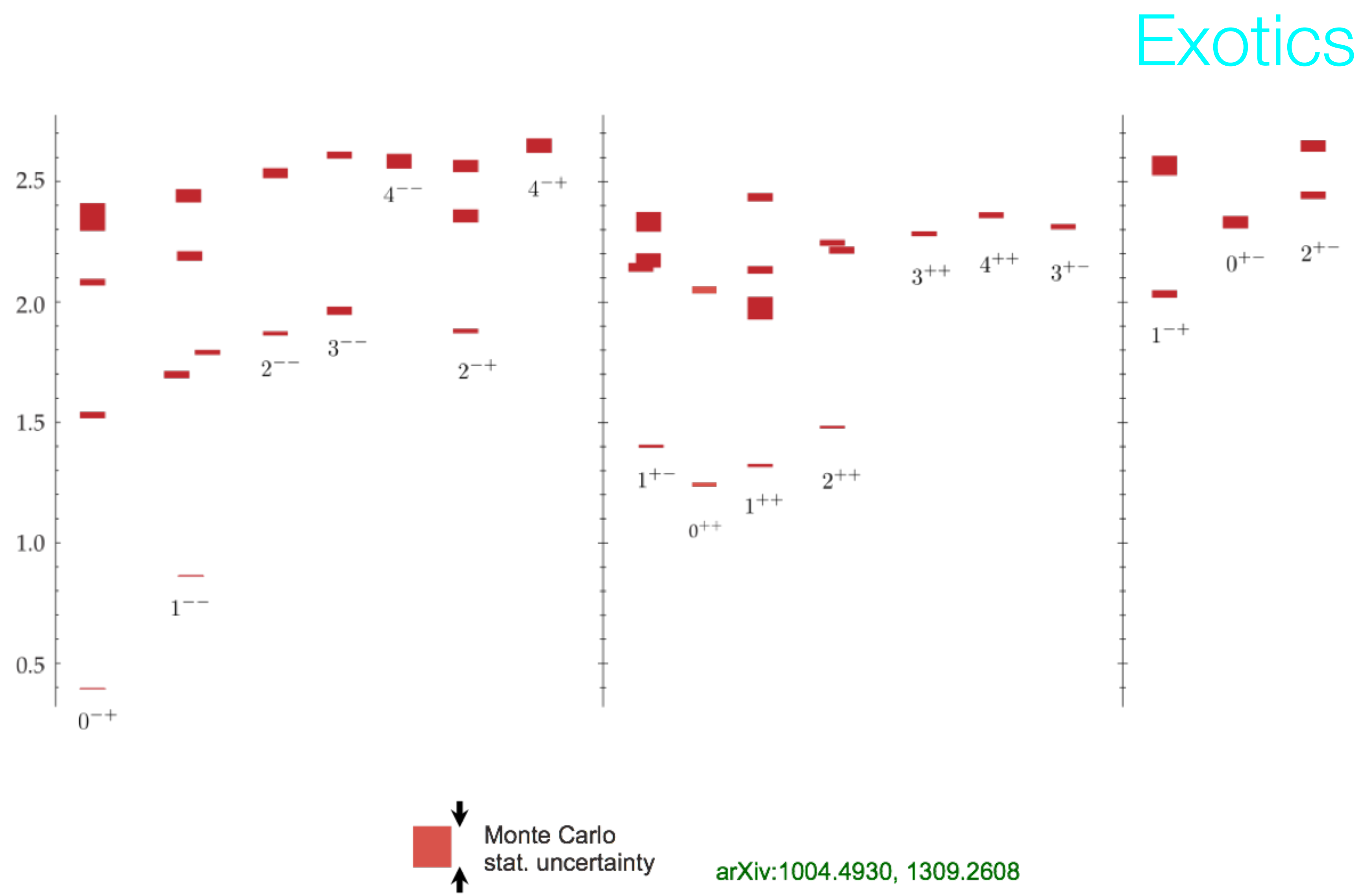
Key Challenges

- ✦ 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 & decays 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 $40^3 \times 256$ grid, with $m_\pi \sim 230$ MeV
- Moving to generate configurations at the physical pion mass on $64^3 \times 128$ grid



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

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
- ✦ We want predictions prior to the experiment to maximize impact and synergy
- ✦ Lattice QCD input is needed to meet several key Nuclear Science Advisory Committee milestones
- ✦ Results are relevant to other experiments such as COMPASS (CERN), BES III (Beijing), ...

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 some production running in our projects, e.g.,
  - Wilson Clover gauge generation runs well on GPUs
  - Decay constant calculations also using GPUs
- ✦ We need large partitions to generate configurations
- ✦ We can run many smaller parallel jobs for 2nd stage

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

Accomplishments

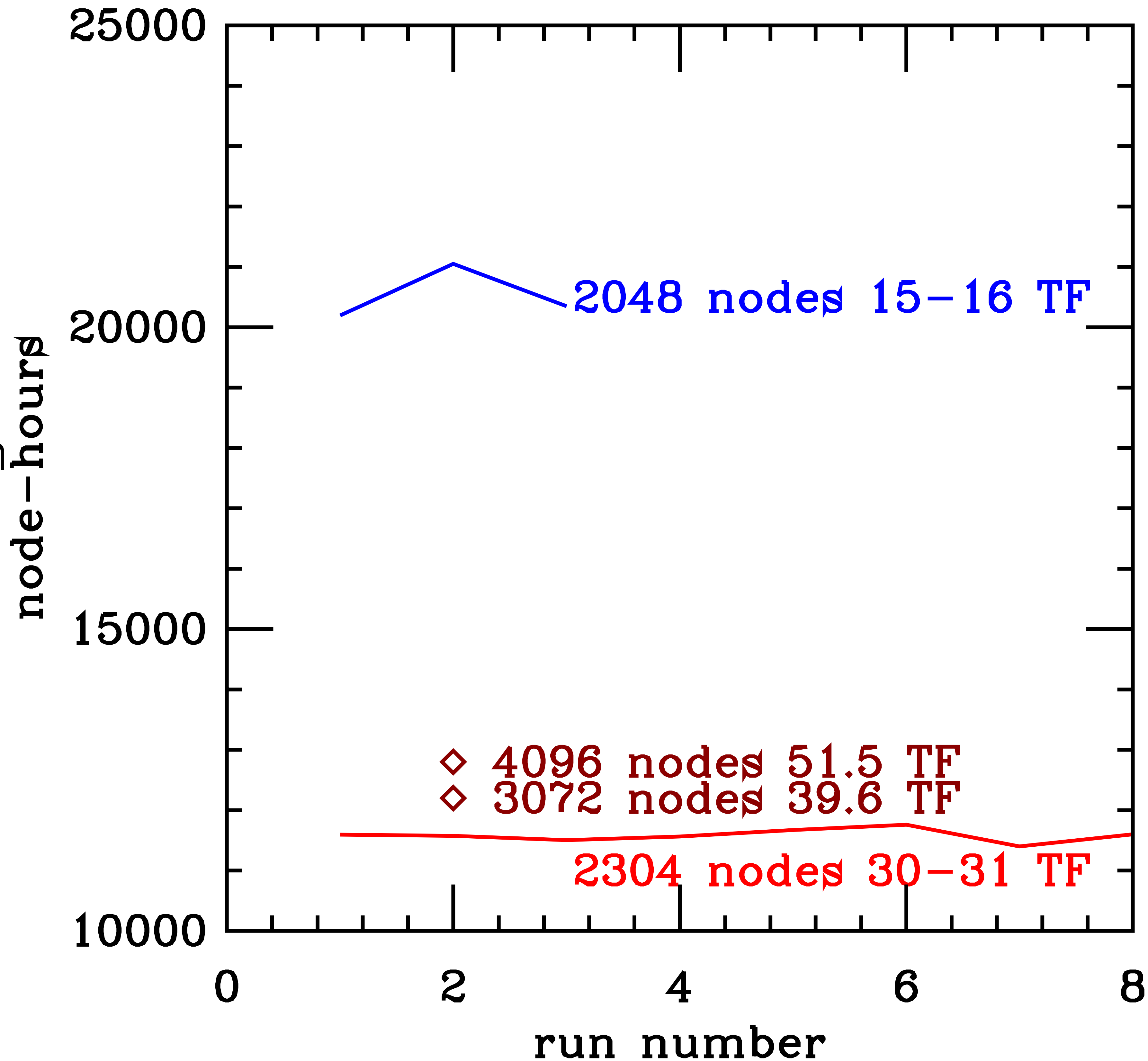
- ✦ Blue Waters has allowed us to produce the most realistic gauge configurations to date
- ✦ These are the most challenging calculations we have ever undertaken ($144^3 \times 288$, physical light quarks, a=0.042 fm)
- ✦ HISQ configurations have allowed us to make the most precise calculations of a number of meson decays
  - 2 *Physical Review Letters (PRL),* 1+ *Physical Review D (PRD)*
  - One *PRL* was designated an *Editors' Suggestion*
- ✦ The Clover quark propagators produced on Blue Waters play a major role in the spectrum calculations described before
  - 485 $32^3 \times 256$ configurations completed, $40^3 \times 256$ in process
  - One *PRL,* one paper in *PRD*

Accomplishments II

- ✦ We owe a great deal of thanks to Bob Fiedler and Craig Steffen for help with topology aware scheduling.
  - details on next slide
- ✦ Just-in-time compilation techniques have been developed to widen the range of code that can be ported efficiently to the GPUs
  - This work appeared in the proceedings of IPDPS '14
- ✦ Additional code development has been done (and will continue) on other parts of the code

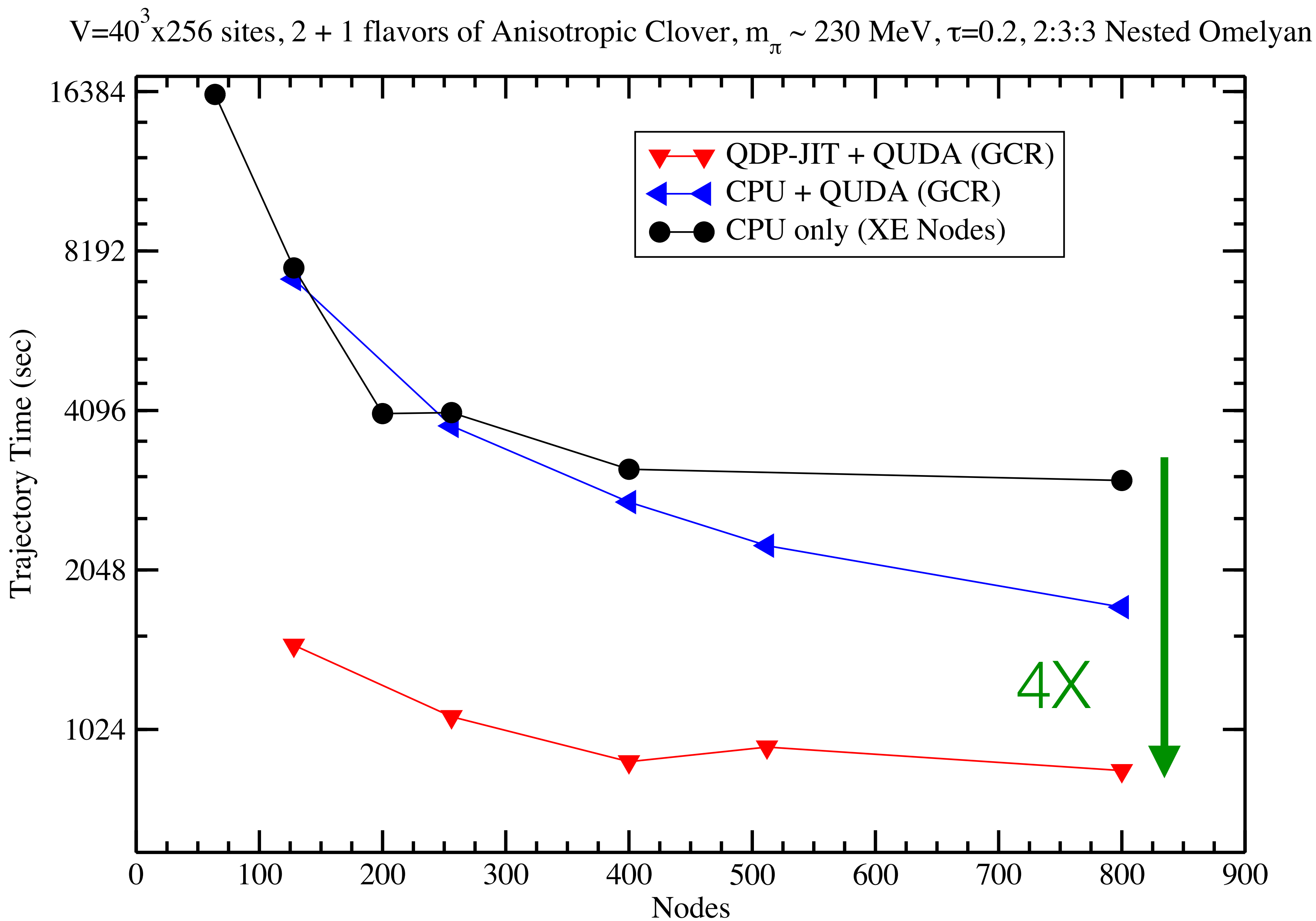
Topology Aware Improvement

- Blue shows three runs without topological awareness
- Red and dark red are results on different numbers of nodes with topology awareness
- Almost a fact of two improvement; and better consistency
- Now trying on GPU jobs where we have seen up to 2× performance variation



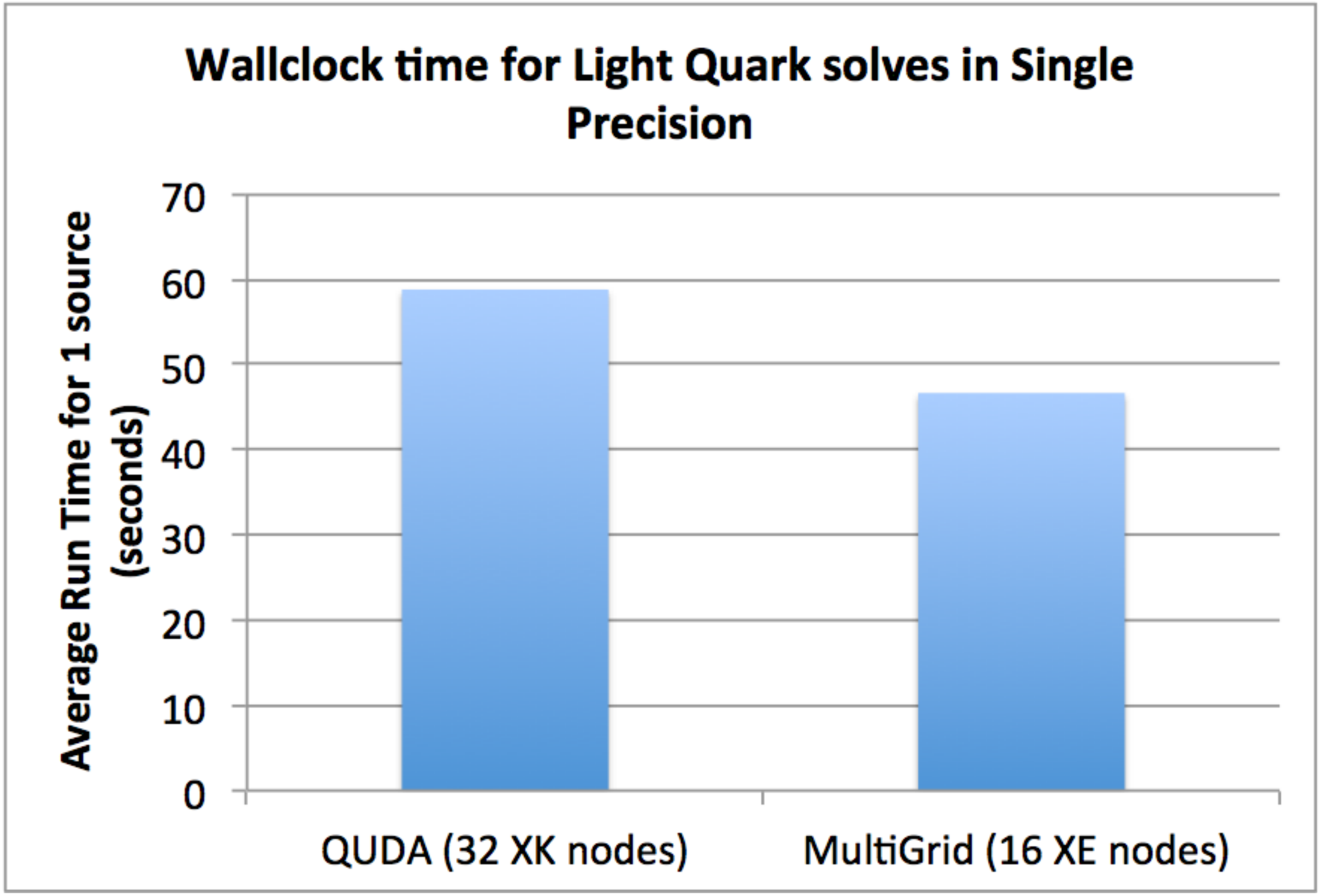
JIT Performance Improvement

- 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 Winter, Clark, Edwards & Joó, IPDPS'14 proceedings



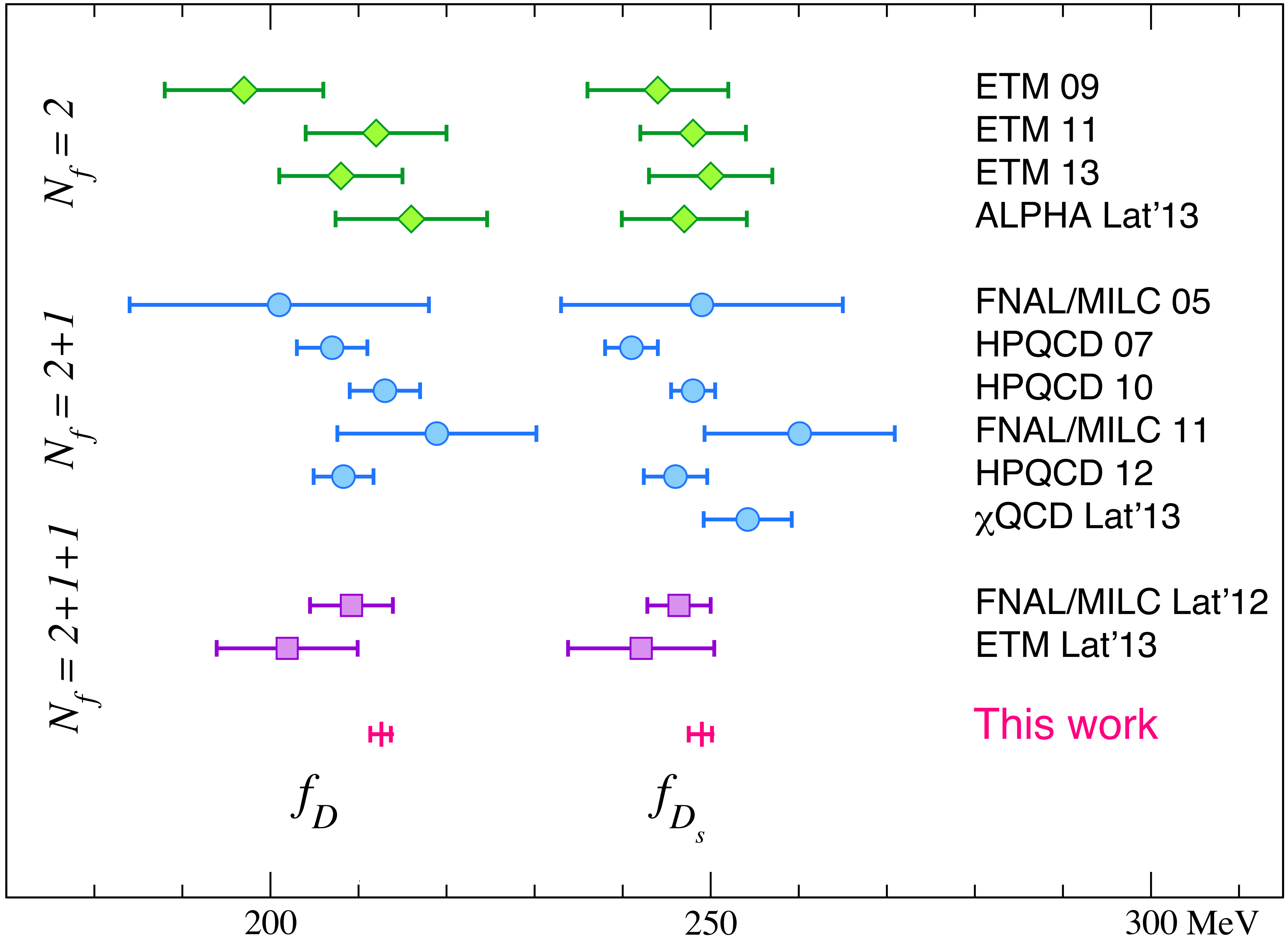
Multi-grid Solver

- 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



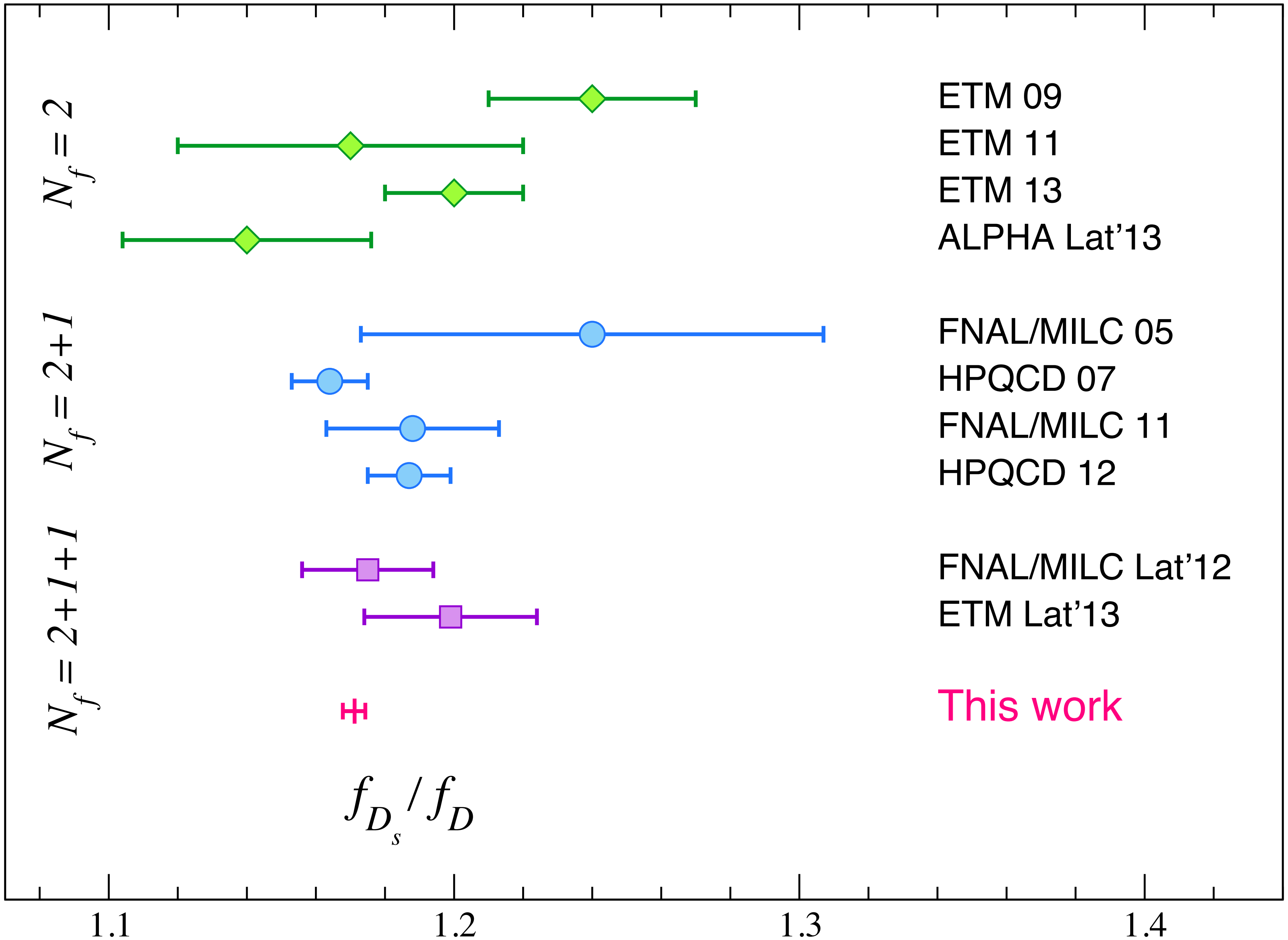
Charm Meson Decay Constants

- Note the progress over the past decade in improving precision
- Blue Waters instrumental for "This Work"
- New results allow much better results for two CKM matrix elements
- Excellent agreement with CKM unitarity.



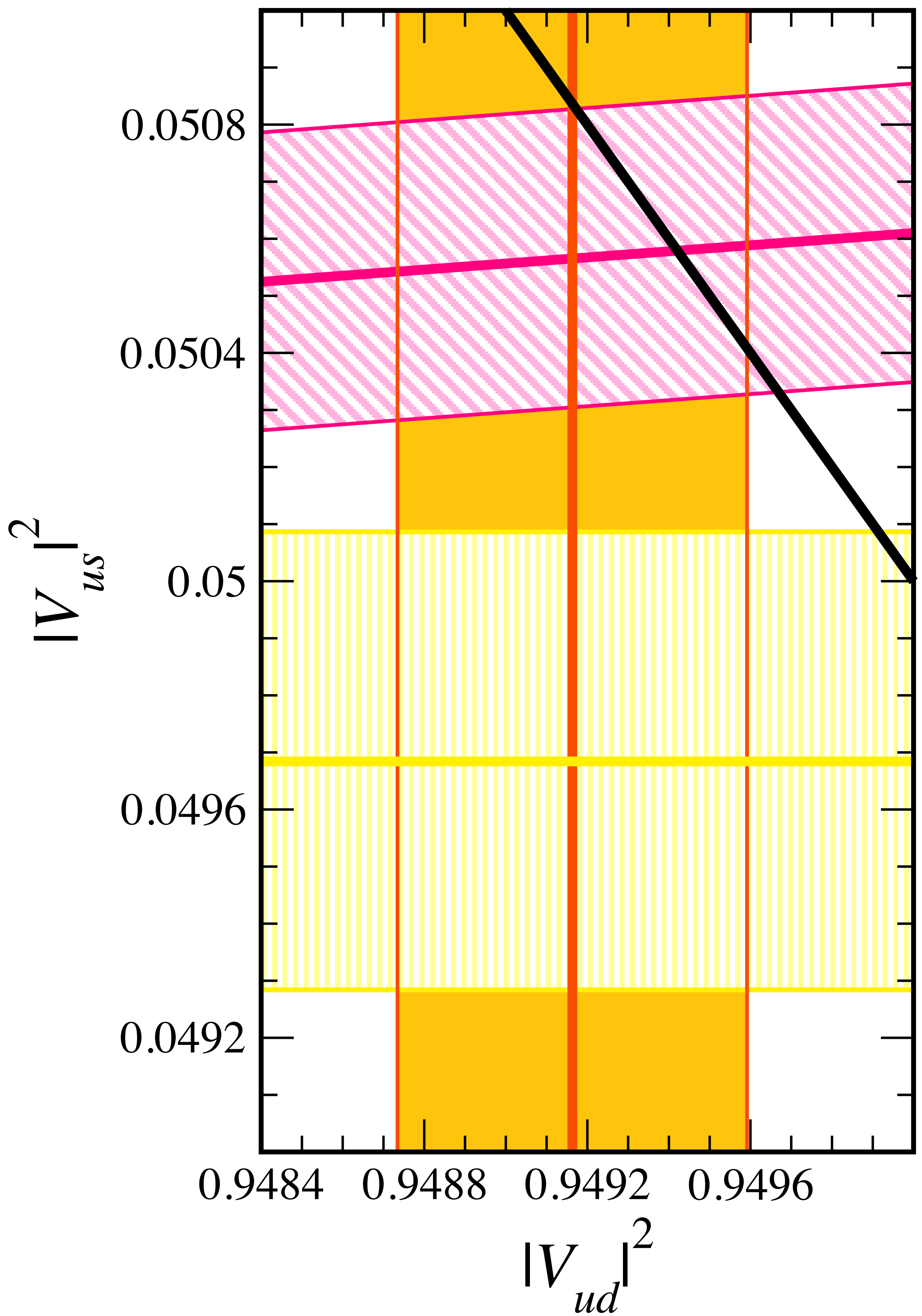
Charm Decay Constant Ratio

- Blue Waters enables a two to four times improvement in ratio of charm meson decay constants



Test of First Row Unitarity

- Magenta diagonal band from f_K/f_π (this work)
- Yellow vertical band from nuclear β decay.
- Black diagonal is unitary condition
- Hatched yellow band from semileptonic decay also on Blue Waters (El Khadra)
- Some tension in latter result



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
- ✦ However, much more work remains to provide the theoretical input required to interpret a large number of experiments