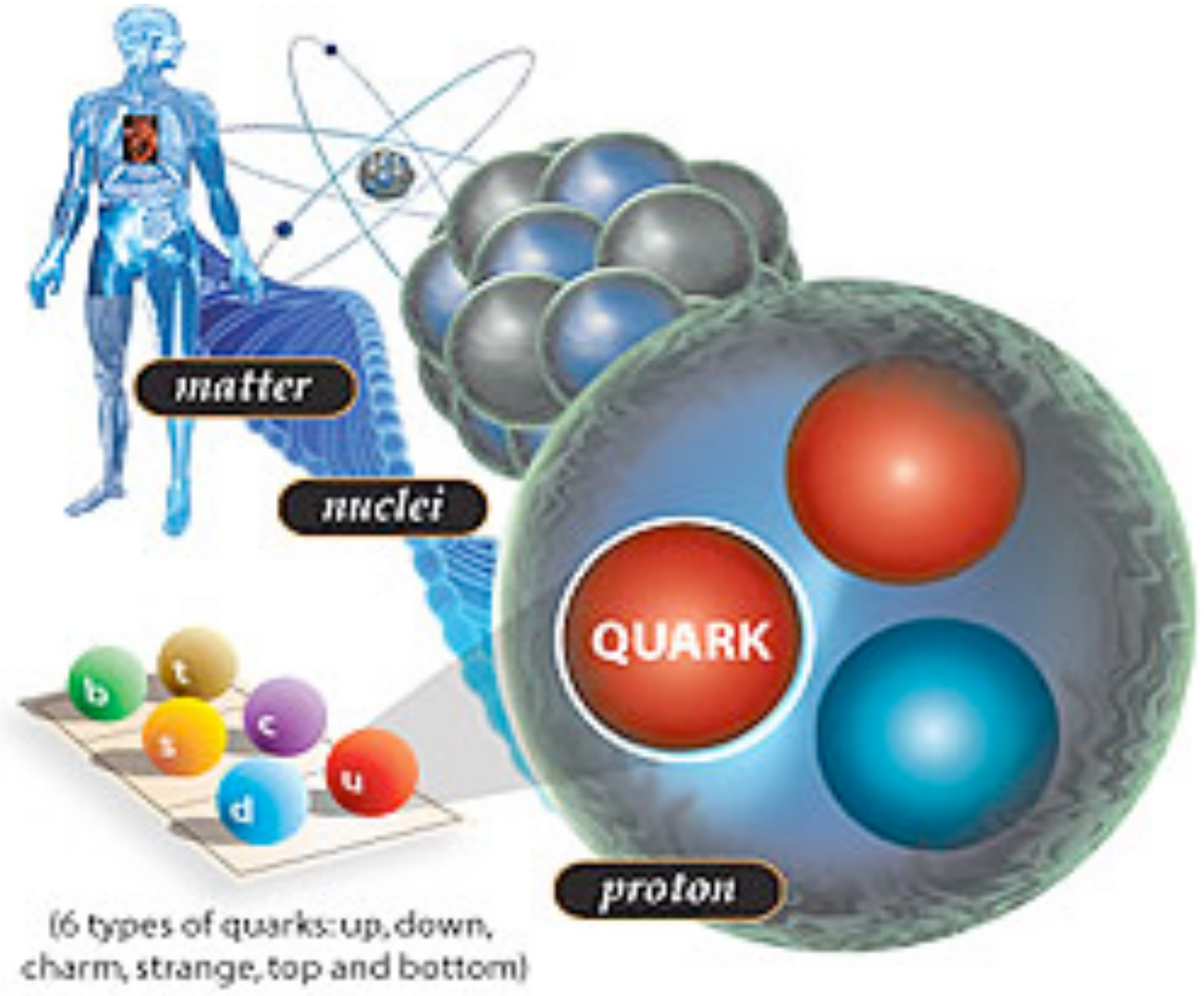
Hadrons, Nuclei and Nuclear Matter from QCD

Bálint Joó, Jefferson Lab
on behalf of the

USQCD Nuclear Physics SciDAC 3 project

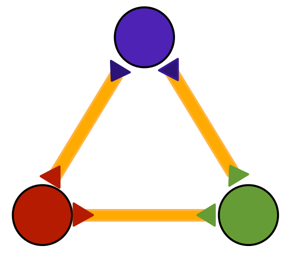
SciDAC PI Meeting, July 22-24, 2015
Bethesda, MD

Introduction

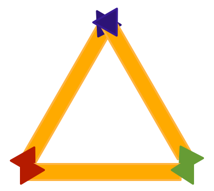


- It is believed that the fundamental building blocks of matter are ***quarks*** bound together by ***gluons***, via the ***strong nuclear force.***
- Quantum Chromodynamics (QCD) is the theory which describes the strong interactions
- Understanding how QCD makes up matter and how quarks and gluons behave is a subject of intense experimental scrutiny
  - < ~20% of the mass of a proton comes from mass of the quarks, rest comes from binding
  - gluon self-coupling and gluon excitations can create ***exotic forms of matter***

meson: 2 quarks



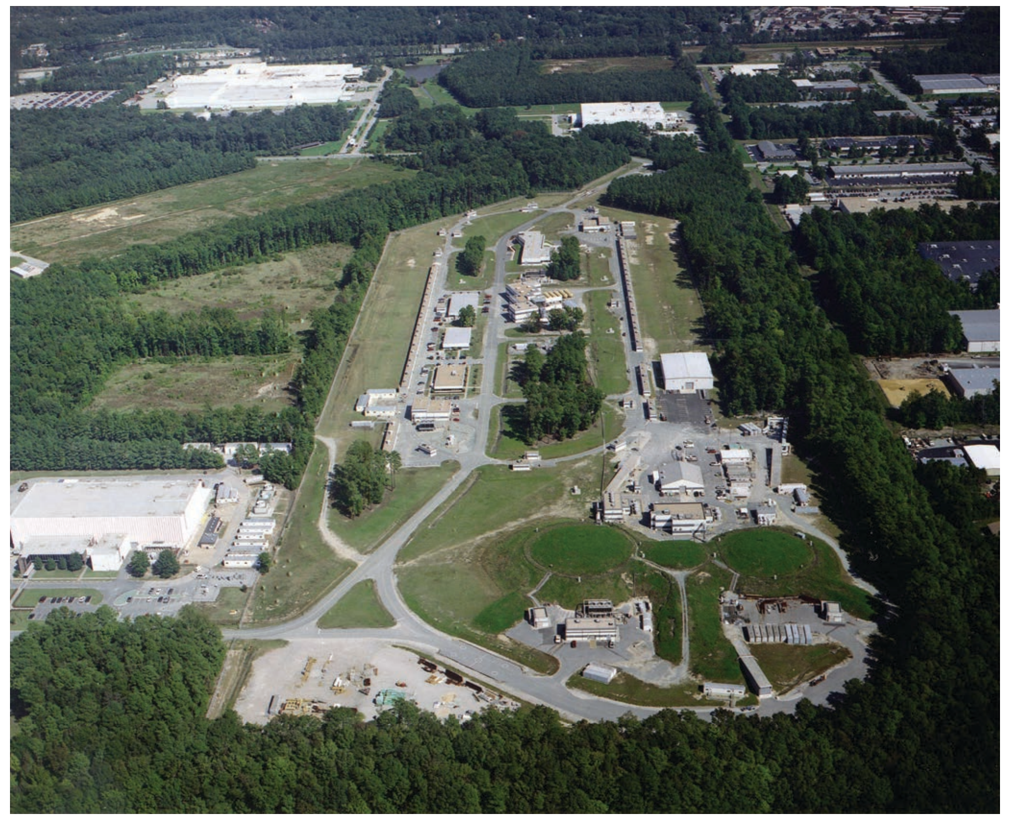
baryon: 3 quarks



glueball: 0 quarks only gluons

GlueX in the new Hall-D of Jefferson Lab@12 GeV. Hunting for exotics!

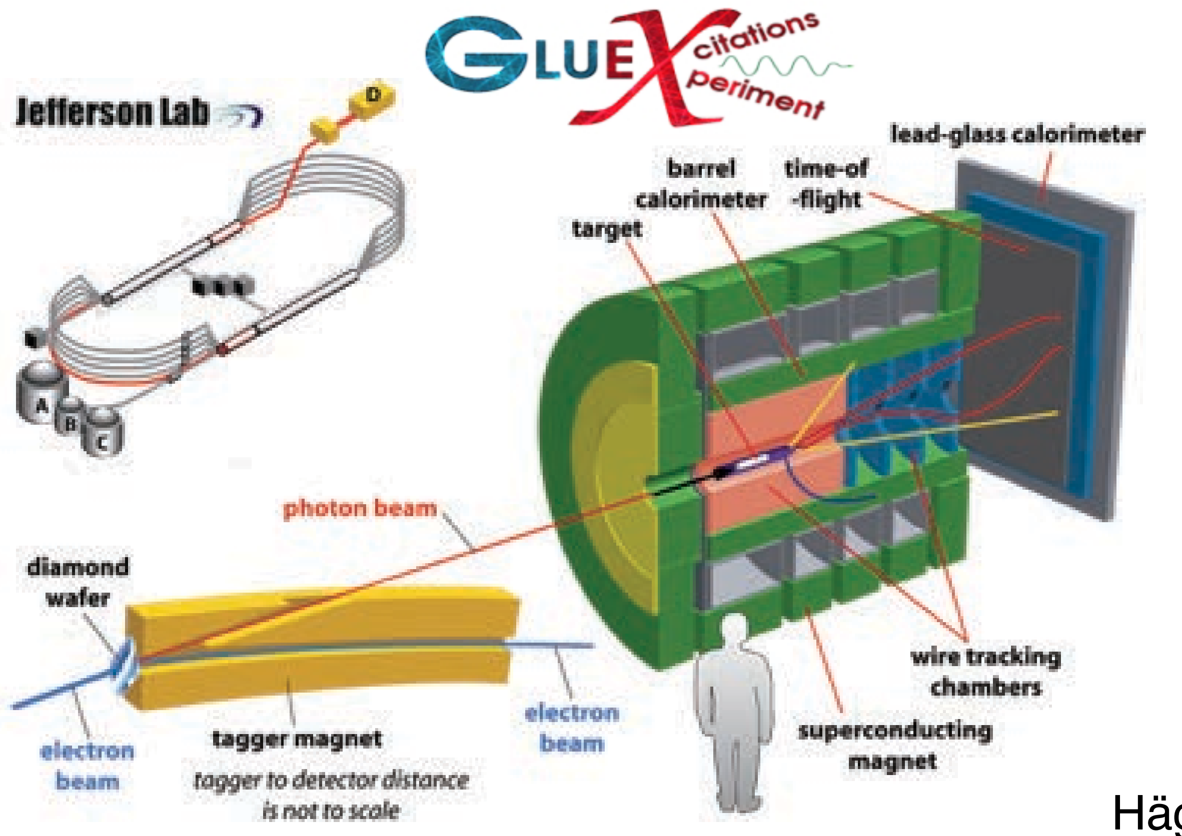
Jefferson Lab

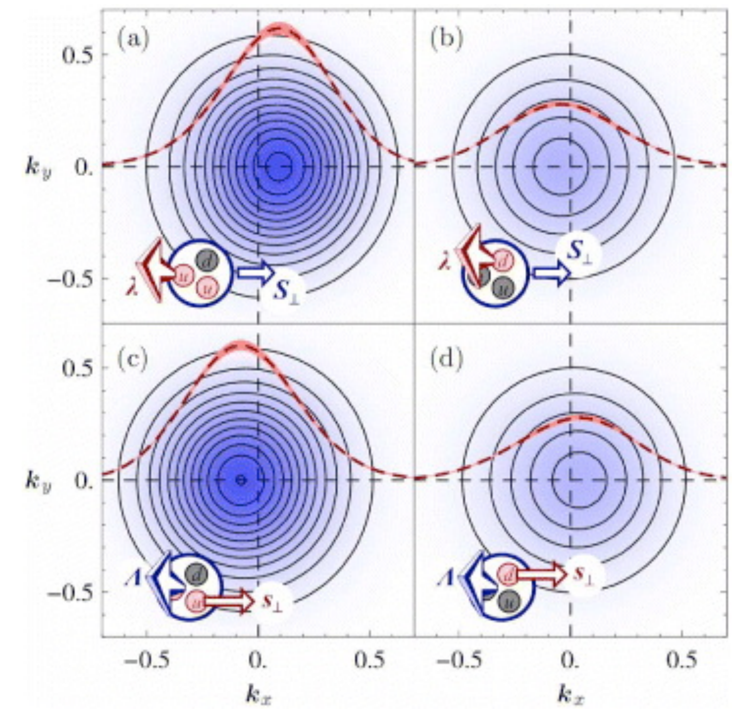


Brookhaven National Lab

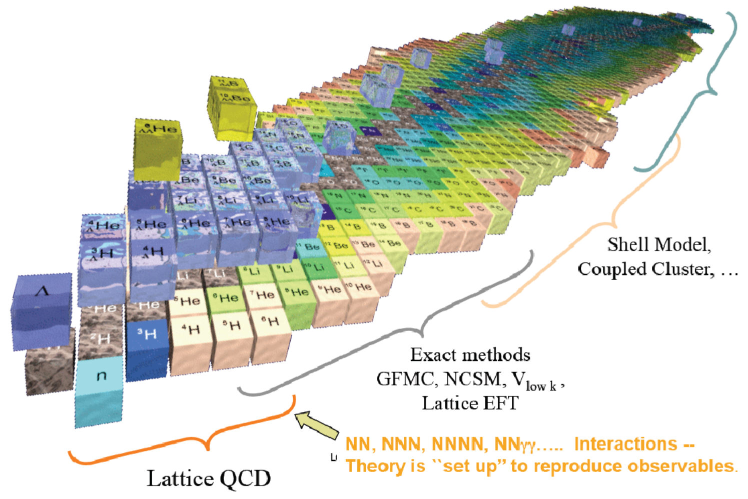
Important questions in Nuclear Physics

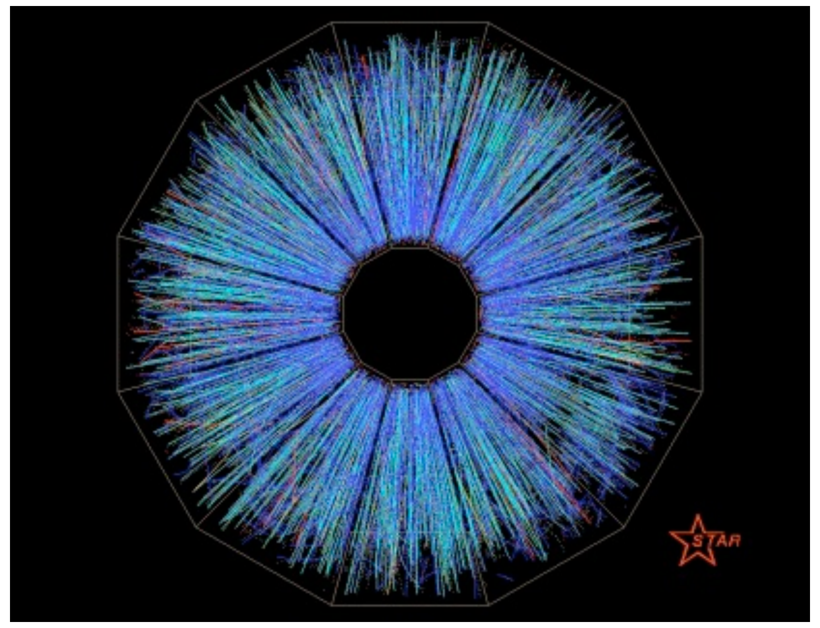
- What observable states does QCD allow?
  - What is the role of the gluons? What about exotic matter?
  - Focus of the Flagship GlueX experiment of $338M Jefferson Lab 12GeV upgrade which will search for exotics
- How does QCD make protons, neutrons?
  - how are quarks & gluons distributed in a proton or neutron ?
  - Focus of JLab 12 GeV, Halls A, B & C, RHIC-spin and proposed future Electron Ion Collider
- QCD must predict properties of light nuclei
  - predict nuclear reaction properties, connect to effective theories
  - $730M Facility for Rare Isotope Beam (FRIB) will investigate nuclear structure and interactions
- How does QCD behave under extreme temperatures & pressures such as in supernovae or shortly after the Big-Bang.
  - Studied in experiments at RHIC at Brookhaven National Laboratory





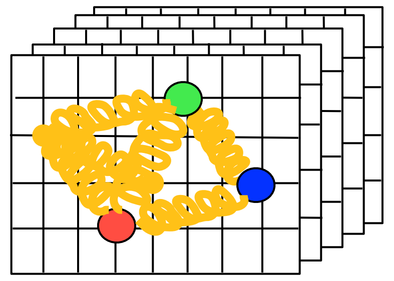
Hägler, Musch, Negele, Schäfer, EPL 88 61001



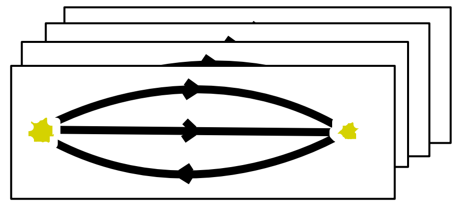


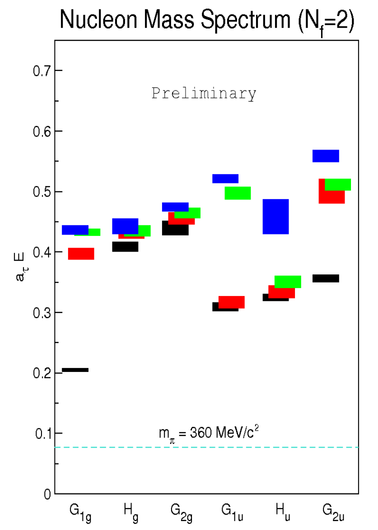
LQCD Calculation Workflow

Gauge Configurations



Propagators, Correlation Functions



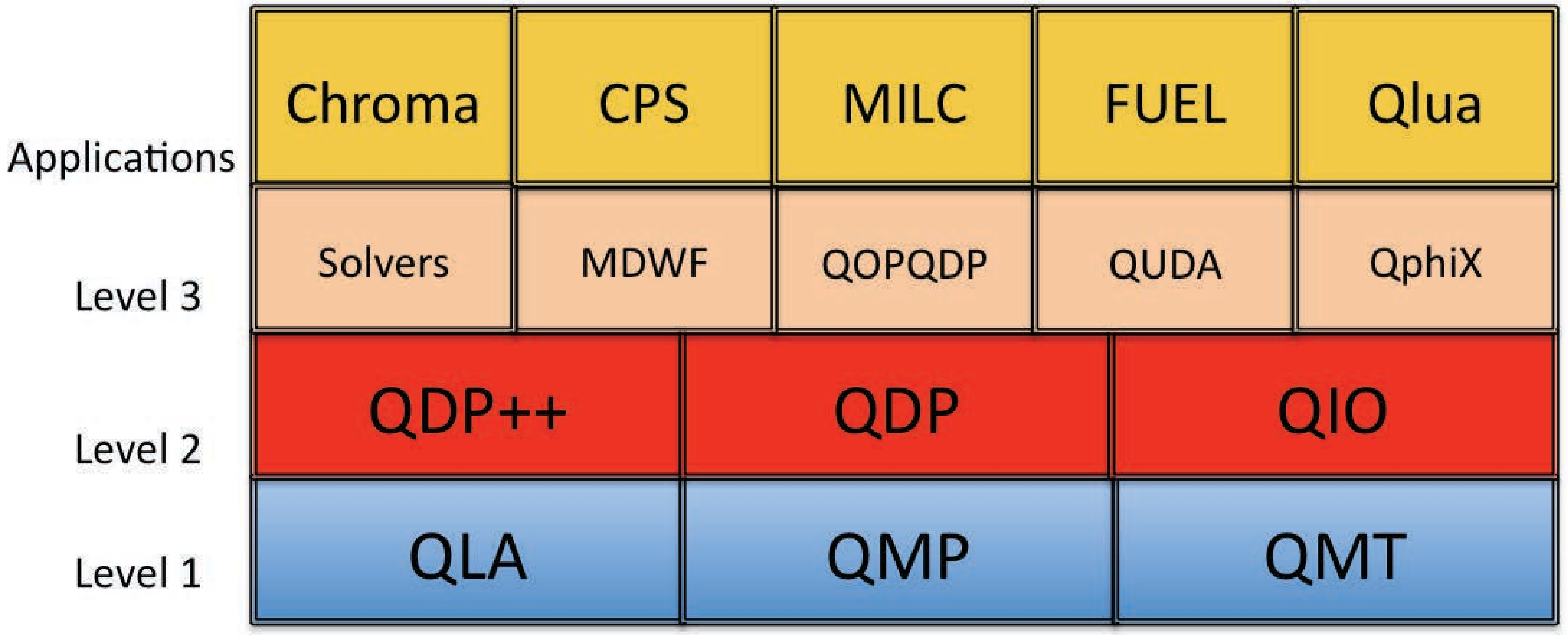


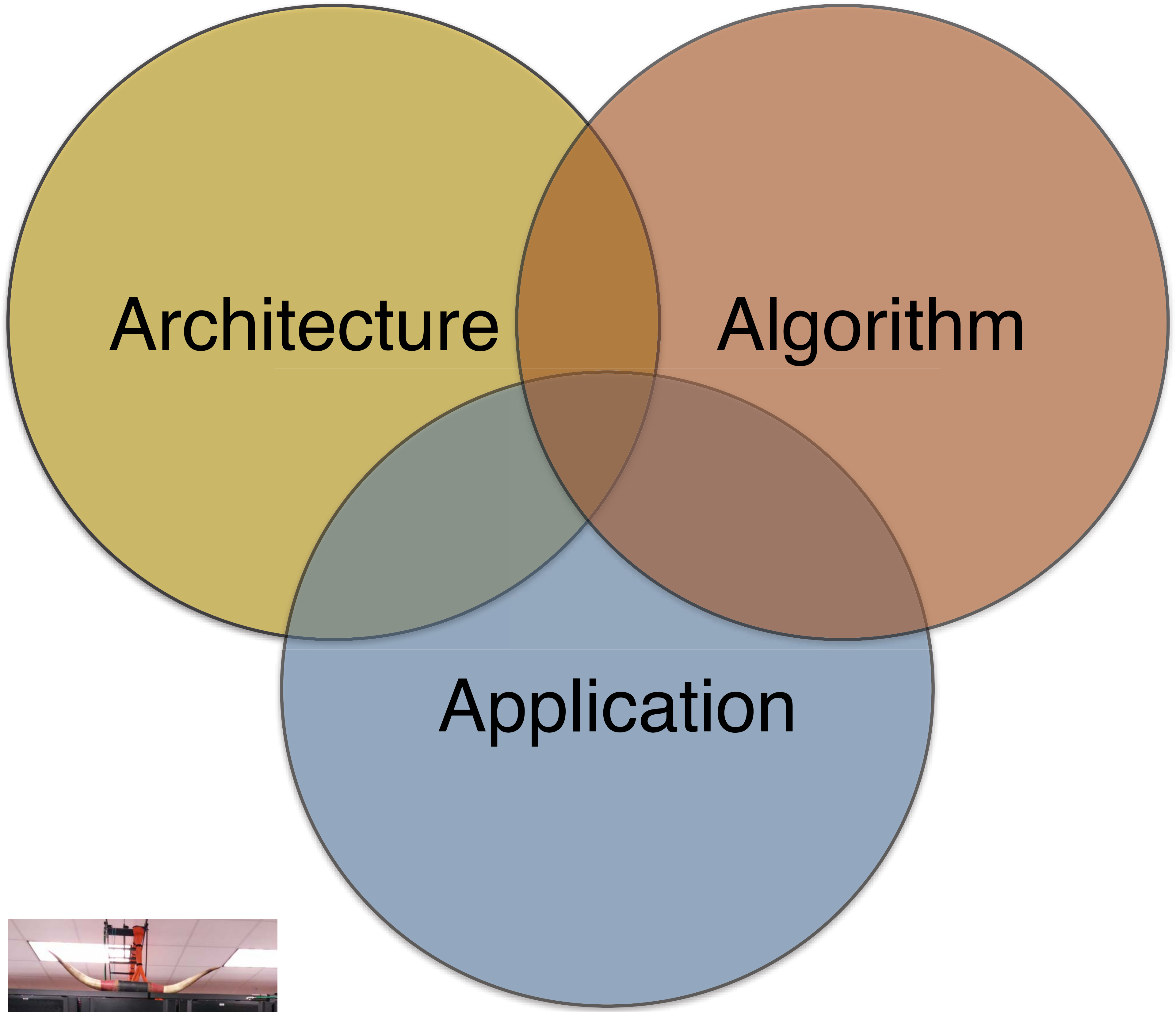
Gauge Generation — Measurement — Fitting — Physics Result

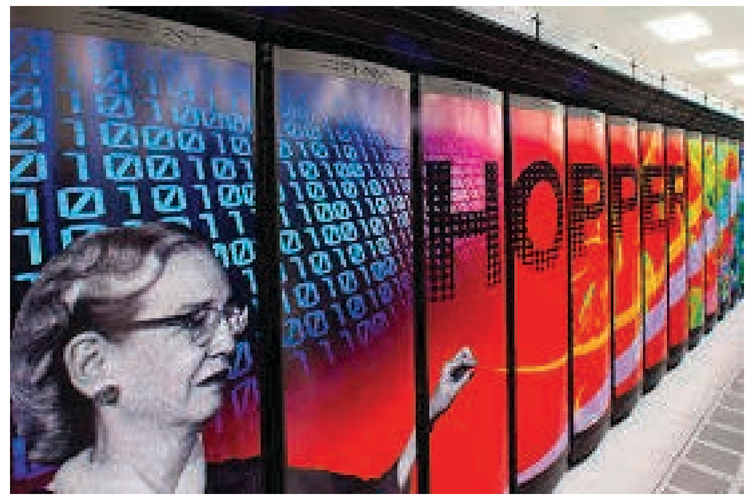
- Gauge Generation: Few independent chains. Strong scaling challenge
  - carried out on leadership computing facilities
- Measurement: Propagator Calculations & Correlation Function Construction (Contractions)
  - Many independent solves, Throughput challenge
  - most cost effective in Capacity mode & on midrange systems (NERSC, USQCD Hardware Project)
  - also on LCFs (through ALCC awards) for high impact, time critical calculations

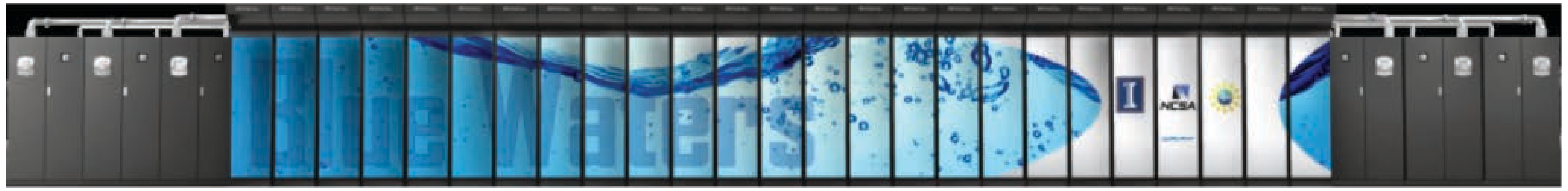
All Phases Require Improved Algorithms and Adaptation to new Architectures!!!

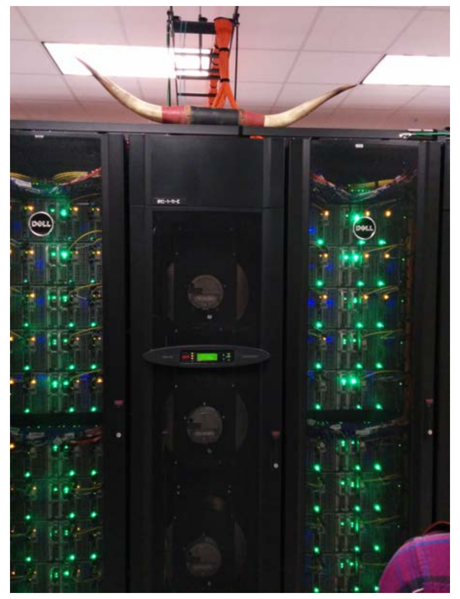
Retrospective





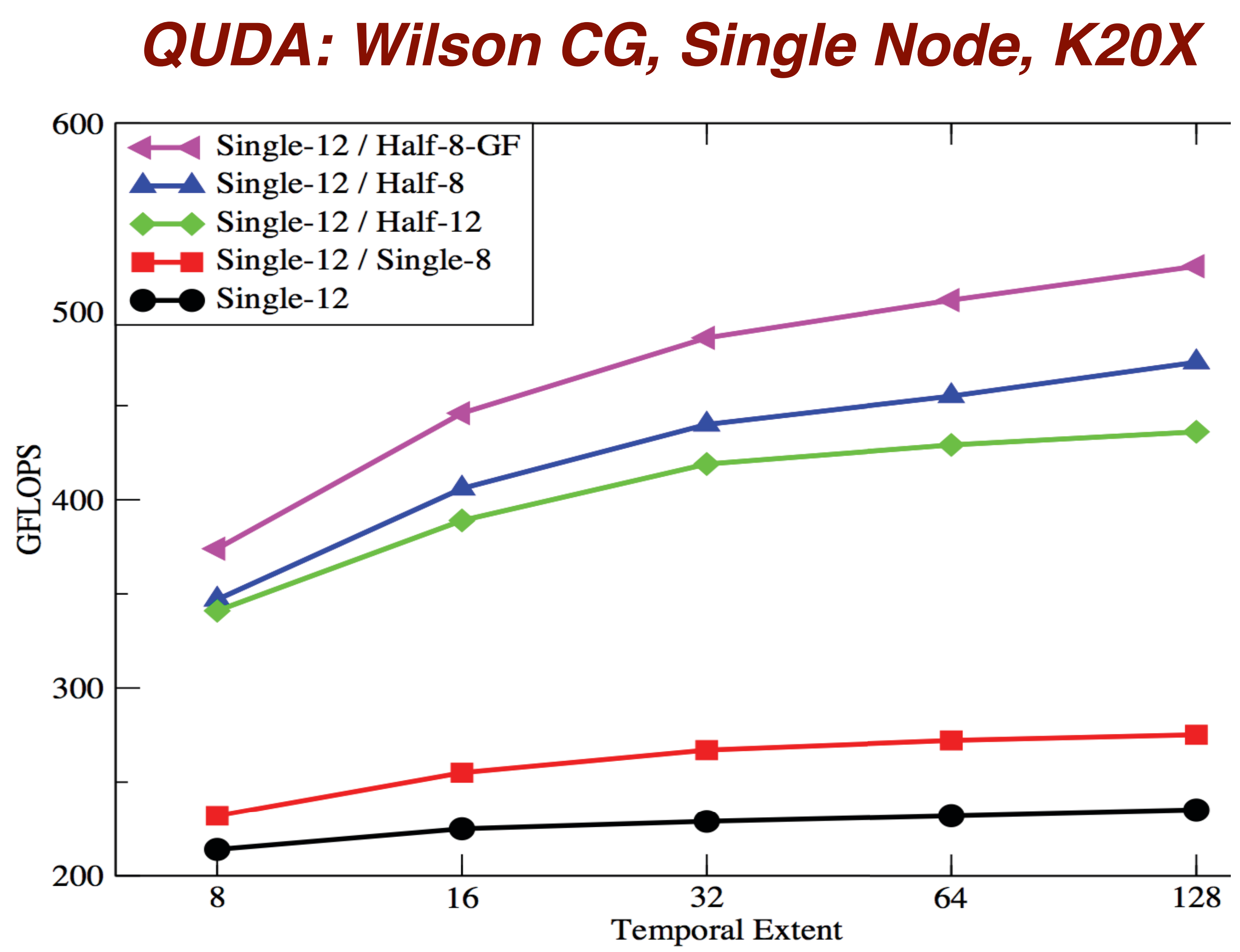


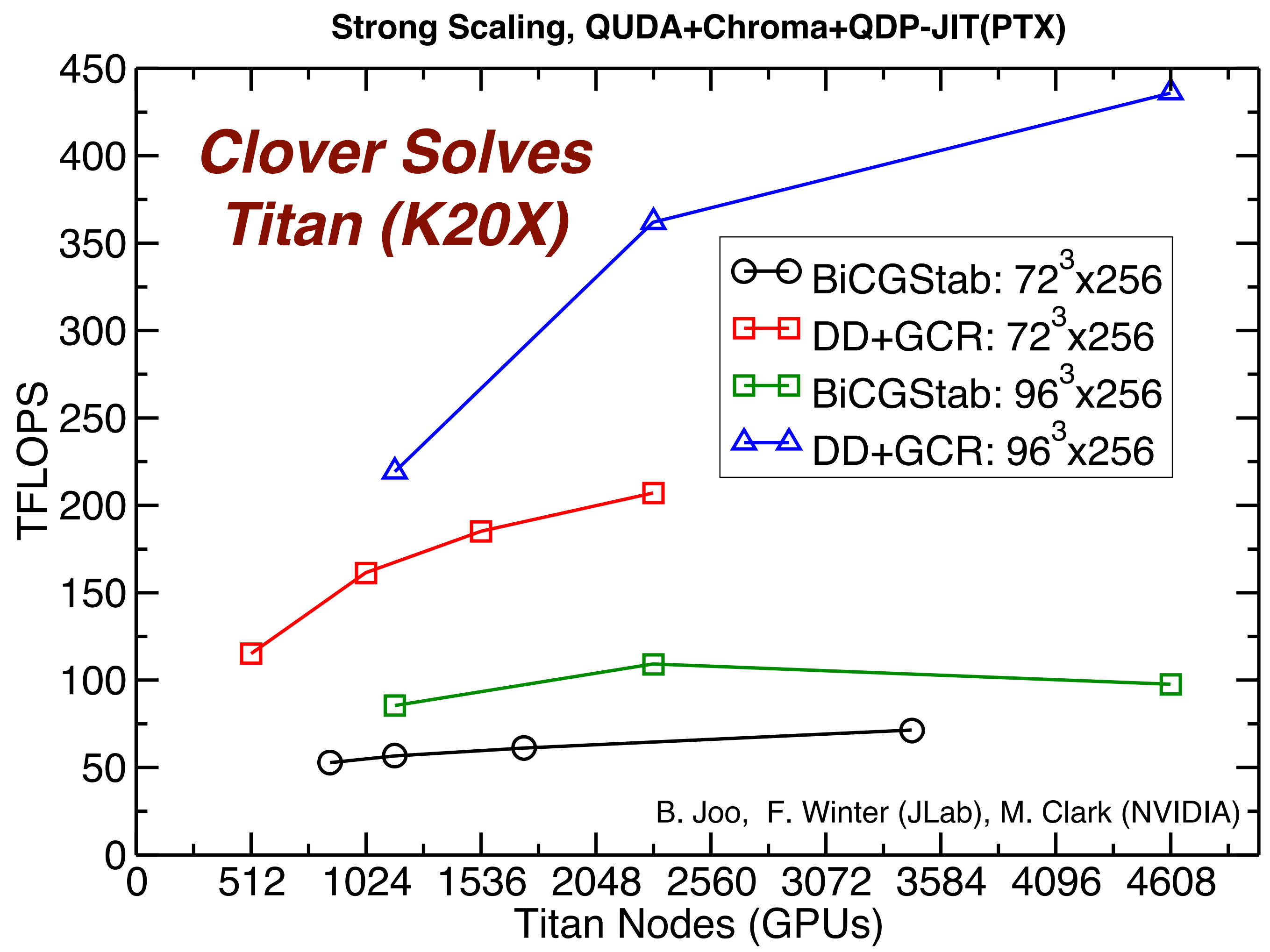


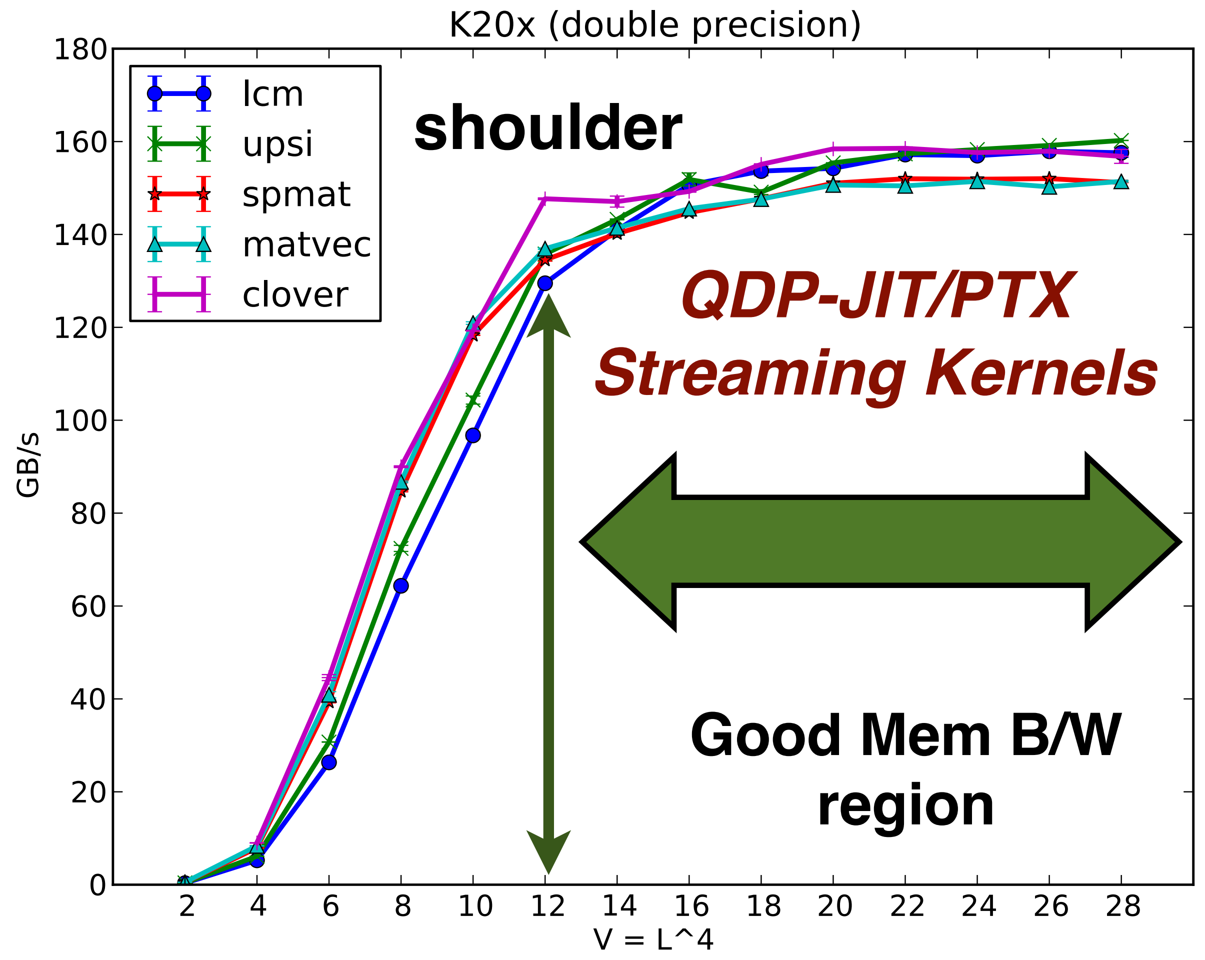


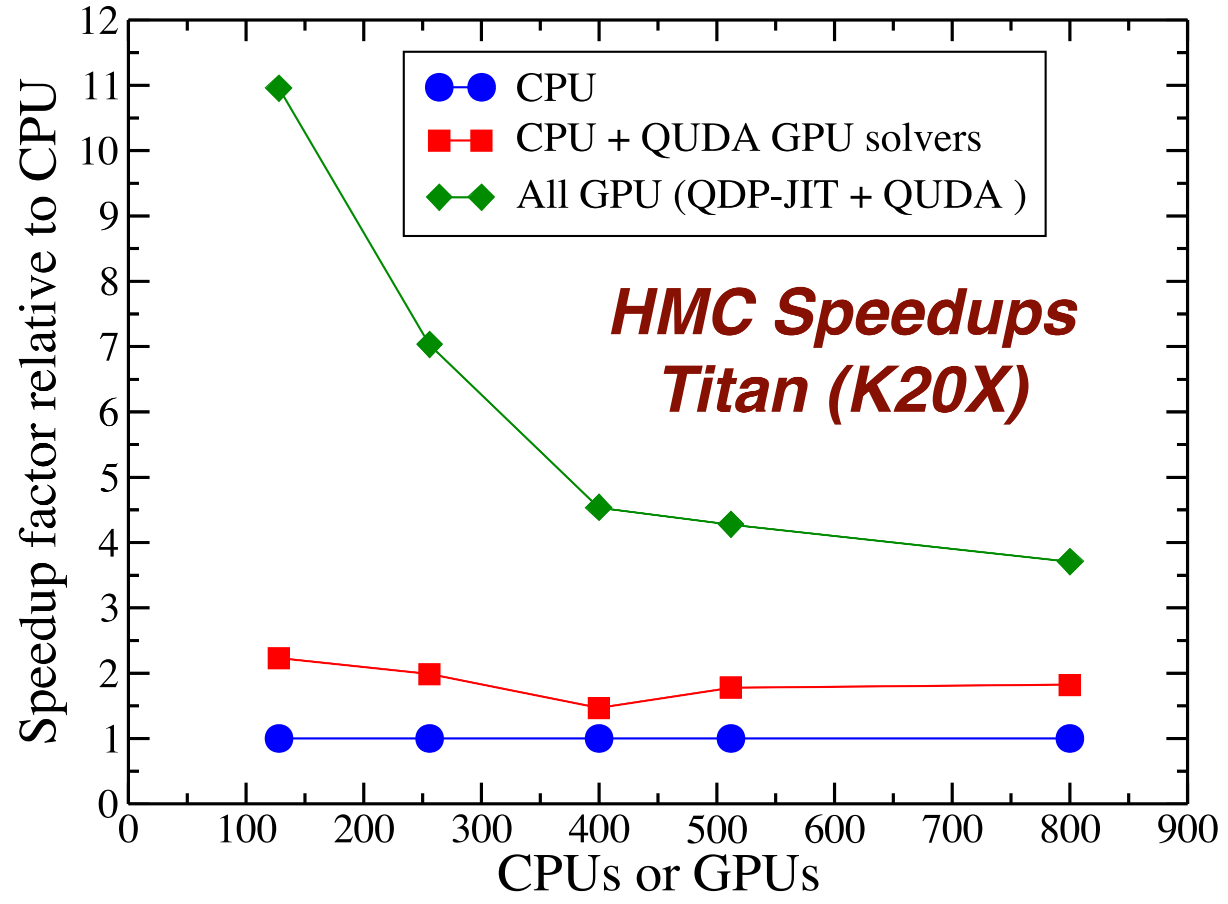
Architectures: GPU

- High performance GPU solvers: QUDA library
  - Maximize memory performance
    - data layout for maximising bandwidth
    - compression/mixed precision
  - Domain Decomposed preconditioners (SC'11)
  - Multi-Grid Implementations are ongoing
  - Strong collaboration with HEP project & NVIDIA
- Fight Amdahl's Law: move more of the application to the GPU
  - Re-developed QDP++ layer of Chroma to generate PTX code for GPUs at run-time: QDP-JIT/PTX (IPDPS'14)
  - Allowed porting all of Chroma to GPUs.
  - Allowed effective use of Titan (& NCSA Blue Waters)
- Transitioning QDP-JIT to use LLVM, to target also CPU based systems (BlueGene/Q, x86, KNL)





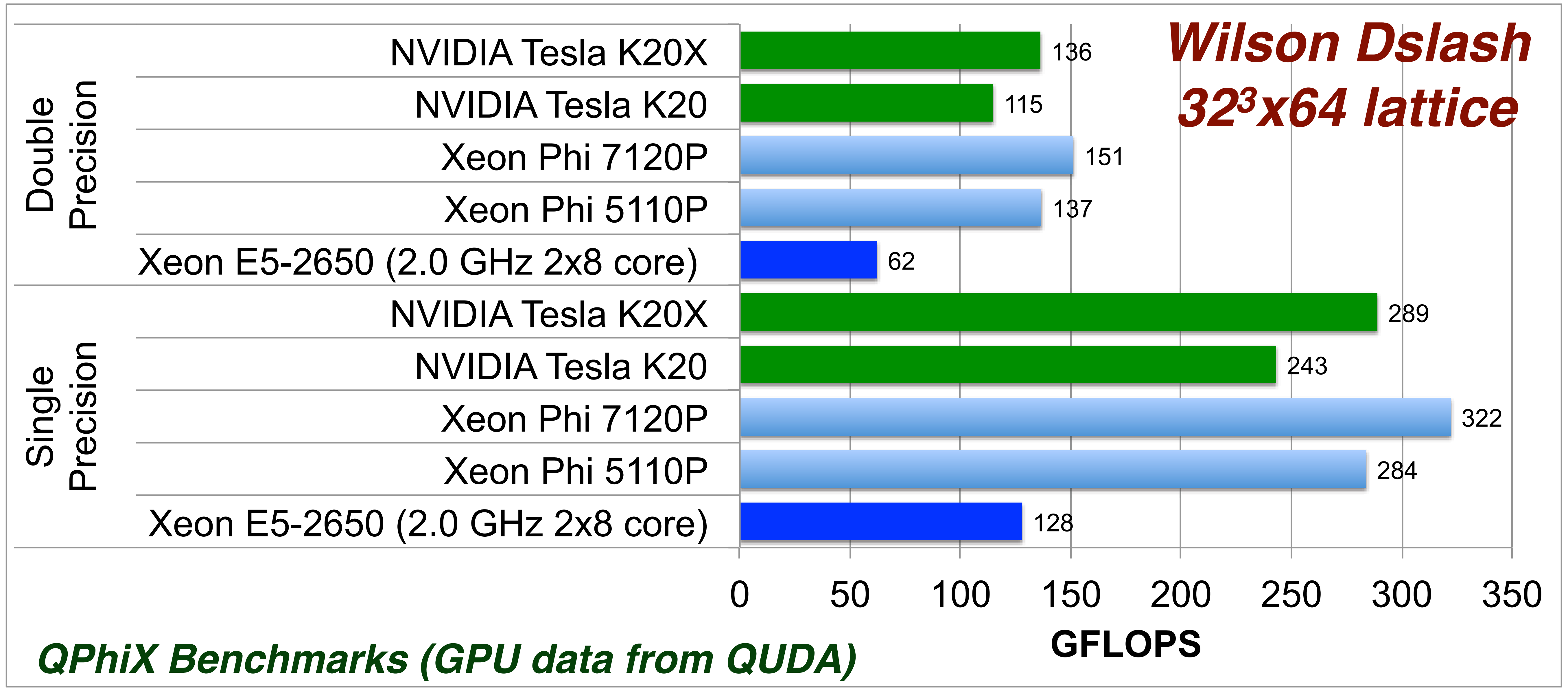


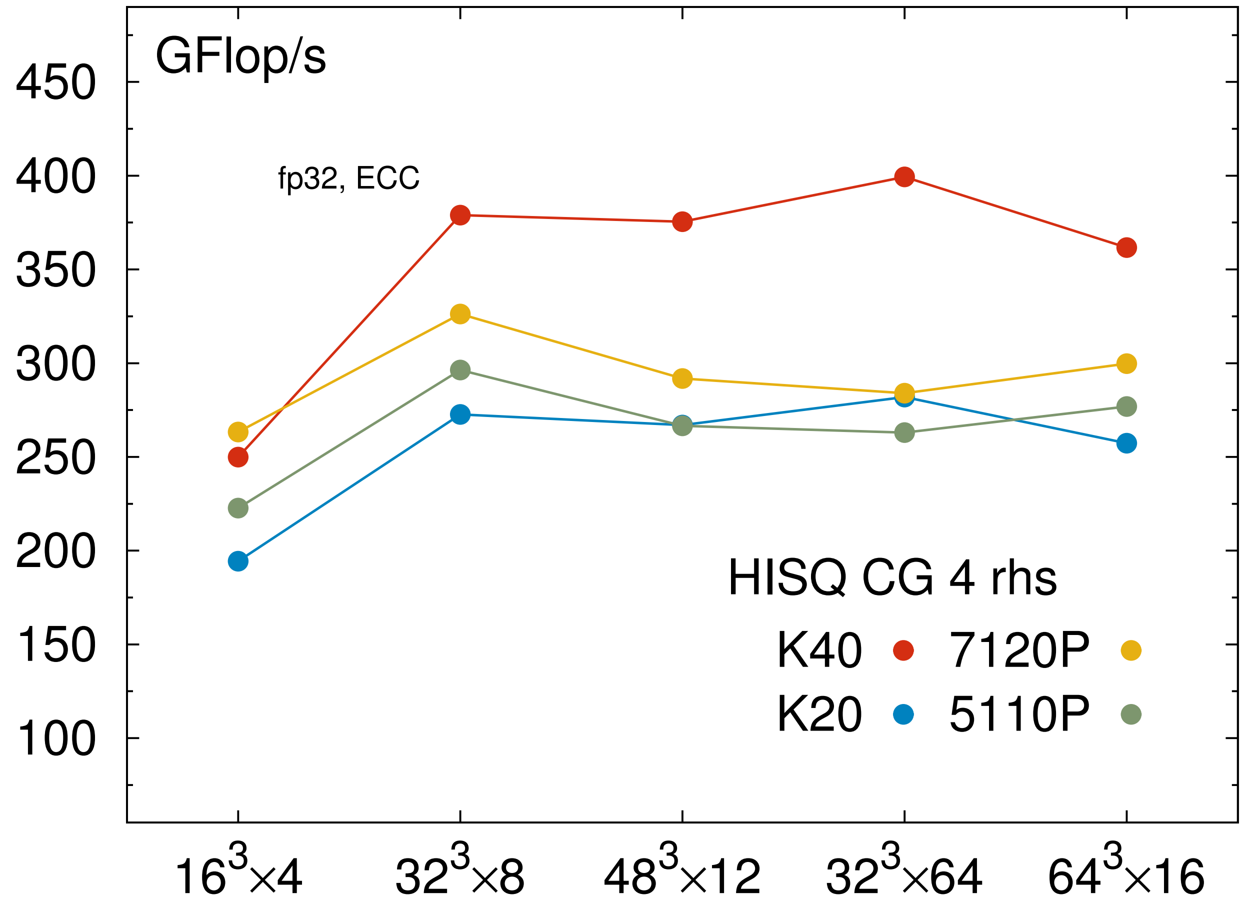


USQCD

Architectures: Xeon Phi & Xeon

- Very Successful Collaboration with Intel Parallel Computing Labs
  - Papers at: SC'11, ISC'13, IPDPS'14
  - Regensburg University & Intel: SC'14
- QPhiX library & code-generator (open source)
  - AVX & KNC for Wilson & Clover fermions
  - BlueGene/Q QPX intrinsics: SUPER Institute
  - HiSQ fermions (S. Gottlieb, R. Li) - HEP project
- Participation in Intel Xeon Phi Users Group
- Other Xeon Phi Efforts
  - RBC-UKQCD, BAGEL code generator
  - BNL HiSQ solver for Xeon Phi & GPU
- NESAP Participation in preparation for Cori:
  - 2 Full (Chroma, BNL) + 1 Affiliated projects (QLua)





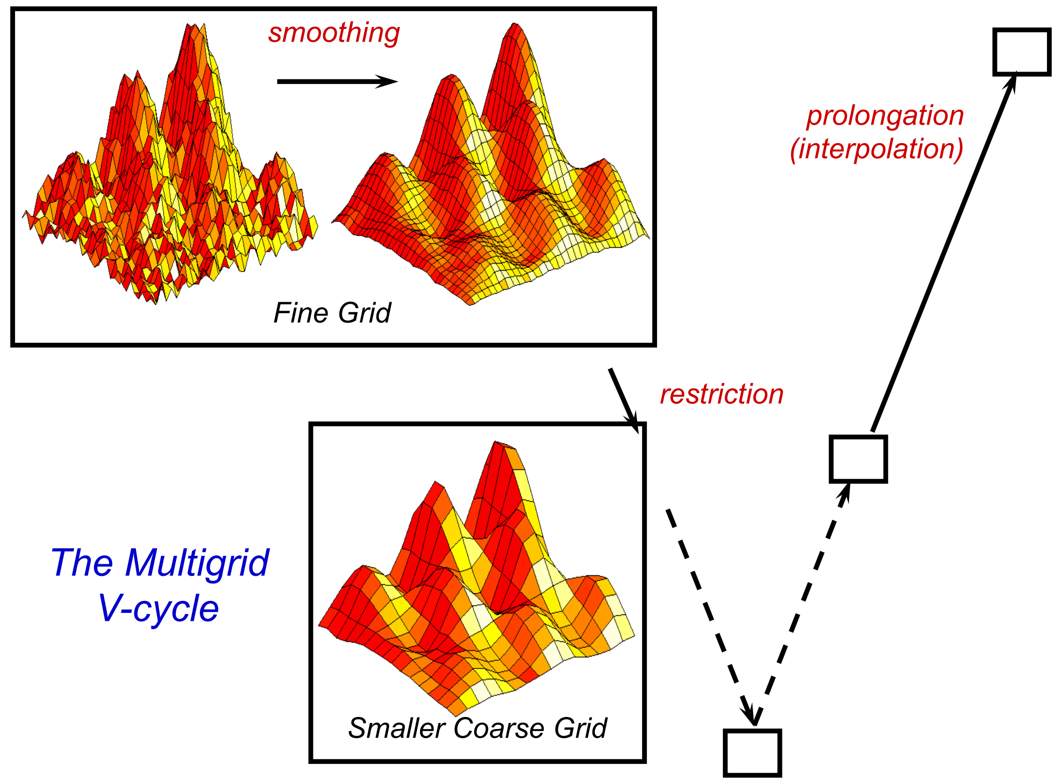
Top: QPhiX Benchmarks. Based on Joo et. al. "Lattice QCD on Intel(R) Xeon Phi(tm) coprocessors", ISC'13 LNCS 7905, 40-54, 2013

Left: Kaczmarek et. al. "Conjugate Gradient solvers on Intel Xeon Phi and NVIDIA GPUs", Presented at "GPU Computing in High Energy Physics", Pisa, arxiv:1411.4439[physics.comp-ph]

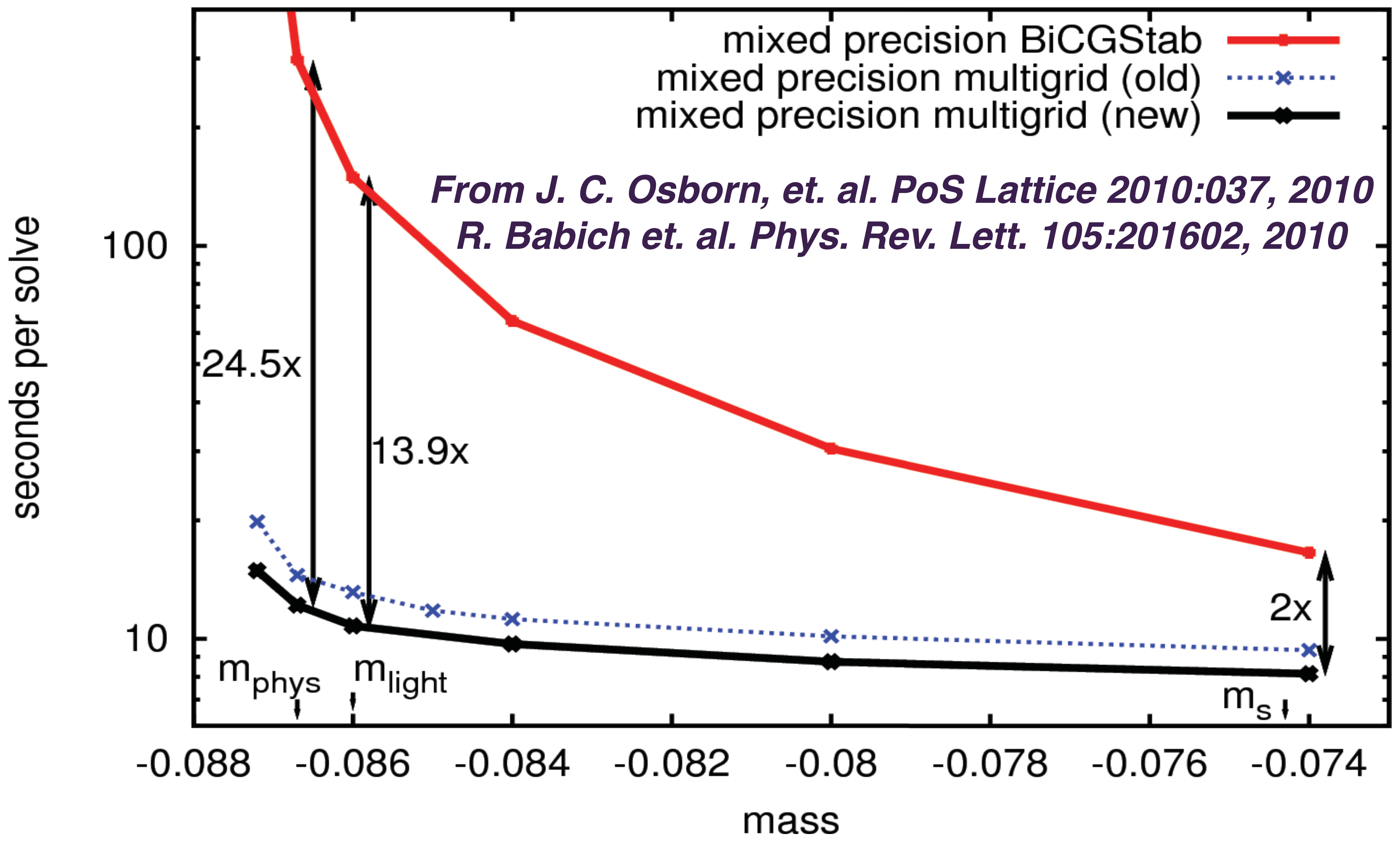
Algorithms: Multi-Grid

- Adaptive Aggregation Algebraic Multi-Grid
  - Method Developed in collaboration with Applied Mathematicians, HEP-USQCD SciDAC project, and NSF funding.
  - CPU Implementation available through QOPQDP library
  - Provides over an order of magnitude improvement over BiCGStab at light quark masses
- Focus of collaboration with FASTMath
  - Extension of HYPRE to allow QCD implementations
  - Integration with QLua package to facilitate algorithmic development
- Current production use:
  - Measurement: spectroscopy calculations with light quarks on CPU based systems
- Ongoing and Future projects
  - Use in Gauge Generation
  - Other Fermion Formulations (DWF, Staggered) in HEP project
  - Need architecture aware implementations for GPUs, Xeon Phi

Image from: http://computation.llnl.gov/casc/sc2001_fliers/SLS/SLS01.html Credit: LLNL, CASC



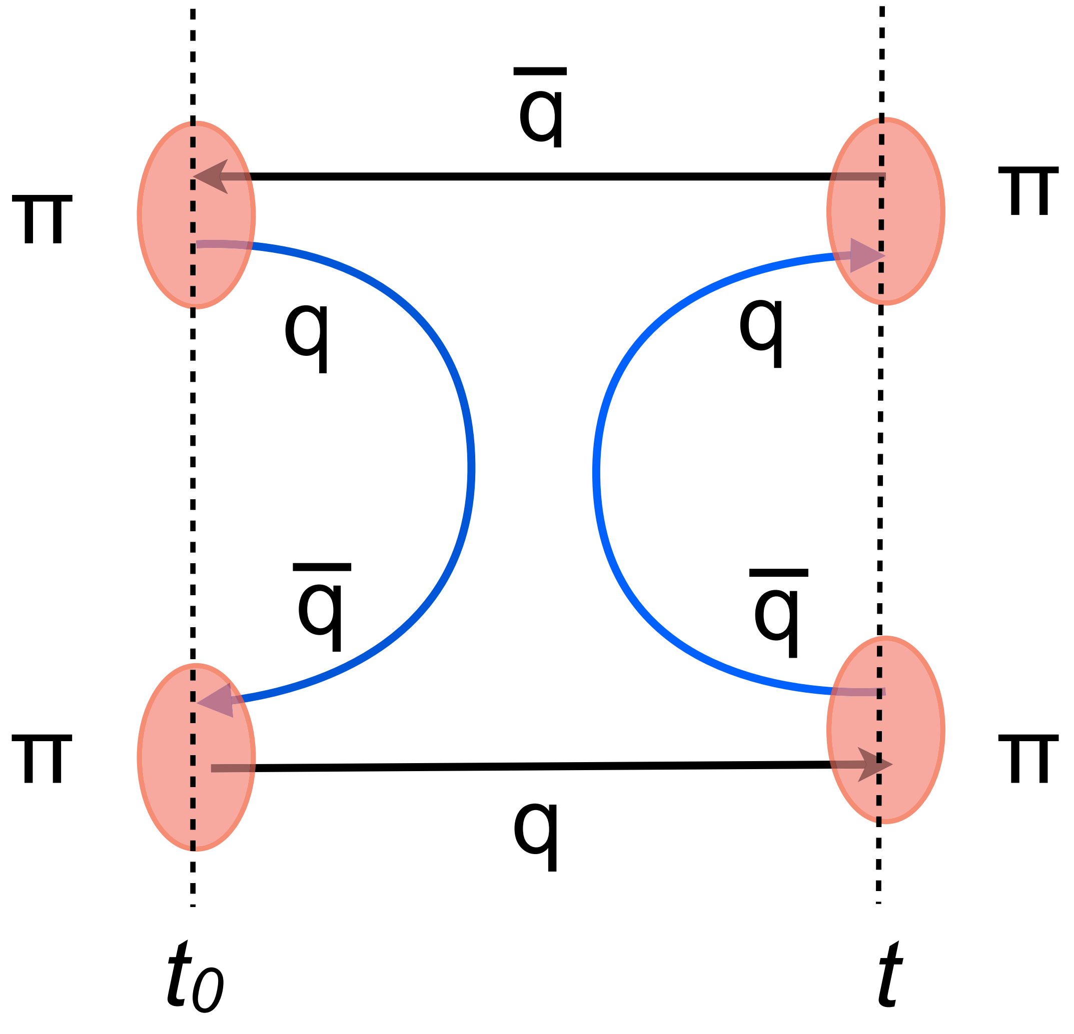
32^3x256 aniso clover on 1024 BG/P cores

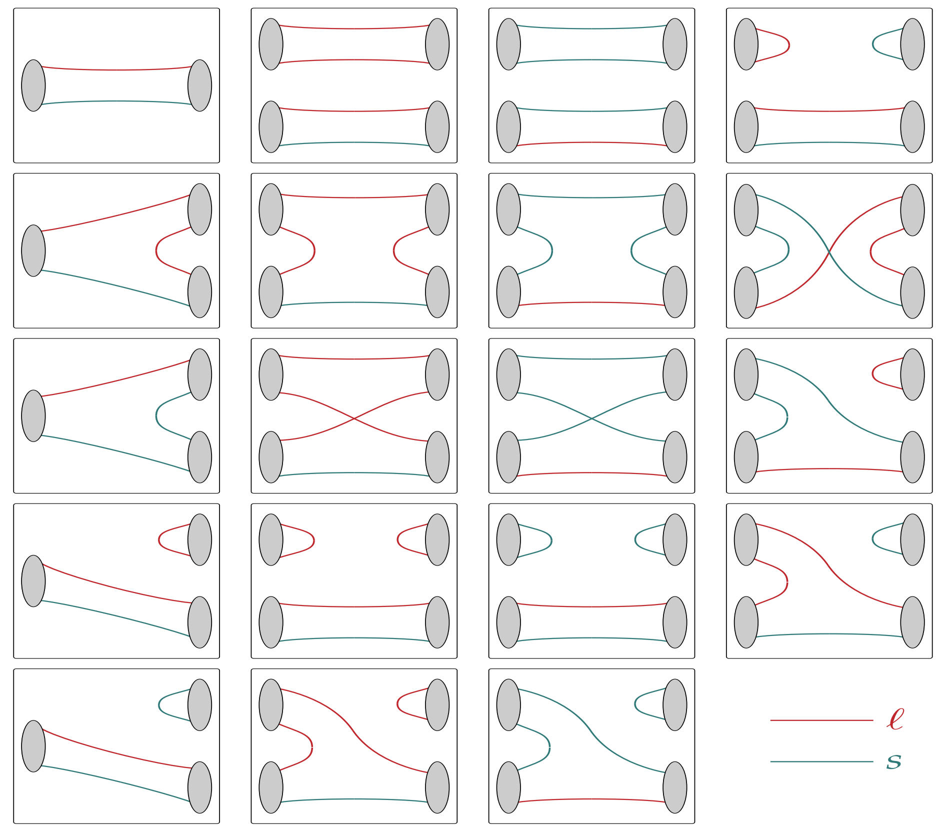


USQCD

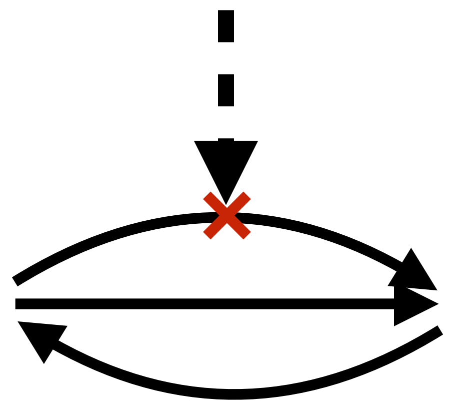
Algorithms for Measurements

- Distillation
  - A way of constructing quark line graphs for multi-particle, scattering systems, currently used in spectroscopy calculations.
  - Implement 'smearing' to enhance low energy states
  - O(10,000) graphs, O(100K-1M) propagator solves per config
  - Need to orchestrate graph evaluation, propagator reuse
    - D. J. Wilson et. al. "Resonances in Coupled πK, ηK scattering from lattice QCD", Phys. Rev. D91, 054008 (2015)
  - To Do: Baryons, and application to hadron structure
- Hierarchical Probing
  - Used in current hadron structure calculations (see later)
  - disconnected contribution has annihilation from current insertion - all frequency modes are allowed - very noisy
  - Variance reduction methods are crucial to resolve signal.
  - Partnership with CS & Applied Maths at College of William and Mary
    - A. Stathopoulos, J. Laeuchli, and K. Orginos, "Hierarchical probing for estimating the trace of the matrix inverse on toroidal lattices" SIAM J. Sci. Comput., 35(5), (2013), S299-S322

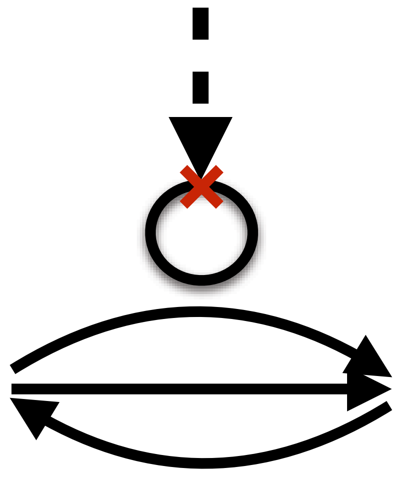




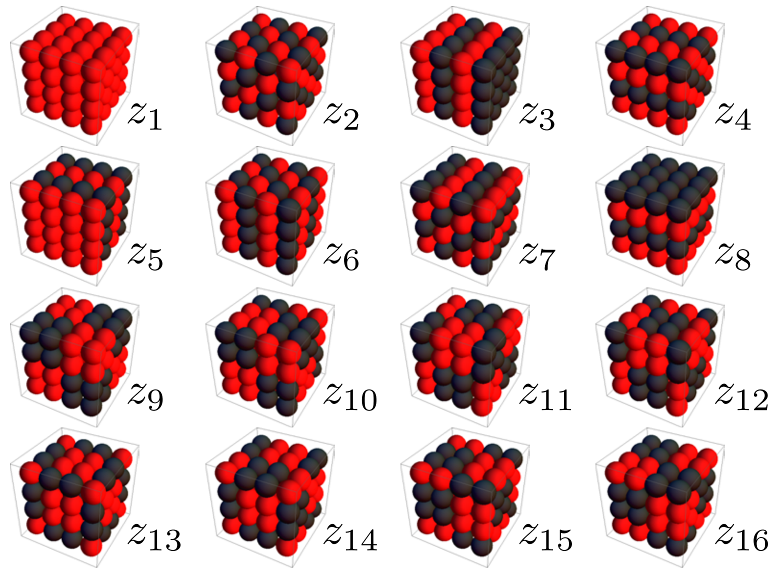
PRD 91, 054008 (2015)



Connected Insertion



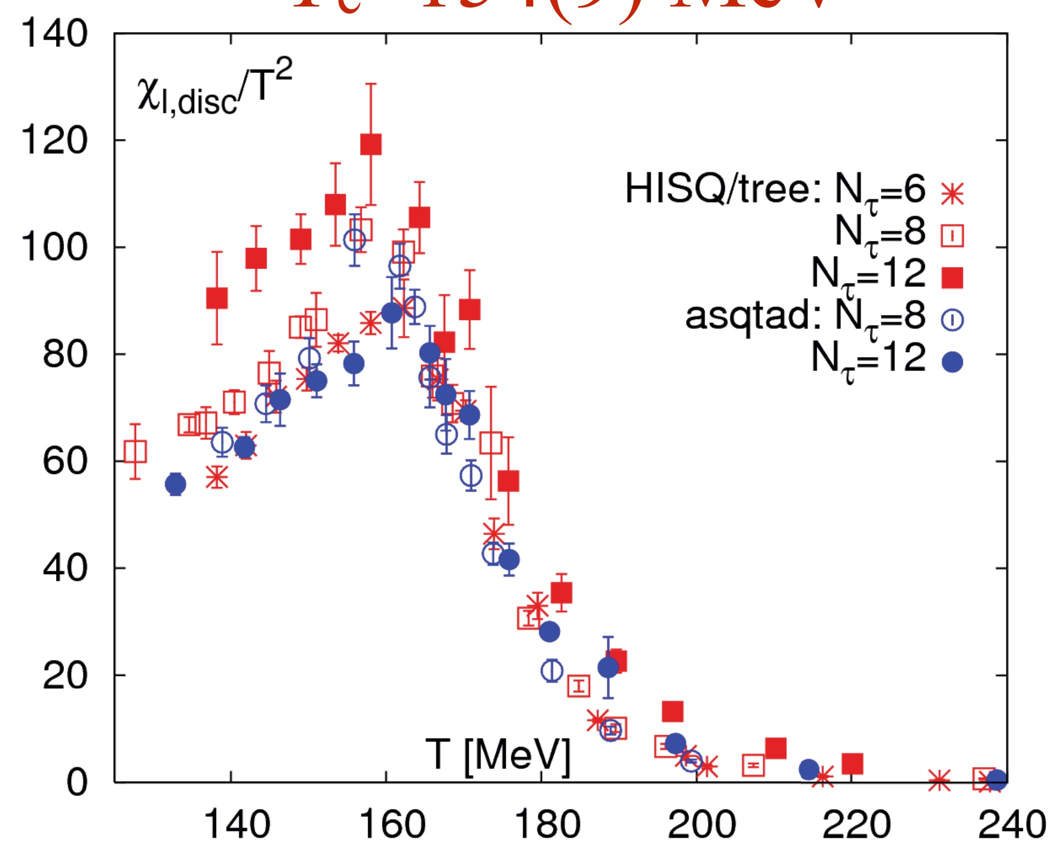
Disconnected Insertion



First 16 Hadamard vectors for hierarchical probing on a 4^3 lattice

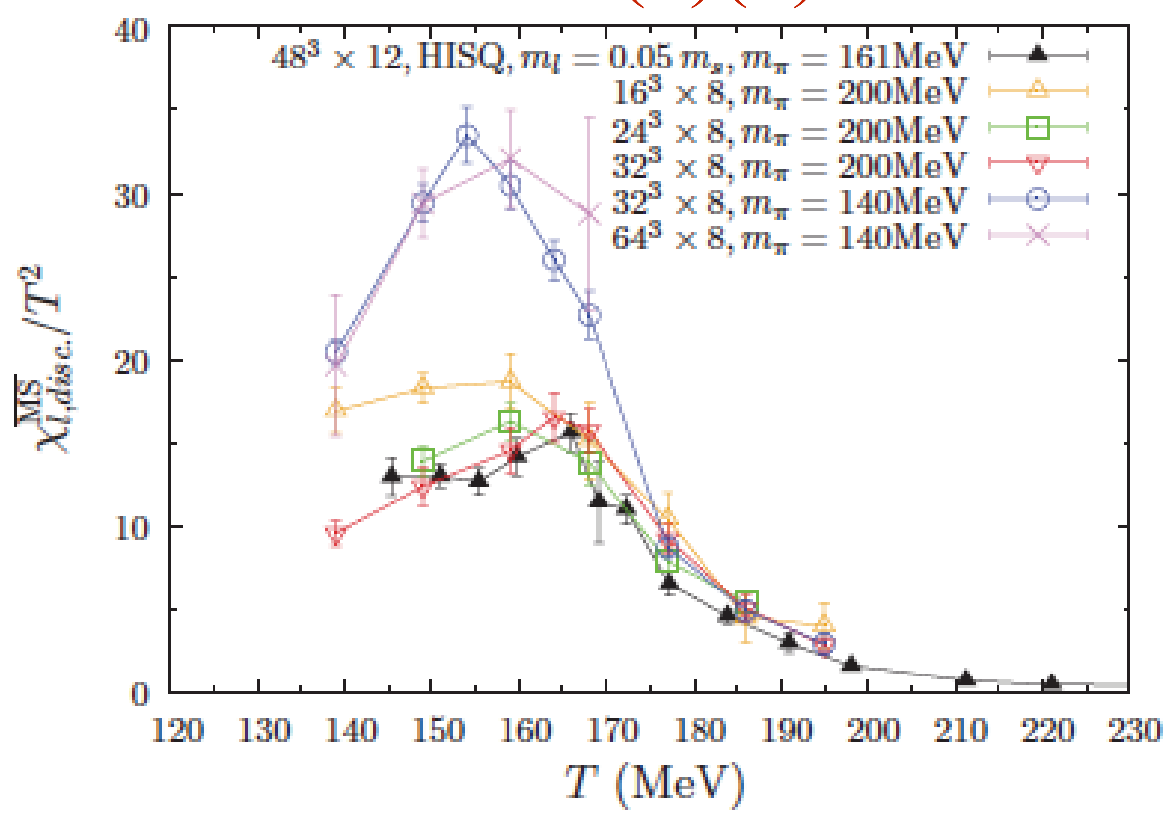
Matter Under Extreme Conditions

T_c=154(9) MeV



A. Bazavov et al. (hotQCD), "The chiral and deconfining aspects of the QCD transition" Phys. Rev. D85, 054503 (2012) (353 cit.)

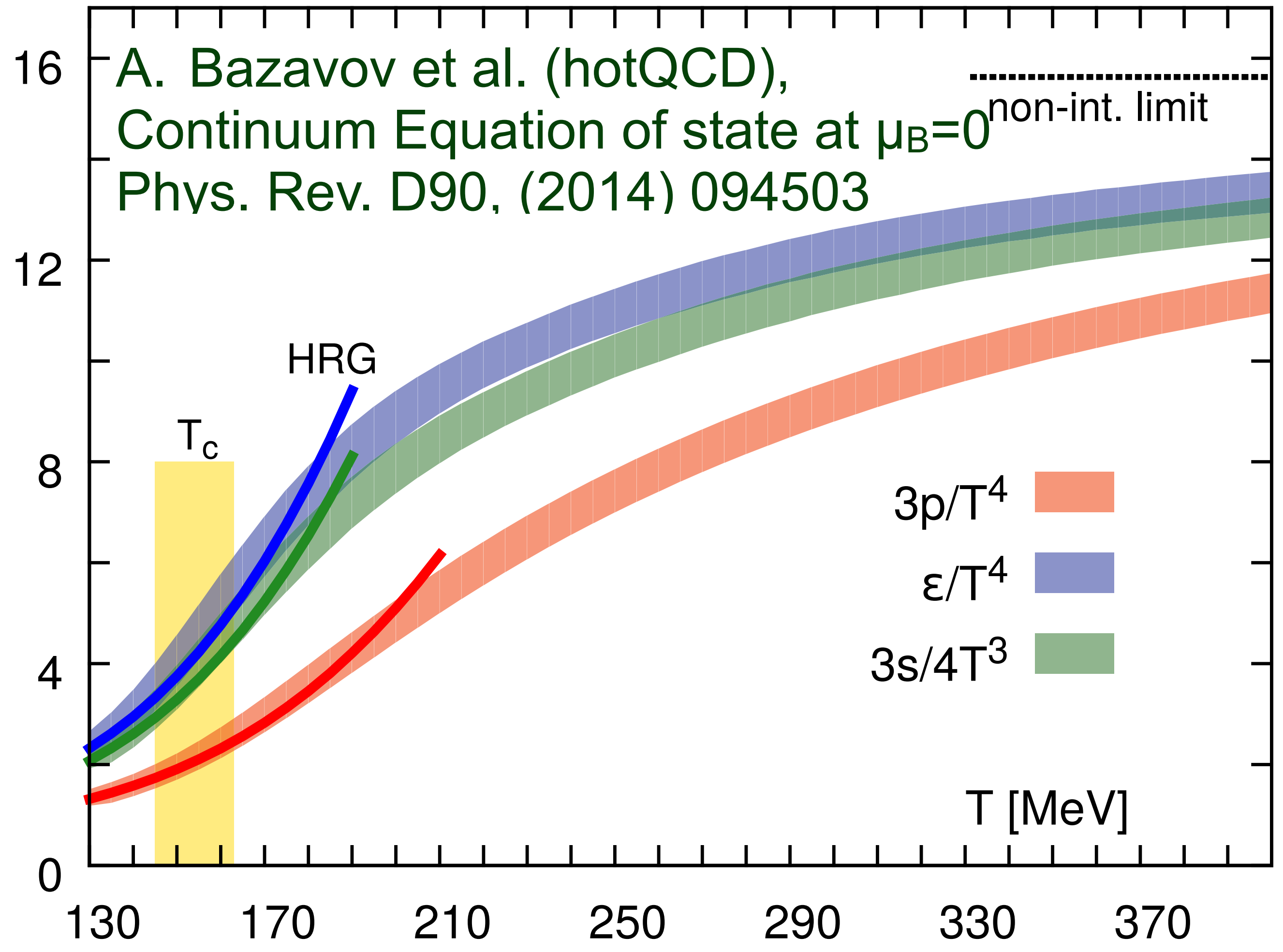
T_c=155(1)(8) MeV

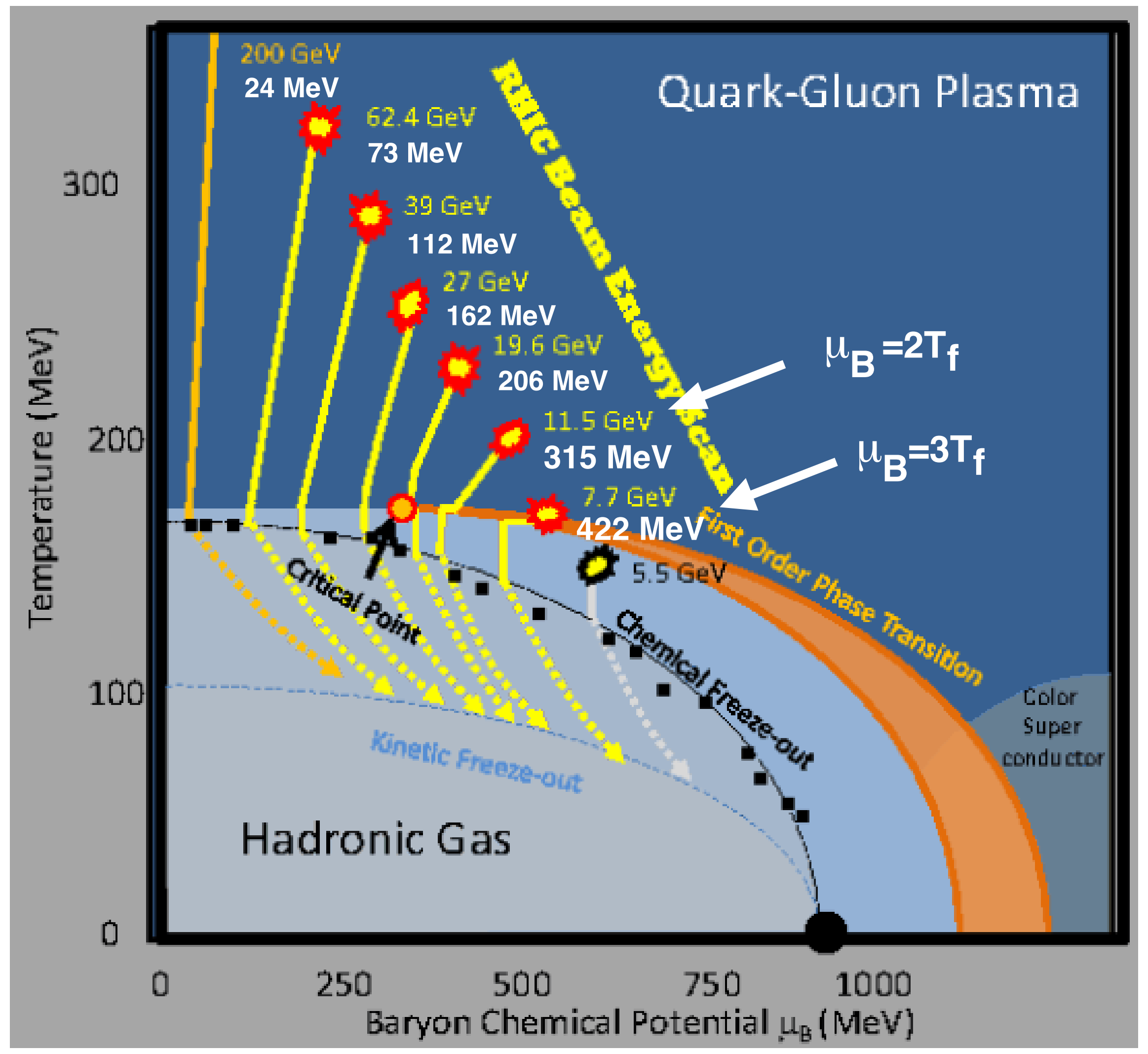


New calculation with chiral quarks

hotQCD Collaboration, Bhattacharya et al, PRL 113, 082001 (2014)

- Deconfinement Phase Transition established
  - T_c=154(9) MeV with HiSQ
  - T_c=155(1)(8) MeV with DWF
  - Good Agreement between formulations
- Continuum Equation of State (EoS) at μ_B=0 established
- Currently Working on EoS up to μ_B=2T
  - covers large range of parameter space probed by RHIC beam energy scan
- Future Goal: EoS up to μ_B=3T
  - aim to cover entire region of RHIC beam energy scan
  - Work to be carried out through 167M core hour Titan ALCC allocation (Mukherjee et. al.)



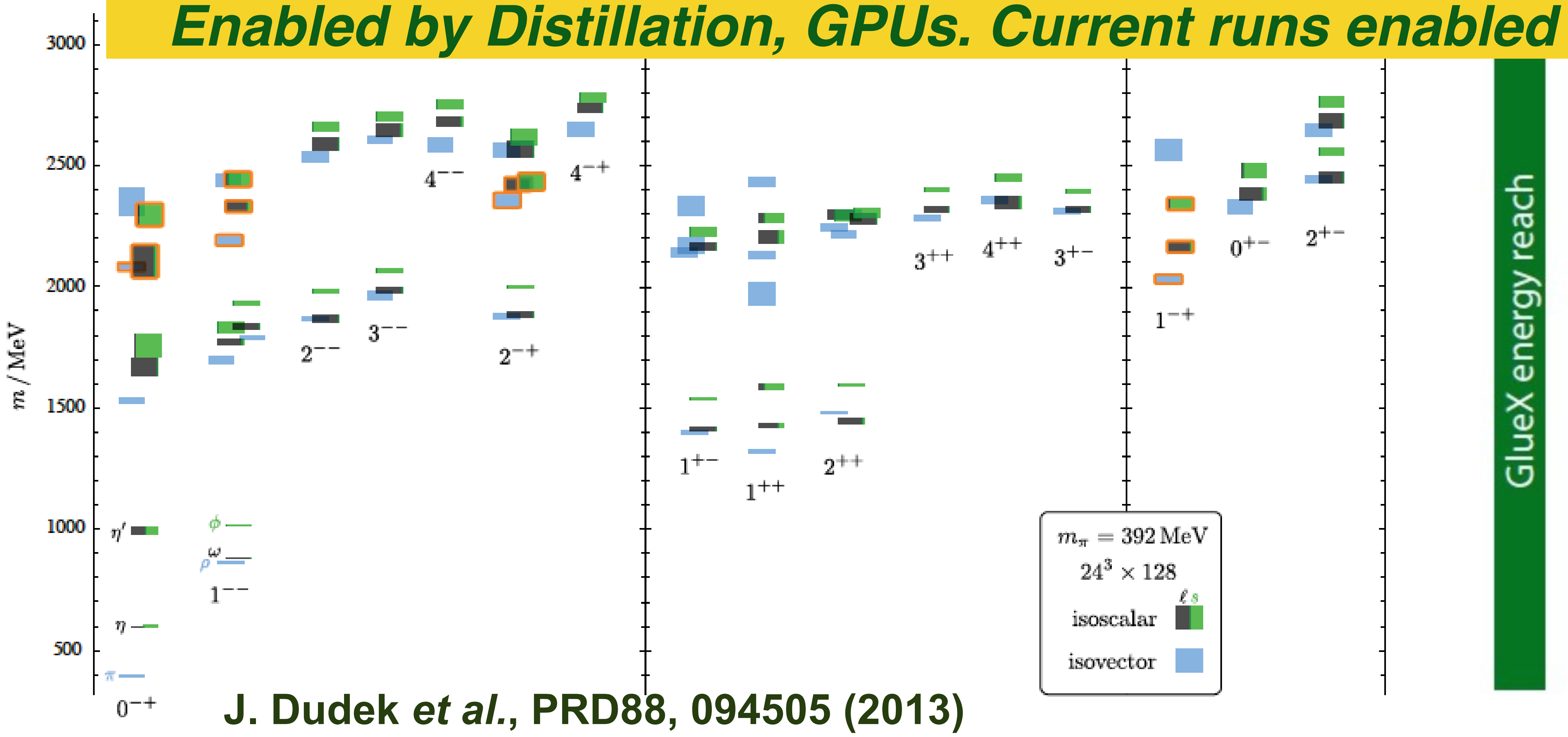


Hadrons, Nuclei and Nuclear Matter from QCD

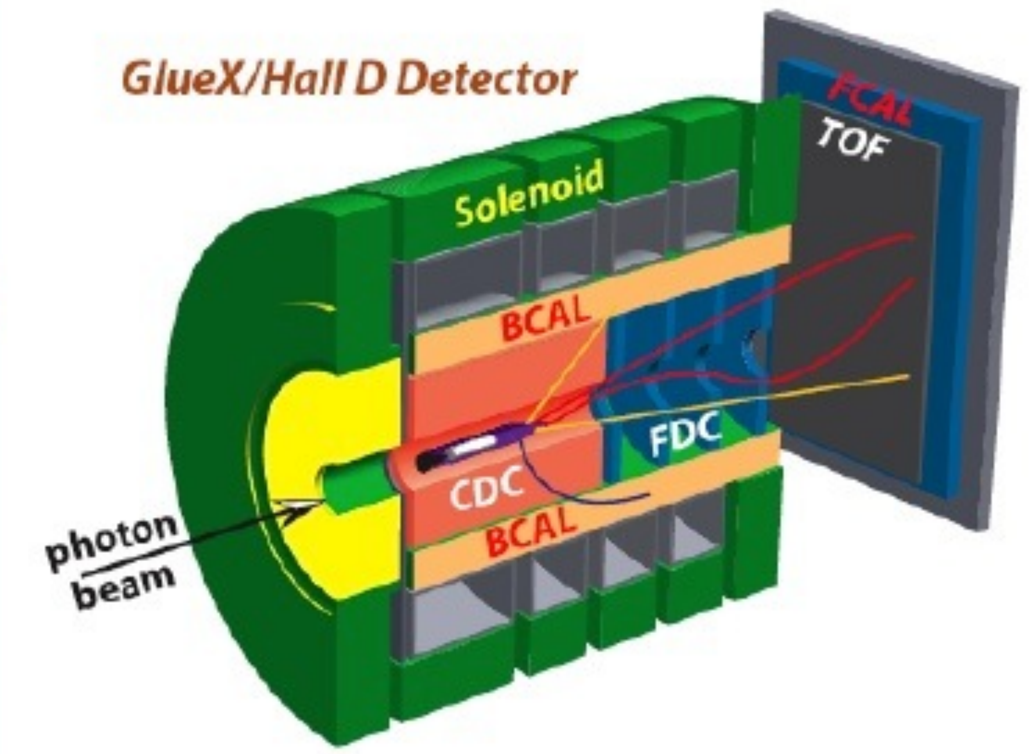
USQCD

Spectroscopy

Enabled by Distillation, GPUs. Current runs enabled by Multigrid

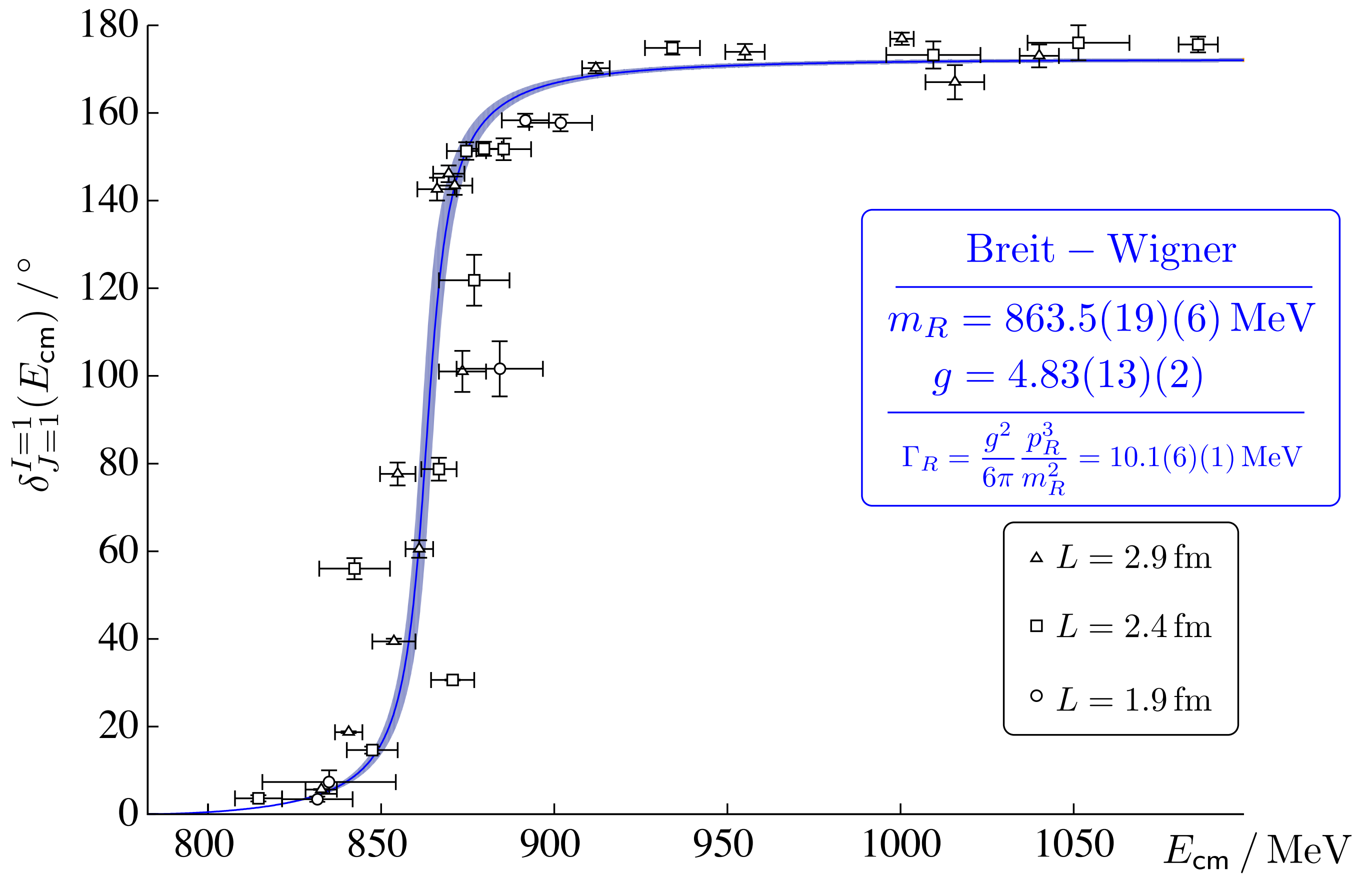


J. Dudek *et al.*, PRD88, 094505 (2013)



Report to NSAC: *Implementing the 2007 LRP*

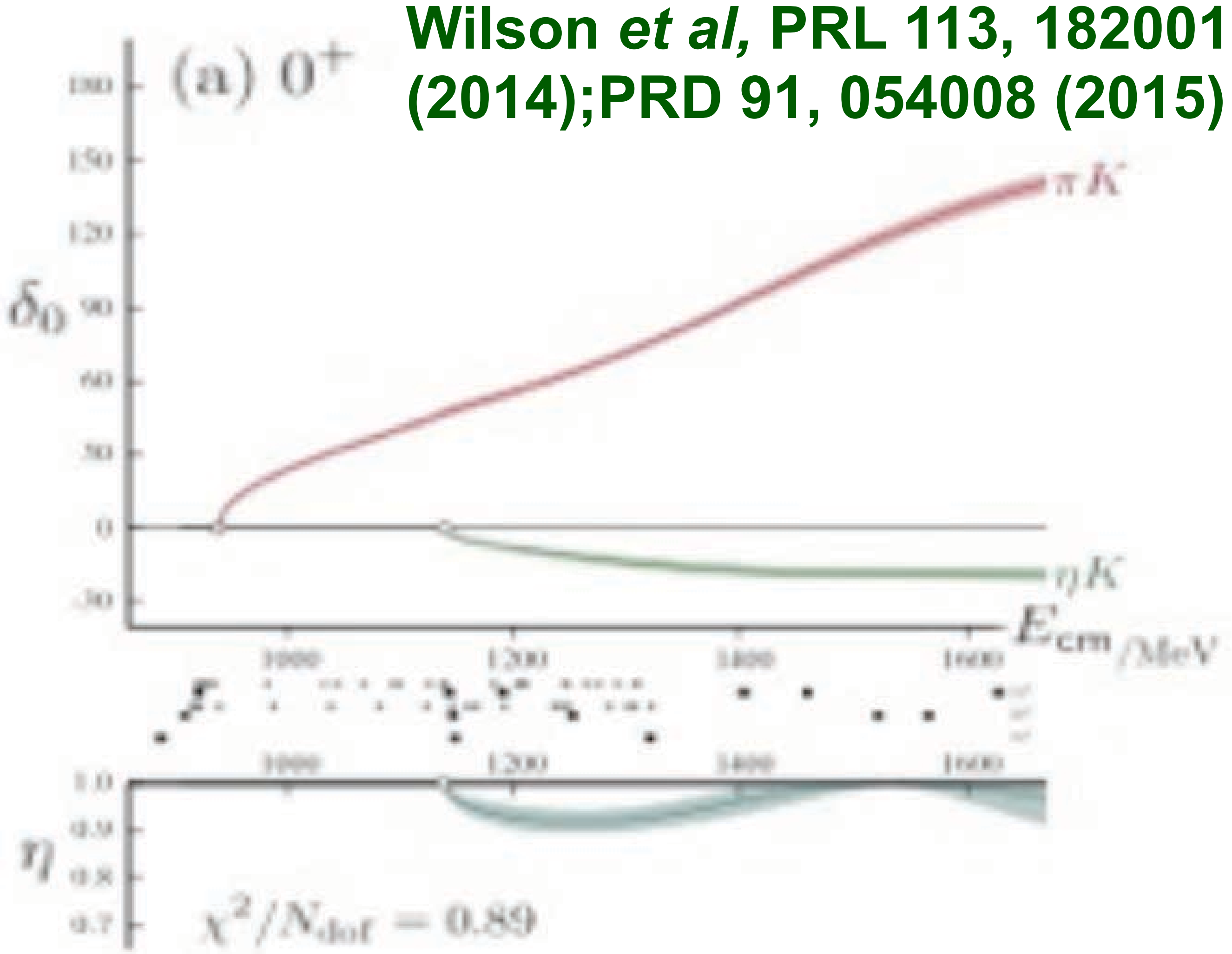
"A key part of the 12-GeV physics program at Jefferson Lab is the ability to produce these exotic hybrid mesons using photon beams, which is expected to generate unprecedented numbers of these particles. The GlueX experiment in the new Hall-D is poised to carry out this program using a detector designed to tackle just this problem. *The GlueX experimental program is coupled with both detailed lattice QCD predictions and the strong support of the Jefferson Lab theory center in analyzing and interpreting the expected new data. This puts the U.S. in a unique position to explore this important new science made possible by the 12 GeV CEBAF Upgrade.... "*



Dudek *et al*, PRD 87, 034505 (2013)

- Top: Spectrum of Isoscalar and Isovector mesons
  - hybrids should be within energy reach of GlueX
  - Pattern of states replicated between isovector, isoscalar and hybrids suggestive of Chromomagnetic Excitation
- Left: Phase Shift in I=1 ρ→ππ scattering
- Right: Scattering amplitudes in inelastic (pK, eK)
  - High fidelity comparison with experiment
  - First ever demonstration of coupled channel scattering directly from QCD

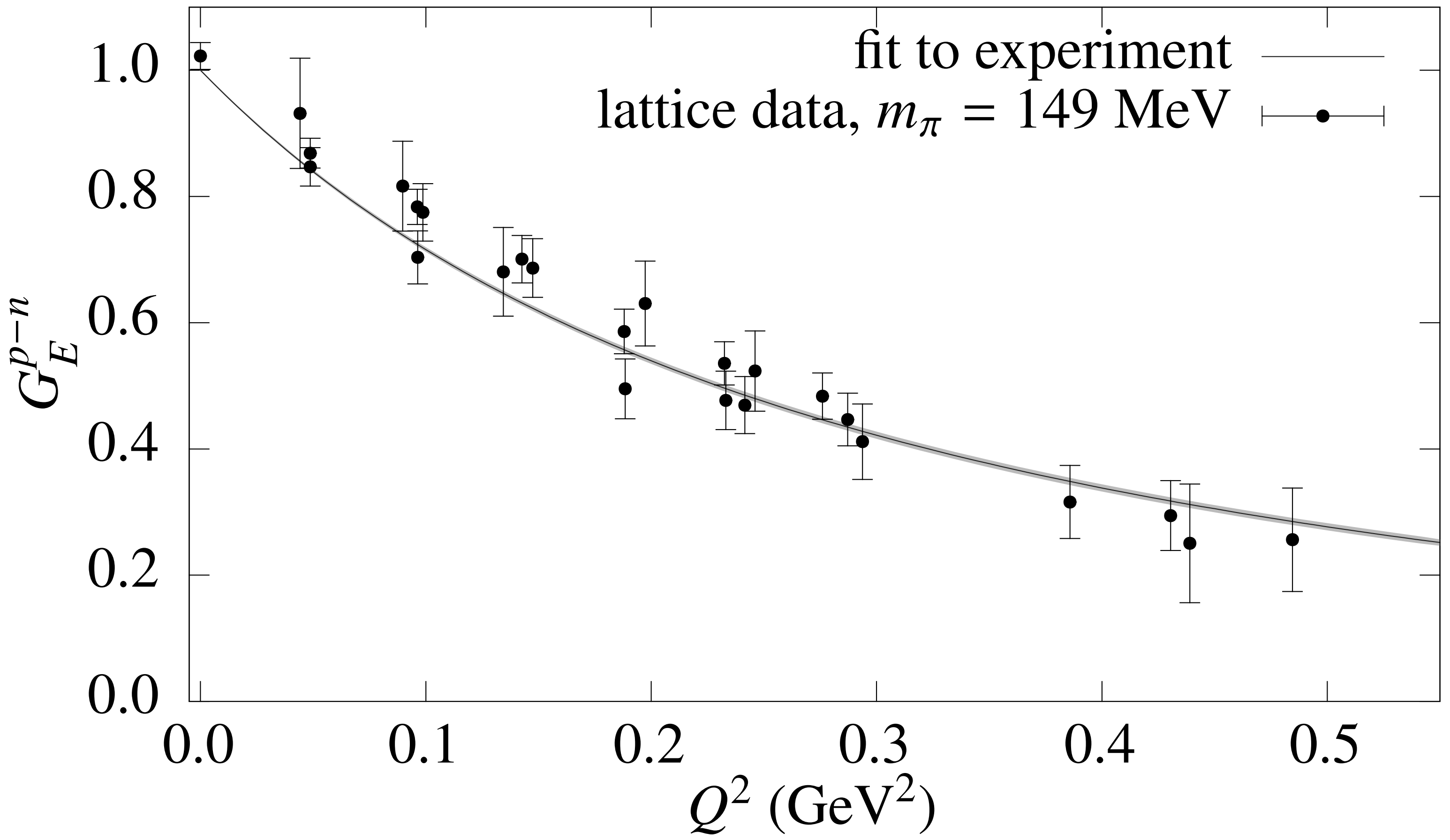
Wilson *et al*, PRL 113, 182001 (2014);PRD 91, 054008 (2015)



USQCD

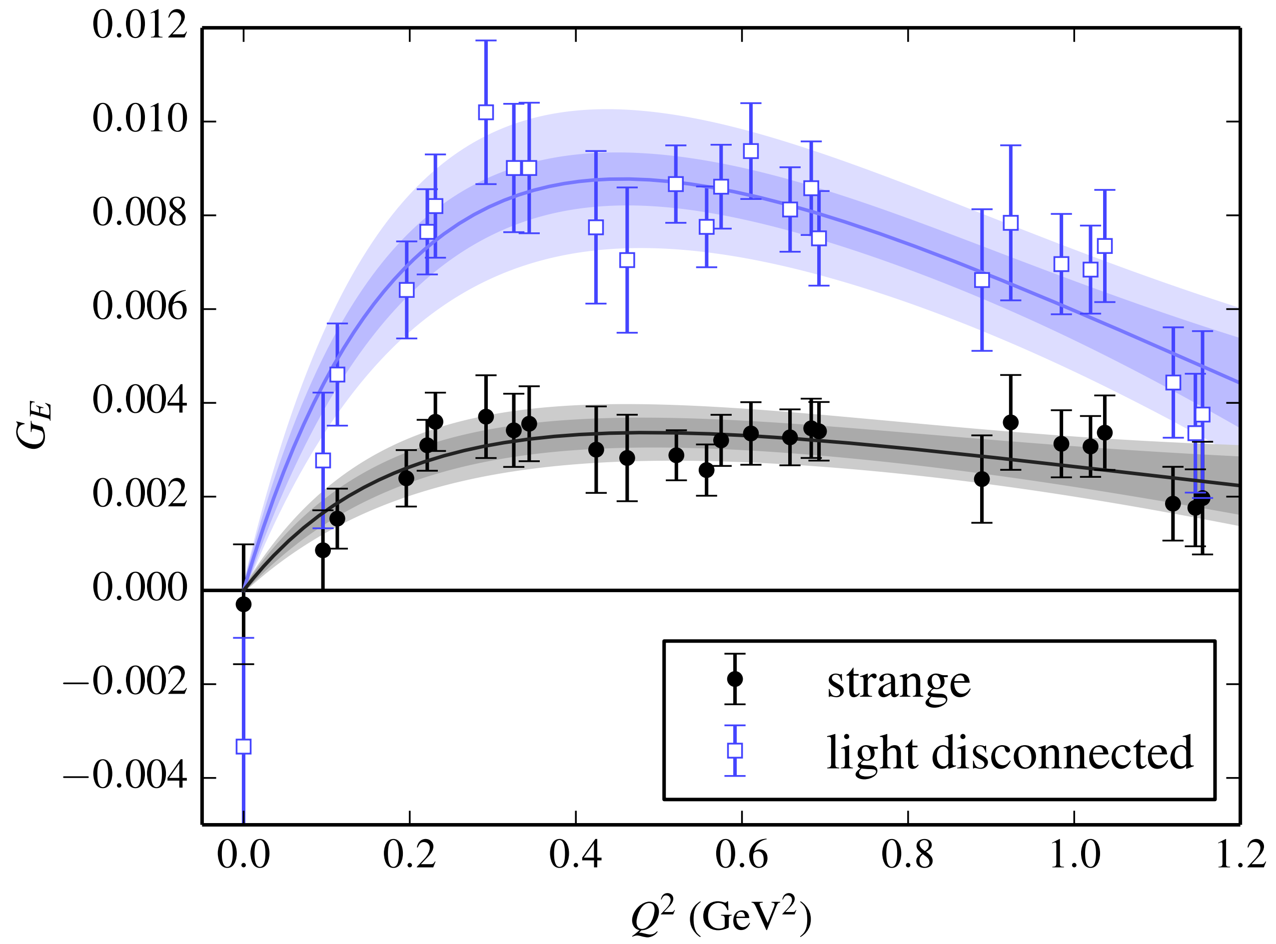
Hadron Structure

Electromagnetic Form Factor

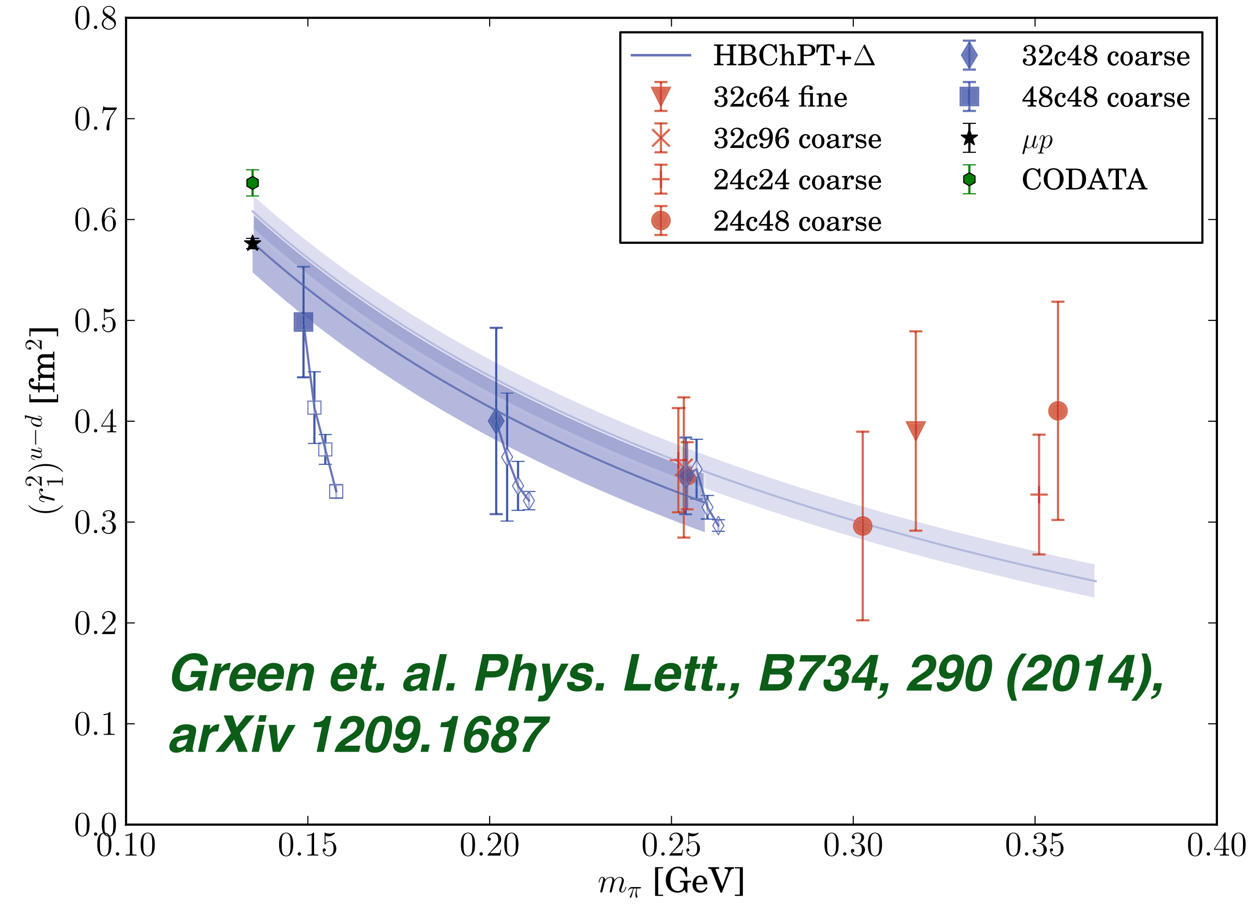


Using Lattices from BMW Collaboration

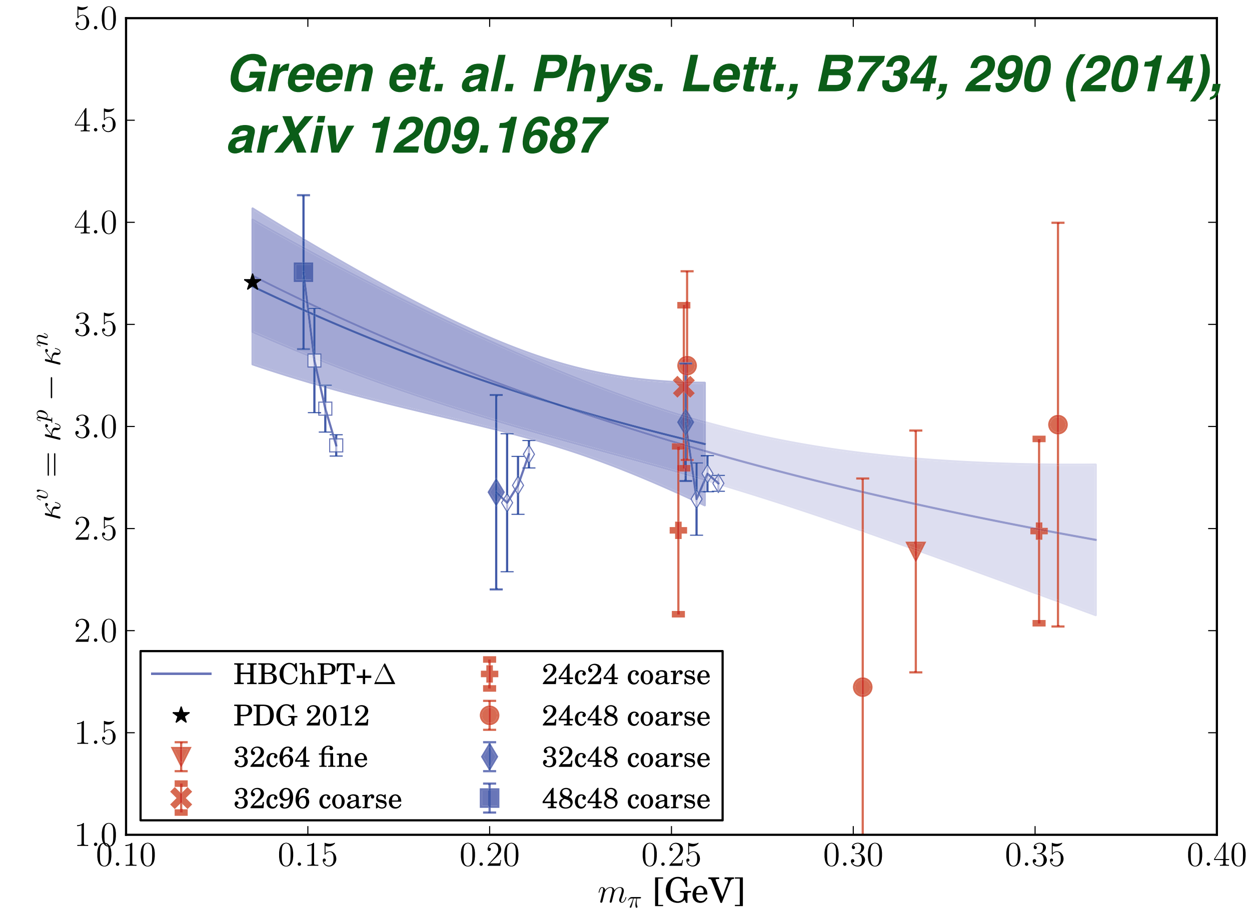
Disconnected contribution to G_E



Charge Radius: r_1^2



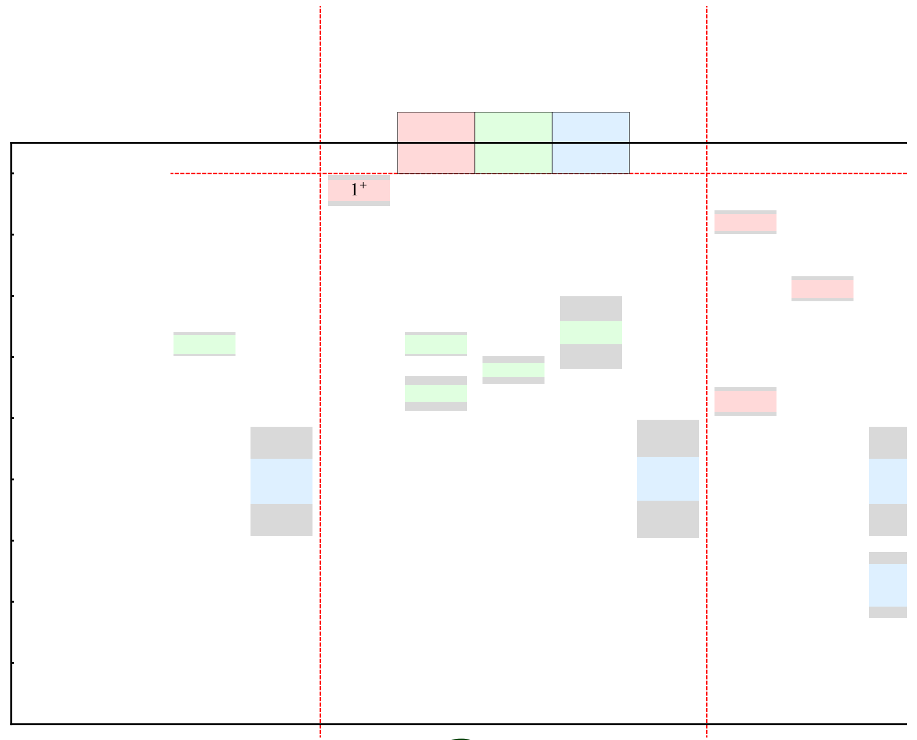
Magnetic Moment: K



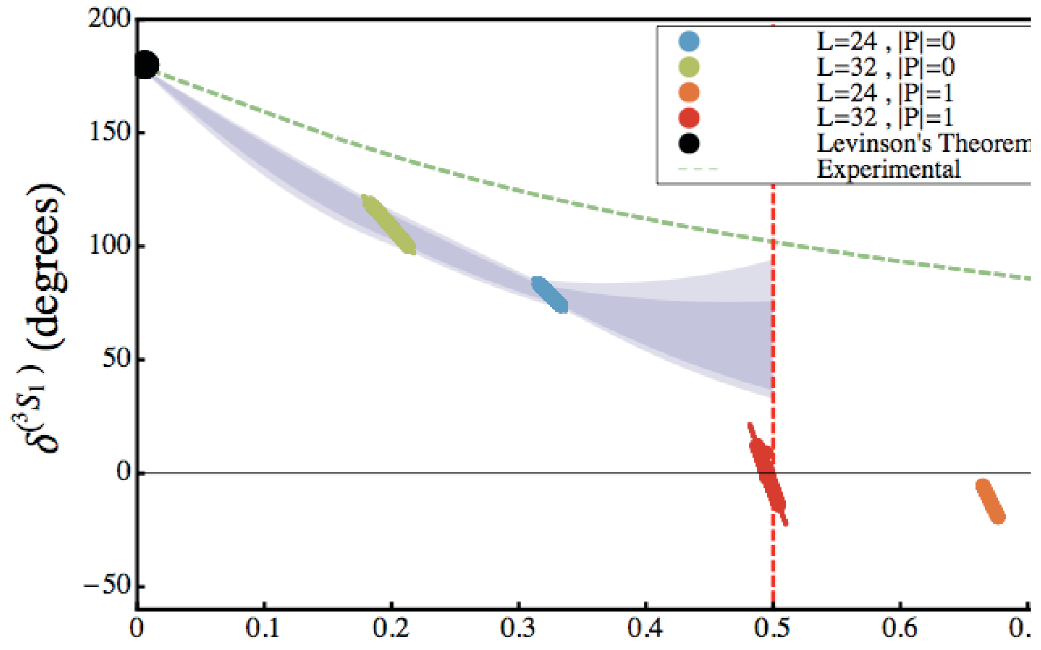
- First lattice calculation including m_π=149 MeV that agrees with experiment for 4 key isovector observables: r_1^2, r_2^2, K, <x>
- First calculation at m_π=149 MeV of isovector $G_E(Q^2)$ and $G_M(Q^2)$, agrees with expt. error band
- First calculation of disconnected light quark contributions to EM form factors, showing non-zero result of ~0.5% of the connected result.
- Calculation of strange EM form factors consistent with expt. and much smaller uncertainty.
  - ***Hierarchical Probing*** proved crucial to reduce noise by 10x and resolve the signal,.
- Challenge: to control systematic errors sufficiently to resolve proton radius puzzle

USQCD

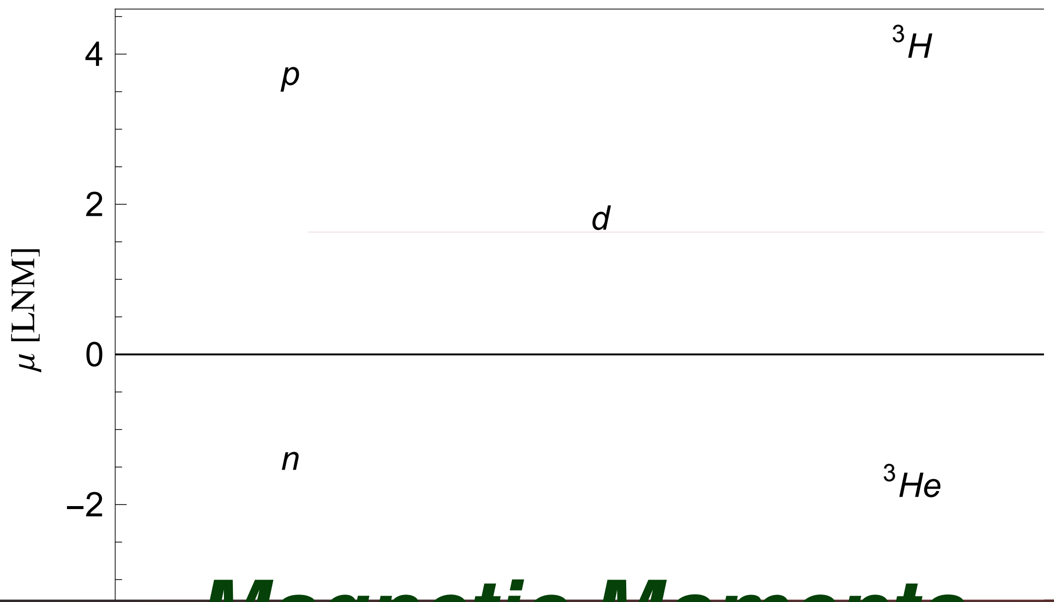
Nuclei from QCD



Nuclear Structure



NN Phase Shifts



Magnetic Moments

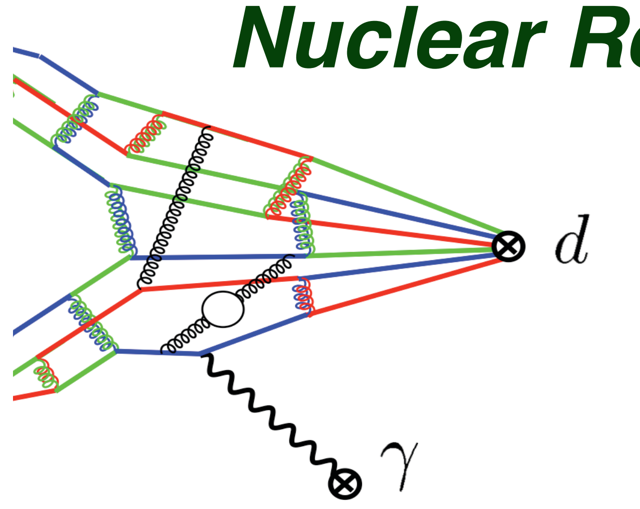
The binding of light nuclei and their properties

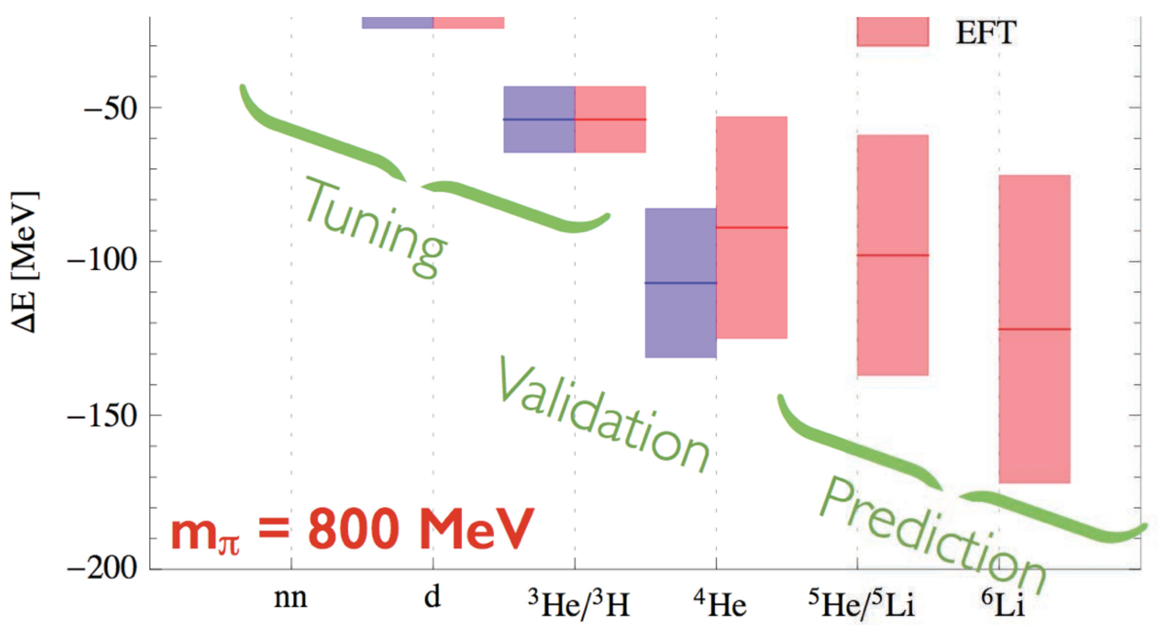
- First calculations of an inelastic nuclear reaction (neutron capture cross section)
- First calculations of the magnetic moments and polarizabilities of light nuclei
- Discovery that the nuclear shell-model structure of light nuclei persists over a large range of quark masses
- Discovery that the magnetic moments of nucleons are generically quark-model
- Used to predict properties of larger nuclei through matching to Nuclear EFT
- Binding of light nuclei
- Nucleon-nucleon scattering phase shifts

Near Future Program:

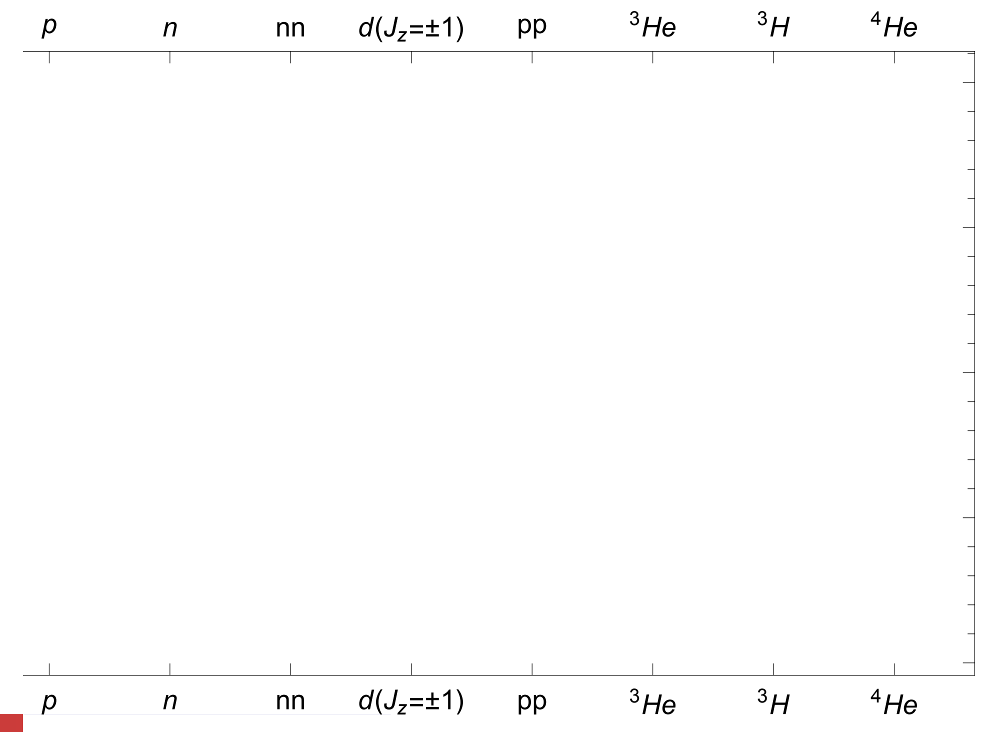
- Properties of multi-neutron systems and the three-body forces
- Axial couplings for neutrino interactions with nuclei and refinement of nuclear shell-model calculations of double beta-decay rates
- Nuclei and exotic nuclei at lighter pion masses
- Magnetic moments and polarizabilities at lighter pion masses

Nuclear Reactions





Refining Nuclear Forces

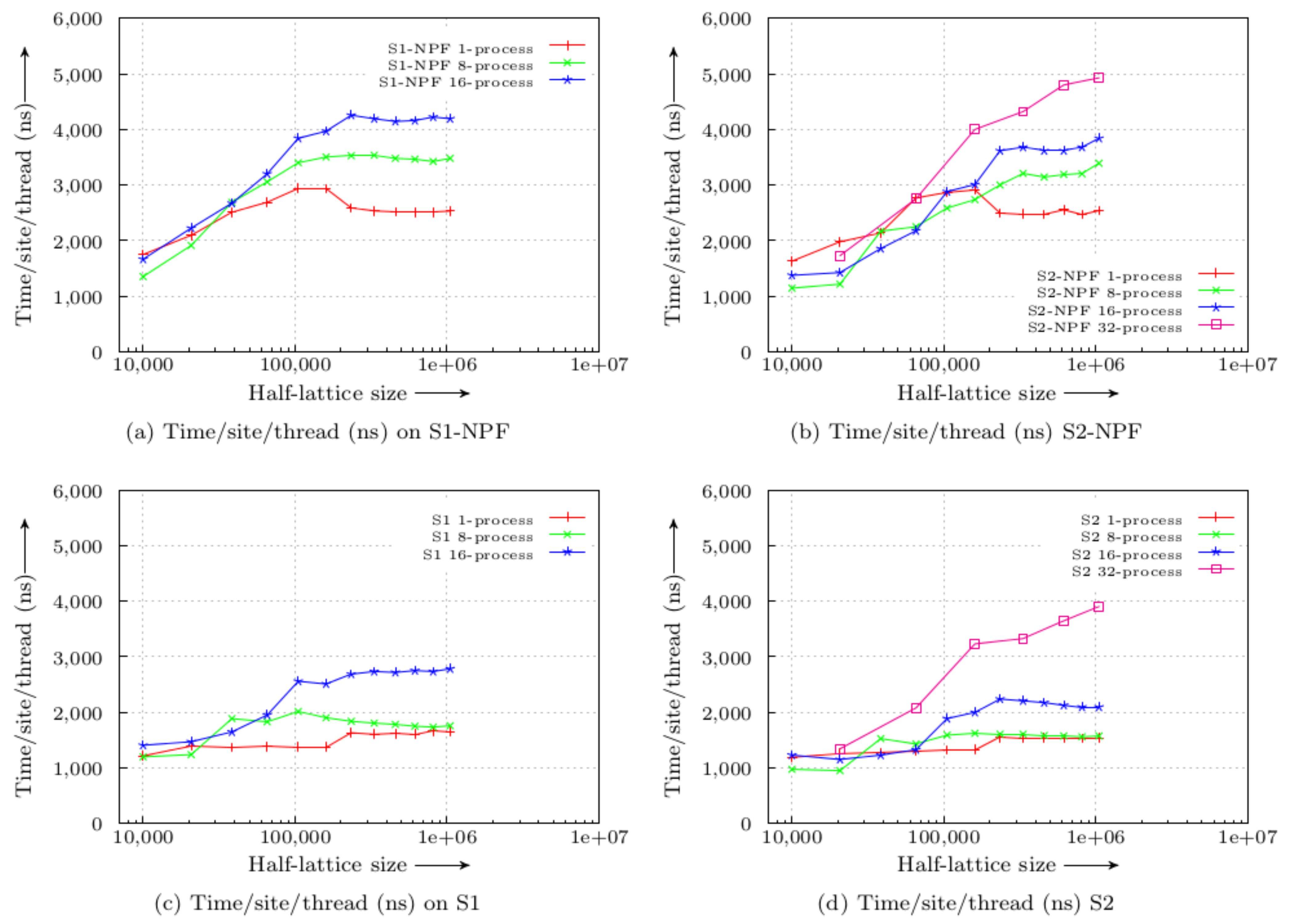


Nuclear Polarizabilities

USQCD

Work With SUPER

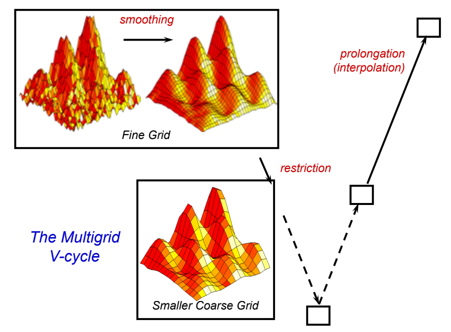
- Aims:
  - Characterize architecture and compiler constraints on the performance of LQCD codes
  - Try to bridge the ‘Ninja Gap’ between ‘productive’ code written in a domain specific framework and highly optimized code like QPhiX for Xeon & Xeon Phi
- UNC Computer Science Ph.D. Student: Diptorup Deb
  - Measured charateristics of QDP++ framework
  - (Back) Ported QPhiX library to BlueGene/Q
  - Ported code to G++ and LLVM/Clang Compilers
  - Summer Intern at Intel - QPhiX and HiSQ (MILC)
  - Expect him back with lots of Xeon Phi experience continue to bridge the ``Ninja Gap” on Cori

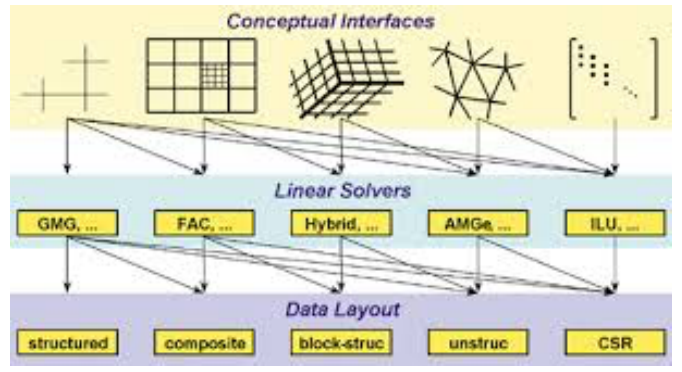


Performance of QDP++ Wilson-Dslash (MPI parallelism) with & without H/W prefetching.
S1: A dual-socket 16-core Intel Ivybridge system with Xeon E5-2650 v2 @ 2.60GHz CPUs.
S2: A dual-socket 36-core Intel Haswell system with E5-2699 v3 @ 2.30GHz CPUs.
S1-NPF and S2-NPF: Same configurations with the hardware prefetching options turned off.

Work with FAST Math

- QCD/Applied Math collaboration has long history: 8 QCDNA (Numerical Analysis) Workshops 1995-2014.
- Fast development framework is being constructed based on the combined strength of the FASTMath's HYPRE library at LLNL and the Qlua software at MIT.
- HYPER enhanced: Complex arithmetic and 4d and 5d hyper-cubic lattices.
- Qlua to HYPRE interface: to important Dirac Linear operators.
- Qlua is enhanced: 4d and 5d MG blocking and general "color" operators
- HYPRE: exploration of bootstrap algebraic multigrid (BAMG) algorithm for Dirac Equation
- Goal to explore multi-scale solvers for Wilson, Staggered and Dirac operators
- Test HYPRE methods at scale in Qlua and port into QUDA and QPhiX libraries.





QUDA

QPhiX

Plans out to 2017

- Application Readiness for New Architectures: Targeting Cori, Laying Groundwork for CORAL
  - Physical mass quarks in gauge generation and measurement
  - Elaborate observables requiring O(1M) propagators
  - Architecture Aware Implementations of Multi-Grid solvers
    - Ongoing Work in community libraries (QUDA for GPU, QPhiX for Xeon Phi)
  - Incorporate New solvers in Gauge Generation
  - Need portable & efficient code outside of solvers
    - Maintain effort on QDP-JIT/LLVM
    - Maintain partnership with SUPER Institute, carrying out research to lower the “Ninja Gap”
- Achieve through:
  - Early Science & Application Readyness programs: 2 full + 1 affiliated NESAP projects
  - Continuing our existing partnerships with LCFs and Vendors
- Pursue scientific aims outlined earlier:
  - INCITE, ALCC, ERCAP, Early Science Programs, USQCD Cluster Facilities and other sources of computer time

Conclusions

- The NP SciDAC Project has made major advances on its core scientific goals
  - supports the mission of the nuclear physics experimental program
  - achieved through successful exploitation of the emerging architectures and through improved algorithms
- Lessons Learned
  - There is a strong need for architecture aware implementations of the newest algorithms
  - Important to port and optimize the 'infrastructure' as well as the libraries, for portability, efficiency and productivity.
- Focus for the rest of project
  - Continue to meet scientific goals, and carry out algorithmic R&D needed for these
  - Prepare for the next generation of systems which will arrive in the project time-frame
    - continue our successful collaboration with Vendors, SciDAC institutes and LCFs

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    - clusters at Fermi National Accelerator Laboratory
    - BlueGene/Q system at Brookhaven National Laboratory
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