Understanding the building blocks of matter by solving Quantum Chromodynamics

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Jefferson Lab

Who we are
Why we are
Exploiting new architectures for LQCD
Algorithms for NP calculations
A sampling of Science

SciDAC-3 PI Meeting, Rockville, Maryland
July 26th, 2013

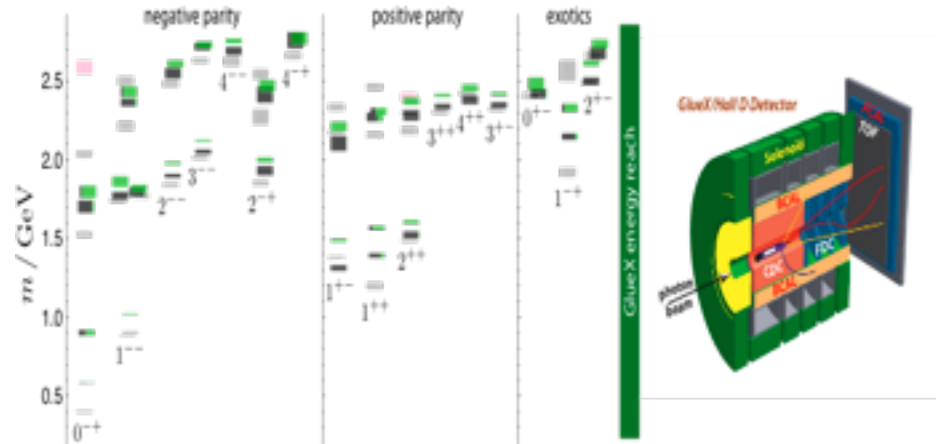
Computing Properties of Hadrons, Nuclei and Nuclear Matter from QCD

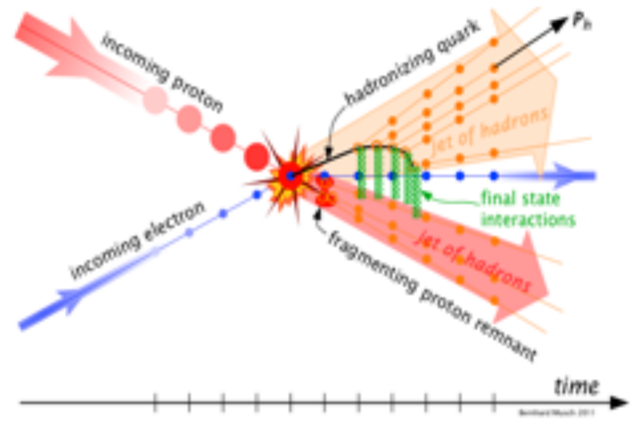
SciDAC-3 Scientific Computation Application Partnership project
Project Director: Frithjof Karsch, Brookhaven National Laboratory
Project Co-director for Science: David Richards, JLab
Project Co-director for Computation: Richard Brower, Boston University

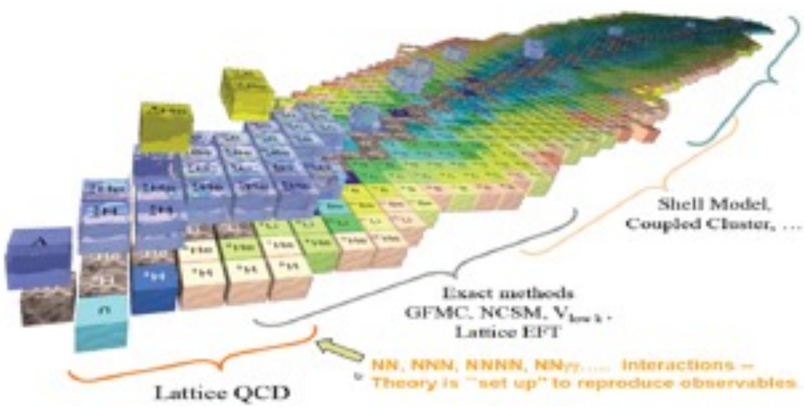
Teams

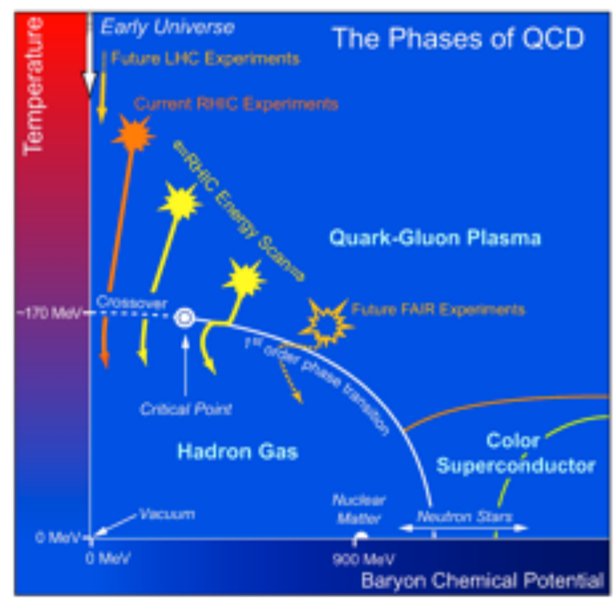
Frithjof Karsch - Brookhaven National Laboratory
Richard Brower -Boston University
Robert Edwards -Thomas Jefferson National Accelerator Facility
Martin Savage -University of Washington
John Negele -Massachusetts Institute of Technology
Rob Fowler - University of North Carolina (SUPER)
Andreas Stathopoulos -College of William and Mary

Lattice QCD for NP: Science









Lattice QCD for NP: Computation

Software + Algorithms

SciDAC
Scientific Discovery through Advanced Computing

SUPER
INSTITUTE FOR SUSTAINED PERFORMANCE, ENERGY, AND RESILIENCE

Leadership-class

\+ Fastmath

Clusters + GPUS + MIC

Multigrid with HYPRE for Lattice QCD, *Andrew Pochinsky*

QDP++ and Chroma on GPUs

AIM: put all of application code on GPU
QDP-JIT - *Just-in-time*

- QDP-JIT/C is production ready.
- QDP-JIT/PTX is fully featured, requires some small integration with QUDA
- Have performed full 2+1 flavor Gauge Generation on Blue Waters with both variants
- JIT/PTX has used Chroma's internal solvers, JIT/C has used QUDA solvers
- Paper Submitted to SC'13.
- Prognosis: Excellent, Tasks will be complete by End of Year

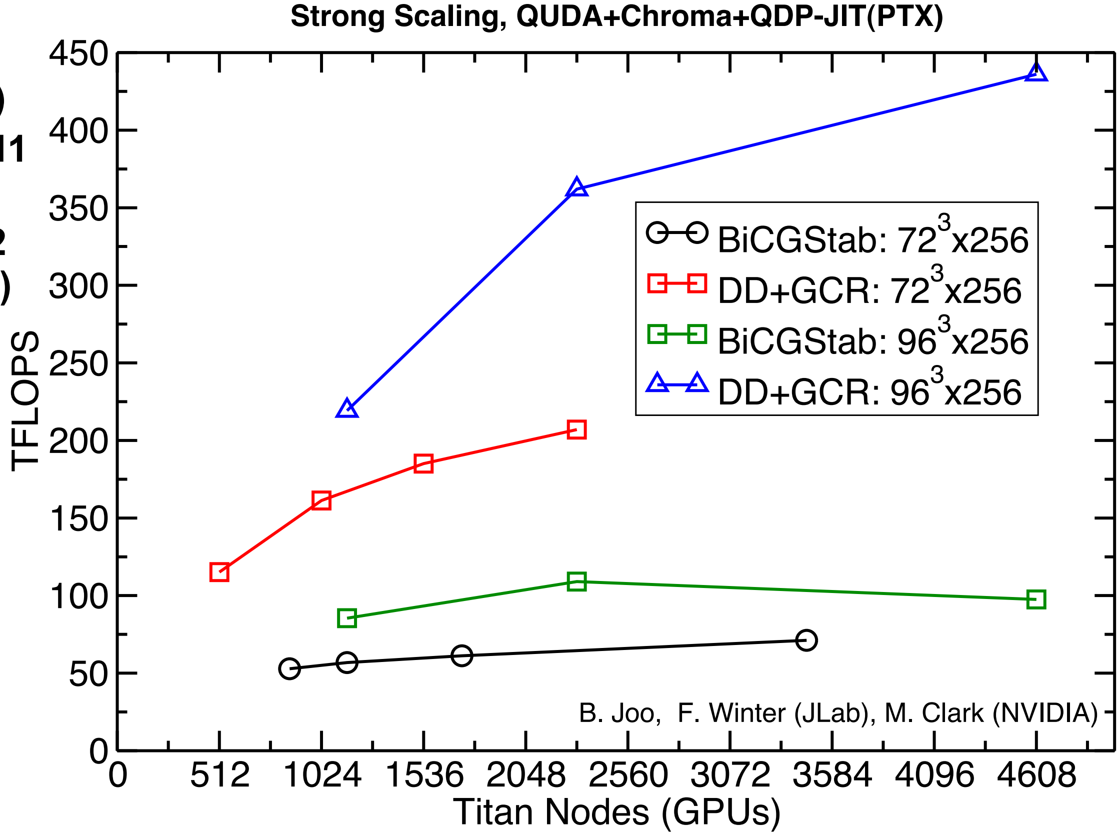
Porting Lattice QCD Calculations to Novel Architectures: Balint Joo, Frank Winter

GPUs and Heterogenous Architectures

Solver performance

- 2010: QUDA parallelized (SC ’10 Paper)
- 2011: 256 GPUs on Edge cluster (SC ’11 Paper)
- 2012: 768 GPUs on TitanDev (ACSS ’12 Contribution, Invited APS Contribution)
- 2013: On BlueWaters (NVIDIA GTC Contribution)

DD: domain-decomposed solver - *architecture-aware*

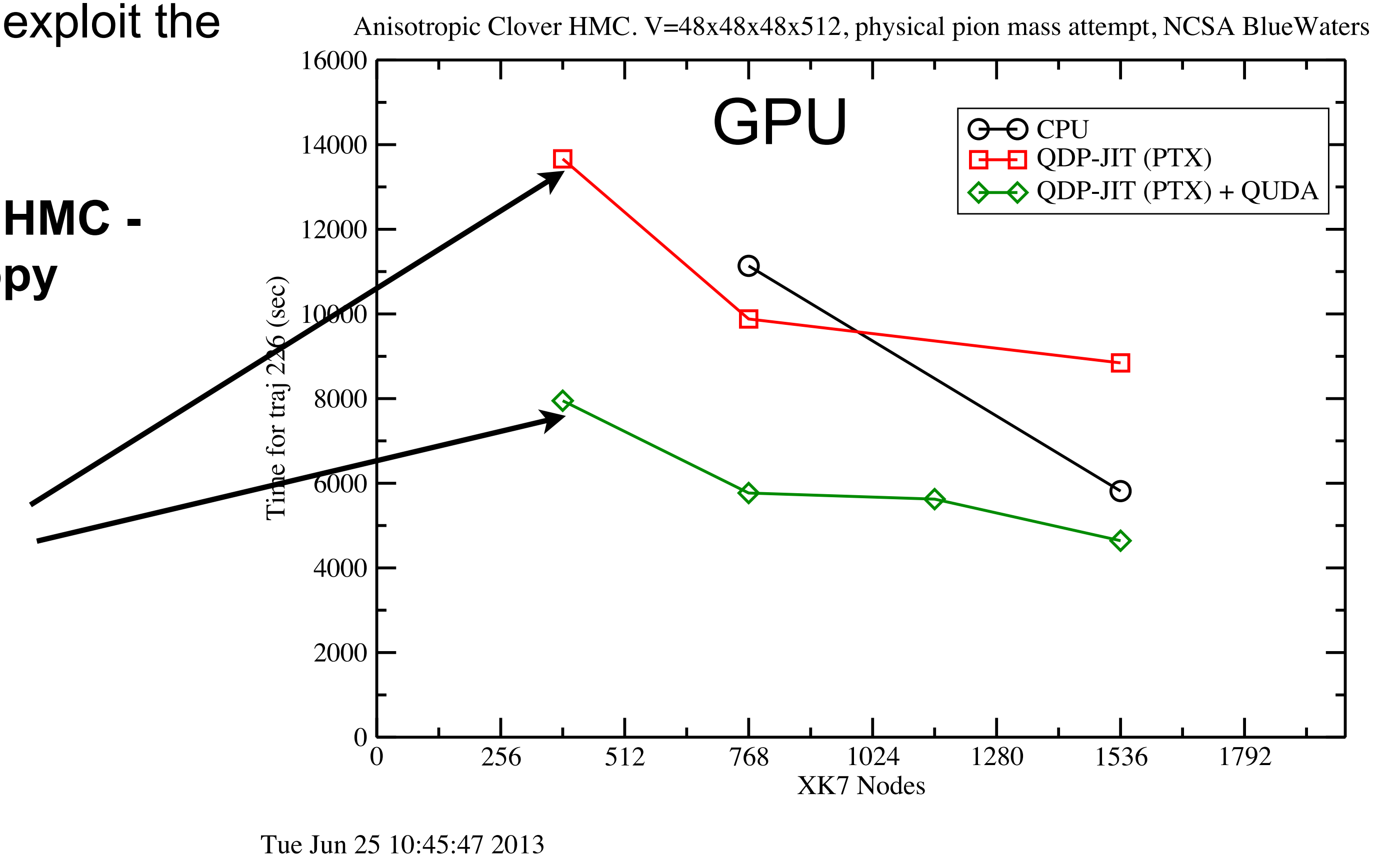


Gauge Generation: HMC - I

Aim: to put the whole of the HMC code so as to exploit the GPU

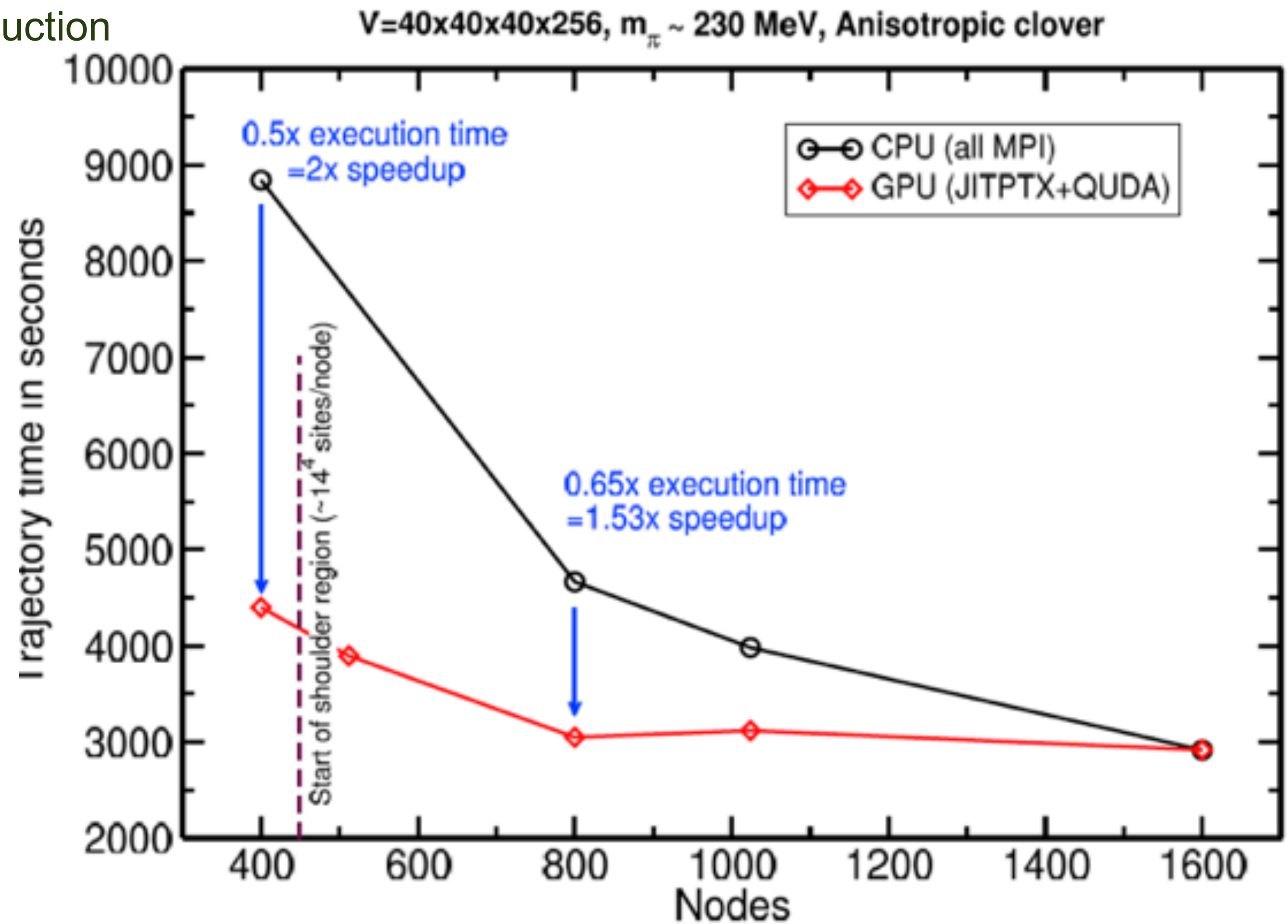
Strong scaling for anisotropic clover HMC - key for spectroscopy *48^3.512*

QUDA solver



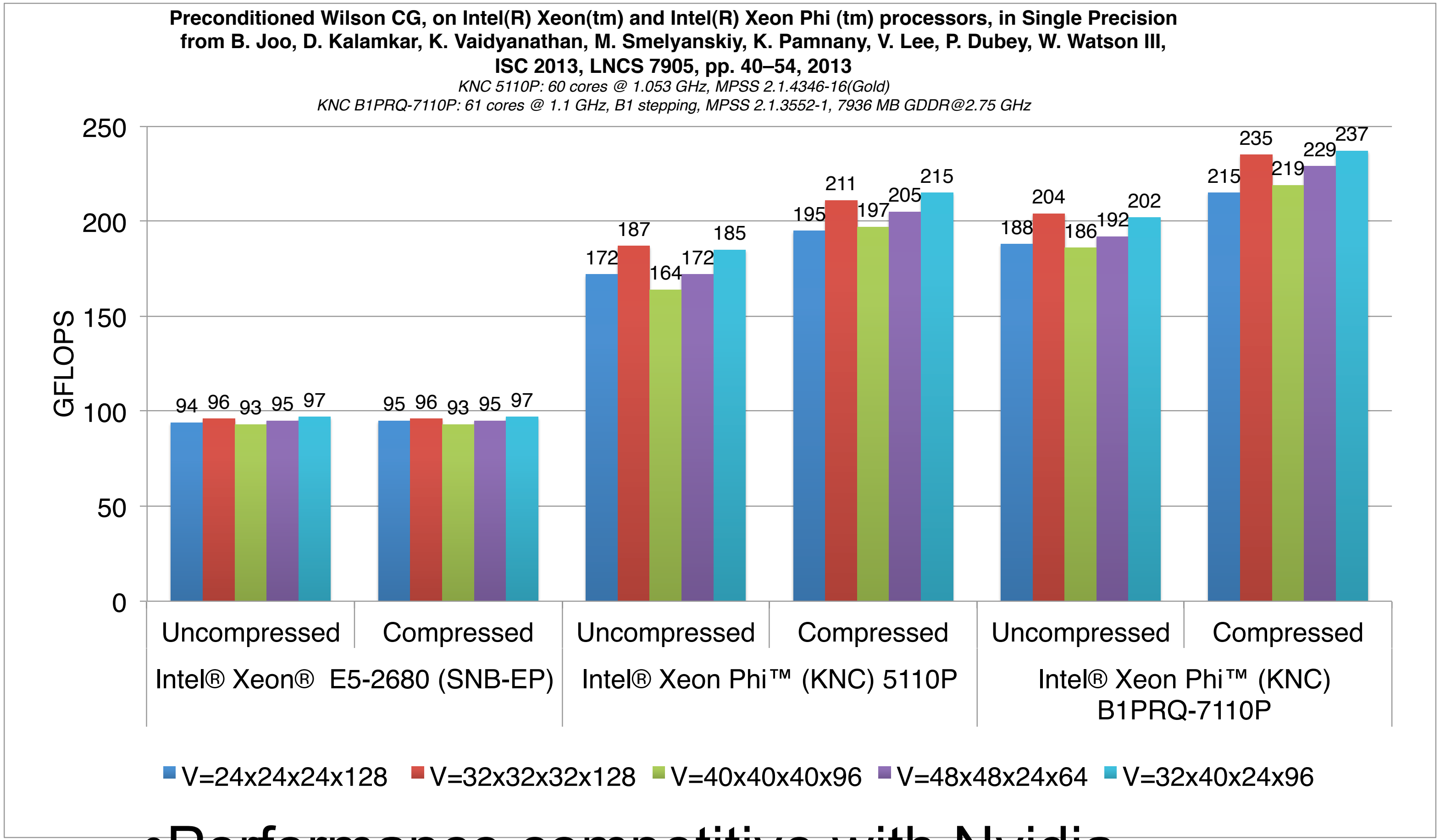
Gauge Generation: HMC - II

Current production running



Intel Xeon-Phi

Collaboration with *Intel Parallel Labs*

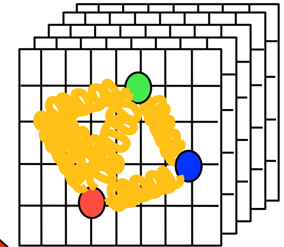


- Performance competitive with Nvidia
- Exploit e.g. Stampede

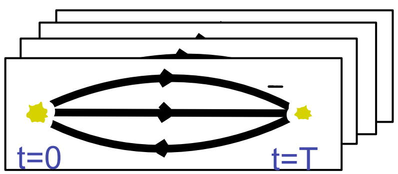
Typical LQCD Workflow

Generate the configurations

- Leadership level



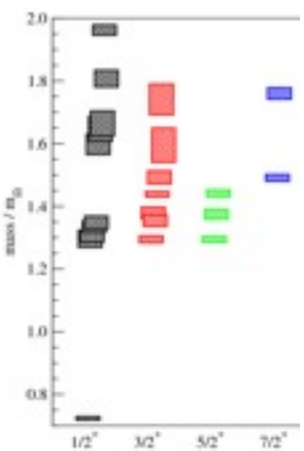
Few big jobs
Few big files



Analyze

- Typically mid-range level

IMPORTANT FOR NP



Extract

- Extract information from measured observables

Many small jobs
Many big files

I/O movement

Correlation functions: Distillation

- Use the new "distillation" method.
- Observe

Eigenvectors of Laplacian

$$L^{(J)} \equiv (1 - \frac{\kappa}{n}\Delta)^n = \sum_{i=1} f(\lambda_i) v^{(i)} \otimes v^{*(i)}$$

- Truncate sum at sufficient i to capture relevant physics modes – we use 64: set "weights" f to be unity
- Meson correlation function

$$C_M(t,t') = \langle 0 \mid \bar{d}(t')\Gamma^B(t')u(t')\bar{u}(t)\Gamma^A(t)d(t)|0\rangle$$

- Decompose using "distillation" operator as

M. Peardon *et al.*, PRD80,054506 (2009)

$$C_M(t,t') = \mathrm{Tr}\langle \phi^A(t')\tau(t',t)\Phi^B(t)\tau^\dagger(t',t),\rangle$$

where

$$\Phi^{A,ij}_{\alpha\beta} = v^{*(i)}(t)[\Gamma^A(t)\gamma_5]_{\alpha\beta}v^{(j)}(t')$$

Perambulators ⟶ $$\tau^{ij}_{\alpha\beta}(t,t') = v^{*(i)}(t')M^{-1}_{\alpha\beta}(t',t)v^{(j)}(t).$$ GPUs

This is a Capacity-computing task: solver with many RHS

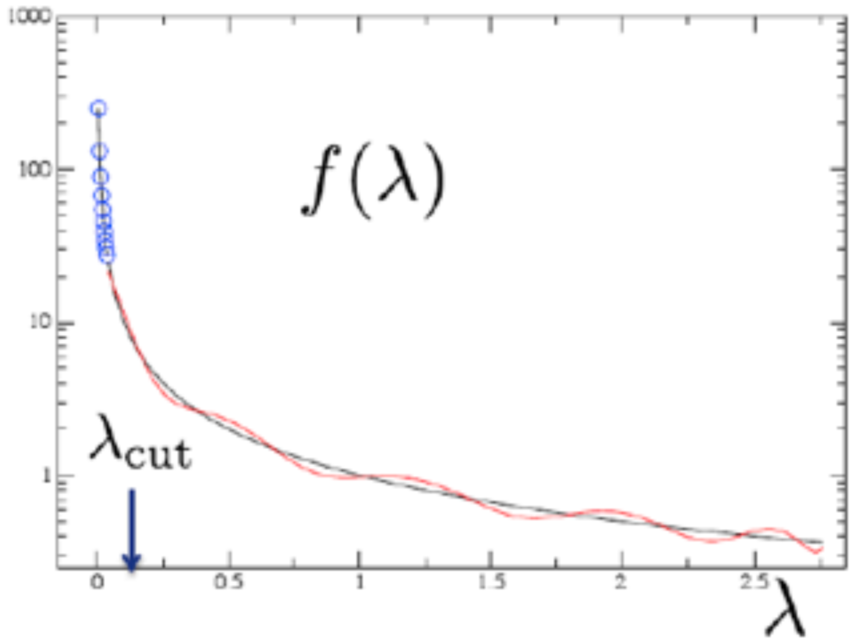
All-Mode Averaging - I

Chulwoo Jung, BNL

$$\mathcal{O}(imp) = \mathcal{O}(rest) + \frac{1}{N_G}\Sigma_g \mathcal{O}^{(approx),g}$$

$$\mathcal{O}(rest) = \mathcal{O}(exact) - \mathcal{O}(approx)$$

Generate preset number of low modes via Implicitly restarted lanczos or EigCG and deflate low modes.
Approx. high modes with CG with relatively large ($\sim 10^{-4}$) stopping condition or polynomial approx.

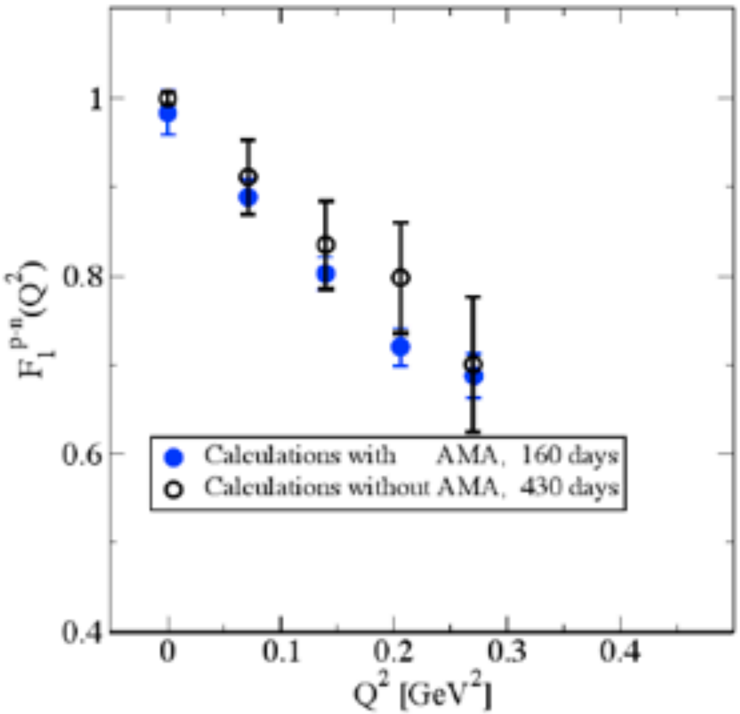


From T. Izubuchi

T. Blum, T. Izubichi, E. Shintani, arXiv: 1208.4349

All-Mode Averaging - II

Electromagnetic form factor of the proton



Without AMA : 150 configs $\times$ 4 sources = 600 measurements 10M core hours (gordon@SDSC)

AMA: 39 configs $\times$ 112 sloppy (5×10^{-3}, Mobius L_s=16) (4 exact) $\sim$ 4400 measurements, 3.9M core hours

exact(68%)+Lanczos(%12)+sloppy(%20)

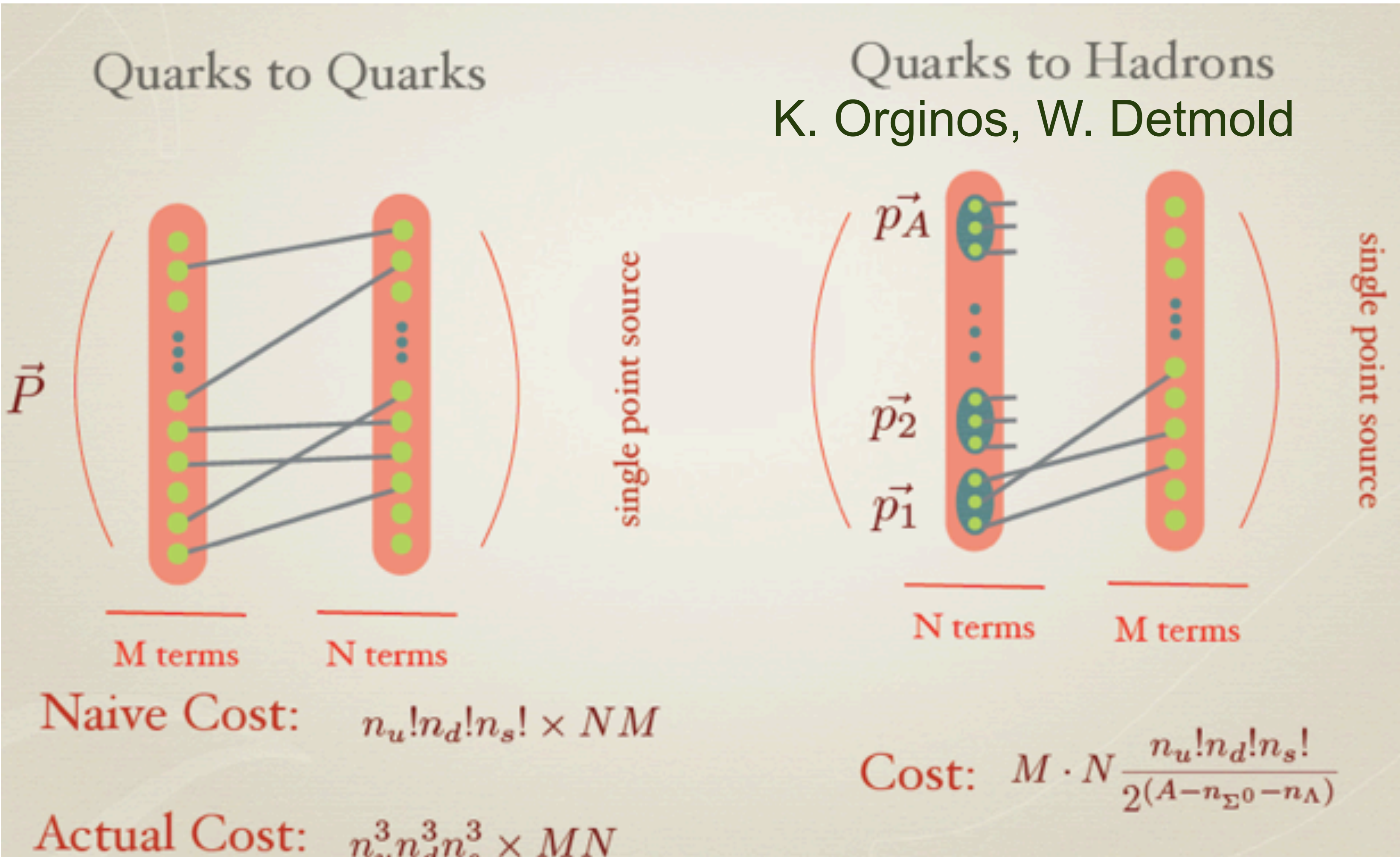
Error bar $\times$ 2 - 2.7 $\sim \sqrt{\frac{4400}{600}} \rightarrow$ all AMA measurements nearly independent.

Even with inefficiency from exact measurements, cost reduction $= \frac{10}{3.9} \times \frac{4400}{600} \sim 19.7$

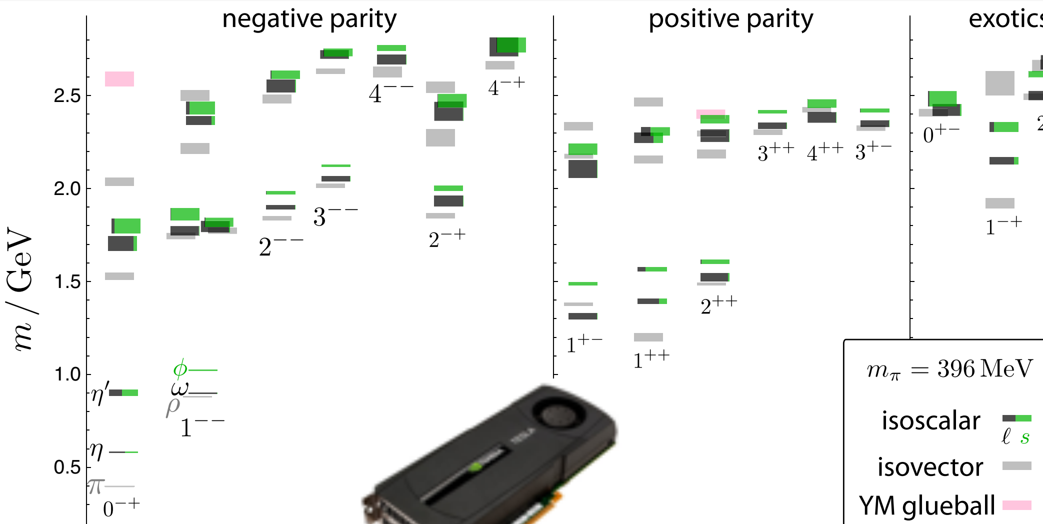
Andreas Strathopolous - AM/CS at William and Mary - development of methods for multiple right-hand sides

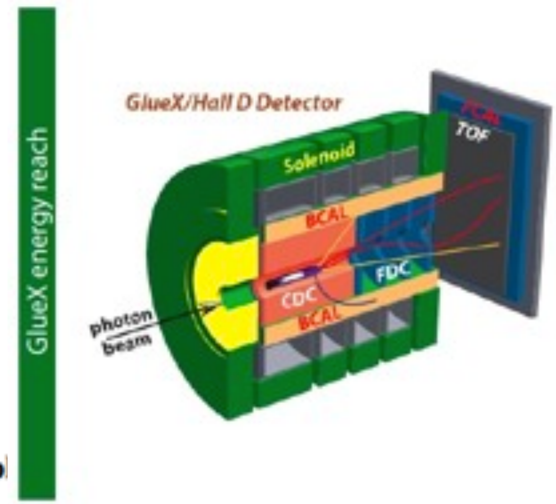
Wick Contraction Methods

Nuclear Physics calculations involve many contractions...



Momentum-dependent Phase Shifts





e p ... m lattice QCD

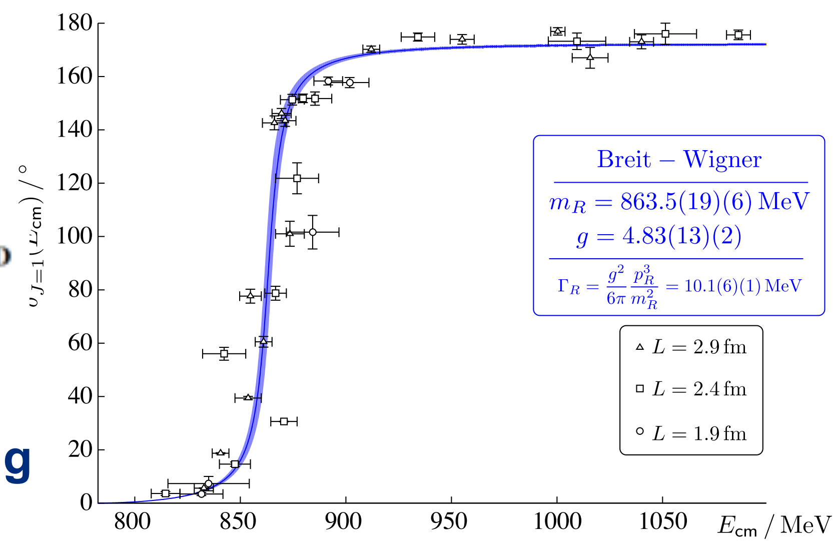
Jozef J. Dudek,[1,2,*] Robert G. Edwards,[1,†] and Christopher E. Thomas[3,‡]

I = 2 ππ elastic scattering

PHYSICAL REVIEW D 87, 034505 (2013)

Energy dependence of the ρ resonance in ππ elastic scattering from lattice QCD

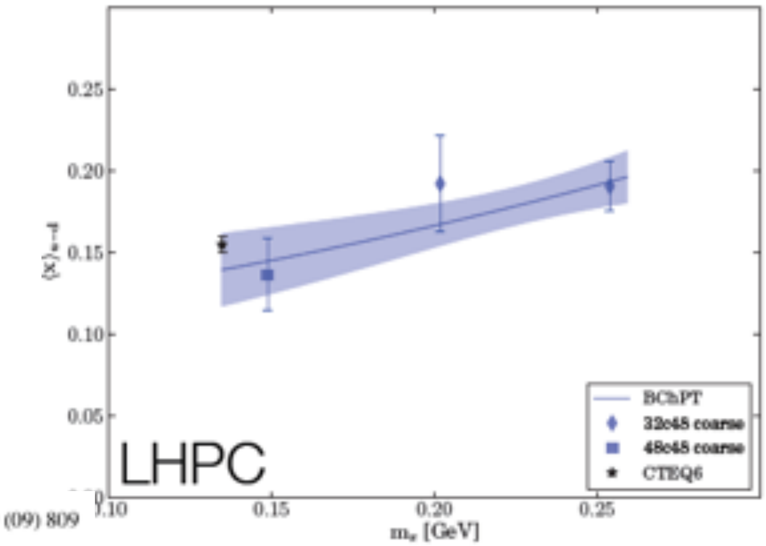
Jozef J. Dudek,[1,2,*] Robert G. Edwards,[1,†] and Christopher E. Thomas[3,‡]

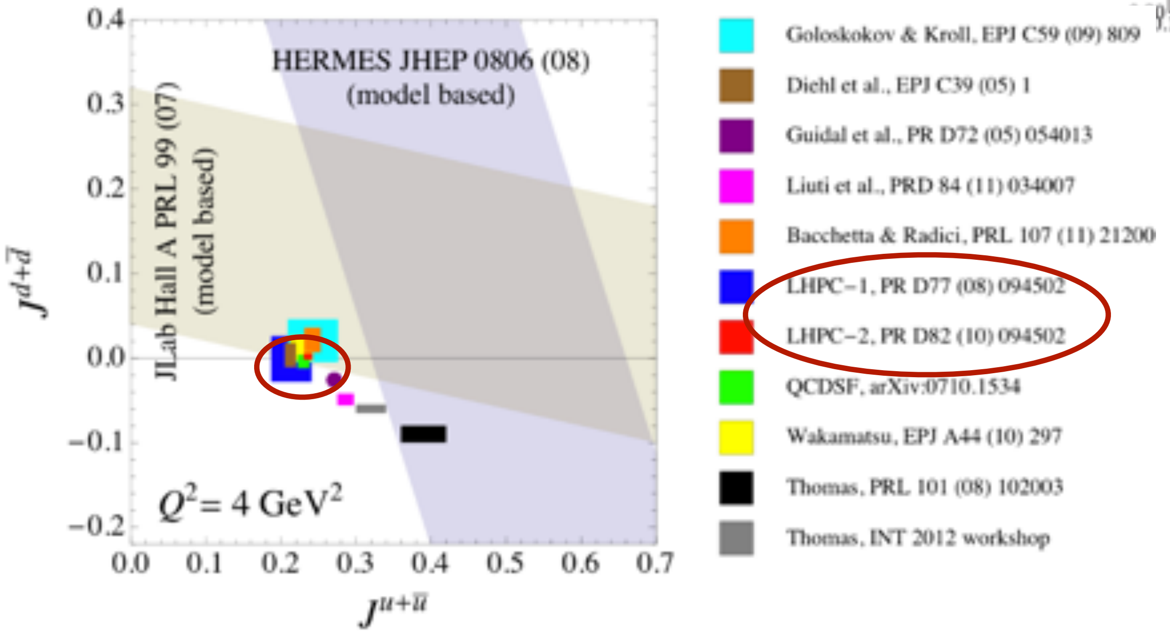


Extension to I = 1 ππ elastic scattering

Hadron Structure

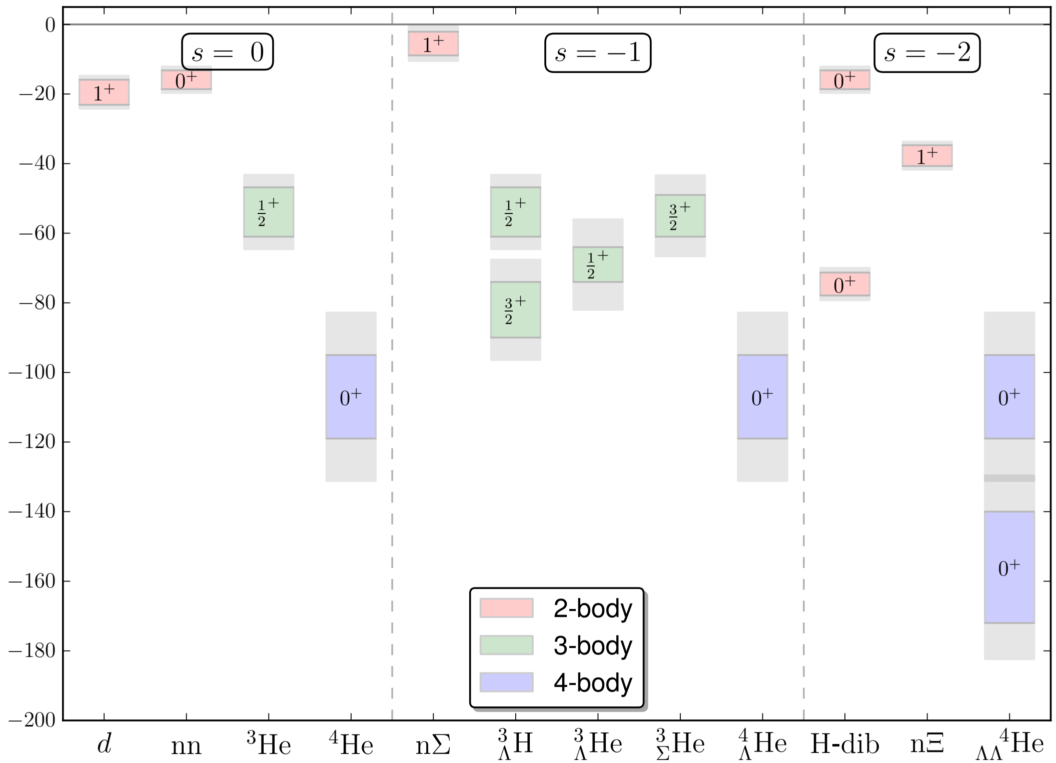
Momentum fraction of quarks in proton

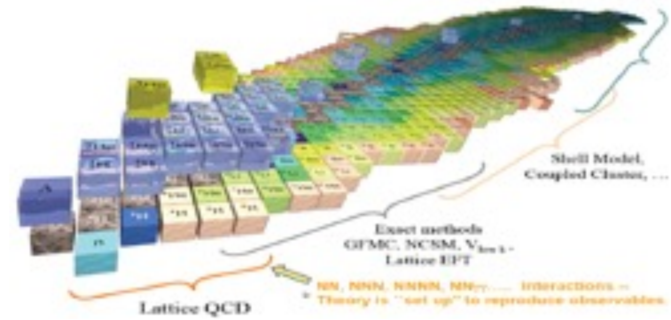




How is spin apportioned in a proton?

Three- and Four-body systems





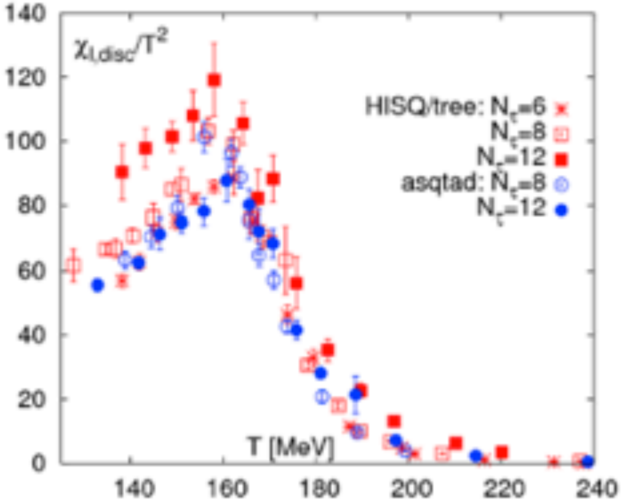
Binding energies at physical strange-quark mass

PHYSICAL REVIEW D 87, 034506 (2013)

Light nuclei and hypernuclei from quantum chromodynamics in the limit of SU(3) flavor symmetry

S. R. Beane,[1] E. Chang,[2] S. D. Cohen,[3] W. Detmold,[4,5] H. W. Lin,[3] T. C. Luu,[6] K. Orginos,[4,5] A. Parreño,[2] M. J. Savage,[3] and A. Walker-Loud[7,8]

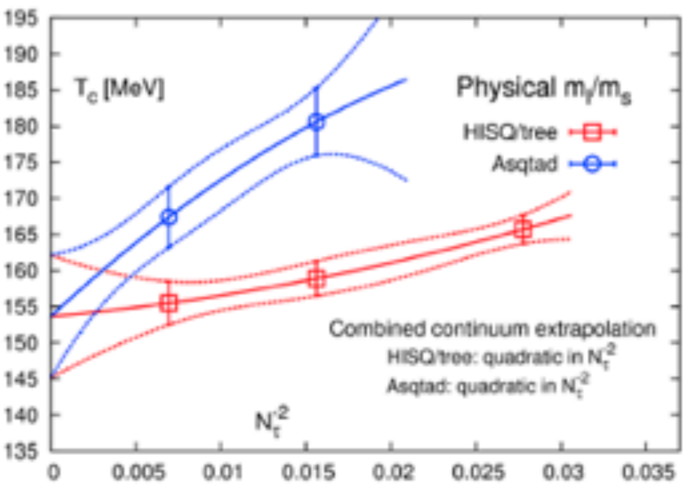
Chiral Transition Temperature



– locate pseudo-critical temperature from chiral susceptibility

$$\chi_{m,l}(T) = \frac{\partial\langle\bar{\psi}\psi\rangle}{\partial m_l}$$
$$= \chi_{l,disc} + \chi_{l,con}$$

– peak location defines pseudo-critical temperature



continuum extrapolation of pseudo-critical temperatures at physical light and strange quark masses for two different lattice discretization schemes

$$T_c = (154 \pm 9)\ \mathrm{MeV}$$

A. Bazavov et al [hotQCD Collaboration] Phys. Rev. D 85, 054503 (2012)

OUTLOOK

- Effective use of JIT to exploit accelerated architectures is basis of work with SUPER to develop domain specific compiler for LQCD. *Apply lessons to other domain-specific frameworks*
- Effective exploitation of Xeon-Phi
- Collaboration with FASTMATH for multi-grid methods
- Lattice QCD for nuclear physics characterised by heavy capacity requirements as well as capability requirement
    - Methods for multiple RHS
      Wick-contraction methods
- Exciting Physics