Computing Properties of Hadrons, Nuclei and Nuclear Matter from Quantum Chromodynamics

Project Director: Frithjof Karsch, Brookhaven National Laboratory

Project co-director for Science: David Richards, Jefferson National Laboratory

Project co-director for Computations: Richard Brower, Boston University

Principal Investigators – Physics:
Frithjof Karsch (BNL)
Richard Brower (BU)
Robert Edwards (TJNAF)
Martin Savage (UW)
John Negele (MIT)

Principal Investigators – Computer Science and Applied Math:
Robert Fowler (UNC)
Andreas Stathopoulos (W&M)

red: attending this PI-meeting

Hadrons, Nuclei and Nuclear Matter

USQCD Nuclear Physics

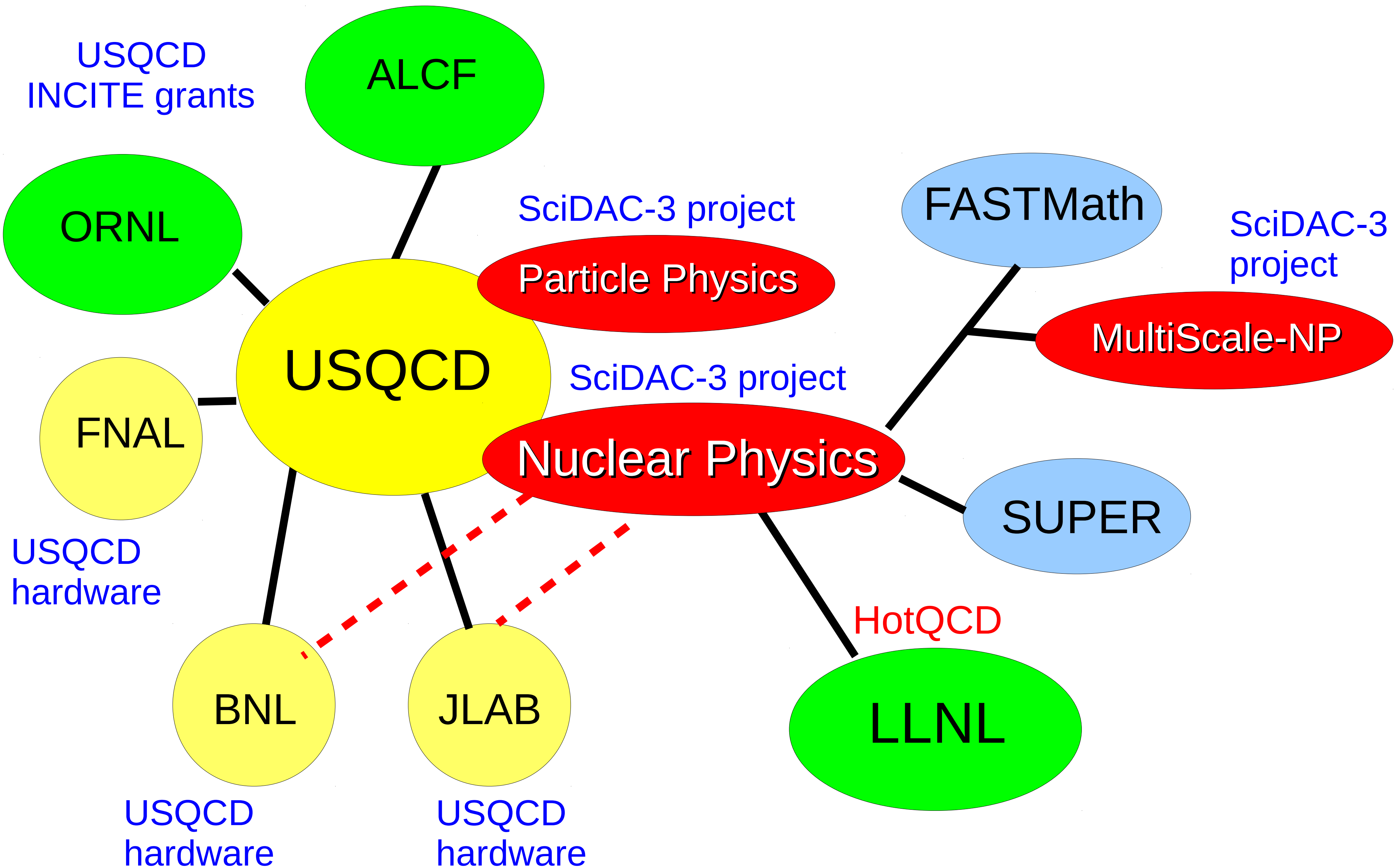
- Quantum Chromodynamics (QCD) is the theory of strong interactions; it describes all properties of hadrons, nuclei and nuclear matter in terms of elementary interactions among the basic constituents of QCD: quarks and gluons

- large experimental programs in the US and worldwide aim at deeper understanding of strong interactions that should provide insight into
  - the existence of exotic hadrons or glueballs
  - properties of nucleons, nuclei, hyper-nuclei and possible multi-quark bound states
  - novel phases of nuclear matter that may have existed in the early universe and may influence the structure of compact stars

- in order to address these problems and arrive at quantitative predictions that can be confronted with experiments, one utilizes numerical techniques that allow to calculate observables of interest within the framework of lattice regularized QCD

Collaborations and Infrastructure

USQCD
Nuclear Physics



Cooperations with Institutes and Industry

USQCD Nuclear Physics

cooperation with SUPER:

- the partnership with the SUPER SciDAC Institute will focus on performance tuning and analysis on current generation hardware, with a planned development of a Domain Specific Language for QCD in later years as a solution to the problem of performance portability in preparation for the exascale and allow the rapid development of highly optimized code

cooperation with FASTMath:

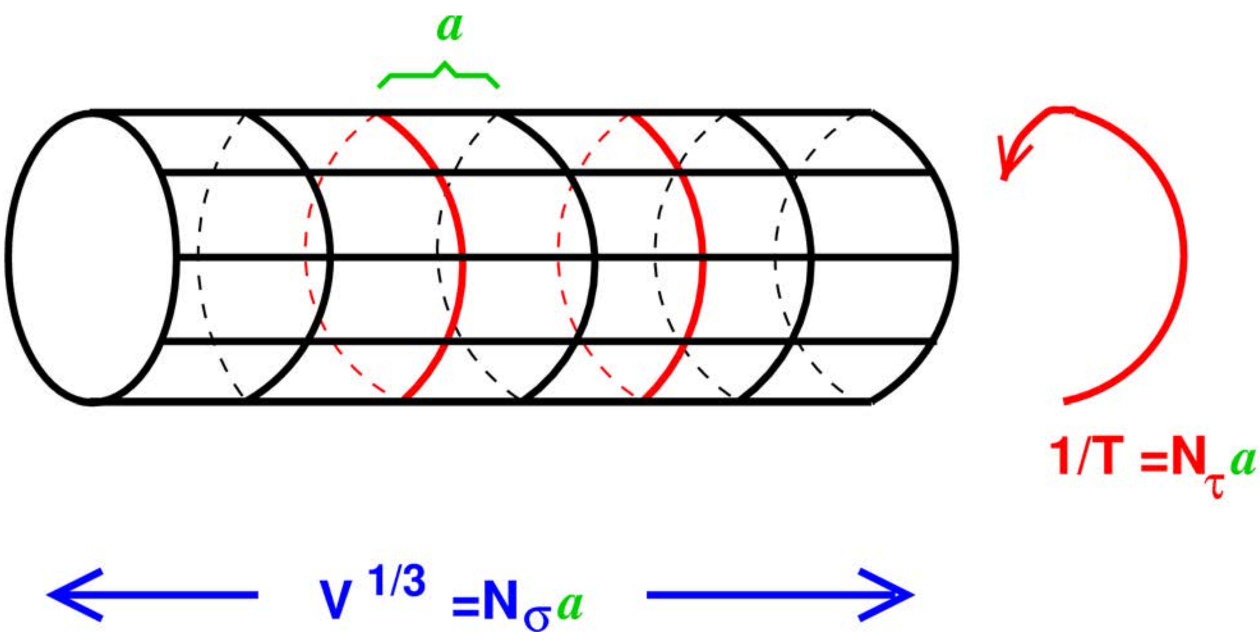
- develop synergy between the MultiScale-NP, the USQCD-NP SciDAC projects and the FASTMath institute
- Perform quantitative tests of alternative implementations of multi-grid algorithm for Wilson Clover operator
- extend multi-grid inverter to staggered and domain wall discretization schemes (jointly with HEP USQCD SciDAC-3 project)

cooperation with NVIDIA Emerging Application group:

- development of efficient code for current and future GPU generations

Simulating strongly interacting matter on a discrete space-time grid (lattice QCD)

USQCD
Nuclear Physics



the lattice: $N_\sigma^3 \times N_\tau$

lattice spacing: a

The fermion determinant: source of all problems

partition function:

$$Z(V,T,\mu) = \int \mathcal{D}\mathcal{A}\; \underbrace{Det M(\mathcal{A}, m_q, \mu)\; e^{-S_G}}_{e^{-S_E} \equiv e^{\mathrm{Tr}\ln M - S_G}}$$

$$S_E = \int_0^{1/T} dx_0 \int_V d^3x \; \mathcal{L}_E(\mathcal{A}, \psi, \bar{\psi}, \mu)$$

$\mathcal{O}(10^6)$ grid points

$\mathcal{O}(10^8)$ d.o.f.

T: temperature   V: volume μ : chemical potential

Simulating strongly interacting matter on a discrete space-time grid (lattice QCD)

USQCD Nuclear Physics

need to control three limits

infinite volume limit: $N_\sigma \to \infty$
continuum limit: $a \to 0$
chiral limit: $m_q \to 0(m_{phys})$

the lattice: $N_\sigma^3 \times N_\tau$

lattice spacing: a

The fermion determinant: source of all problems

partition function:

$$Z(V,T,\mu) = \int \mathcal{D}\mathcal{A} \; \underbrace{DetM(\mathcal{A}, m_q, \mu) \; e^{-S_G}}$$

$$e^{-S_E} \equiv e^{\mathrm{Tr} \ln M - S_G}$$

$$S_E = \int_0^{1/T} dx_0 \int_V d^3x \; \mathcal{L}_E(\mathcal{A}, \psi, \bar{\psi}, \mu)$$

$\mathcal{O}\left(10^6\right)$ grid points
$\mathcal{O}\left(10^8\right)$ d.o.f.

T: temperature V: volume μ : chemical potential

Pros and Cons of different Fermion discretization schemes

highly improved staggered fermions (HISQ):

fast, maintains a U(1) remnant of chiral symmetry,
explicit breaking of flavor symmetry (taste-violations)
– used in state-of-the-art thermodynamics calculations

clover/Wilson fermions:

good control over flavor quantum numbers,
explicitly broken chiral symmetry
– used in state-of-the-art spectroscopy calculations

domain wall fermions (DWF):

'exact' chiral symmetries of QCD even at finite cut-off;
requires the introduction of a 5-th dimension – slow
– becomes increasingly important/usable with improved computing resources

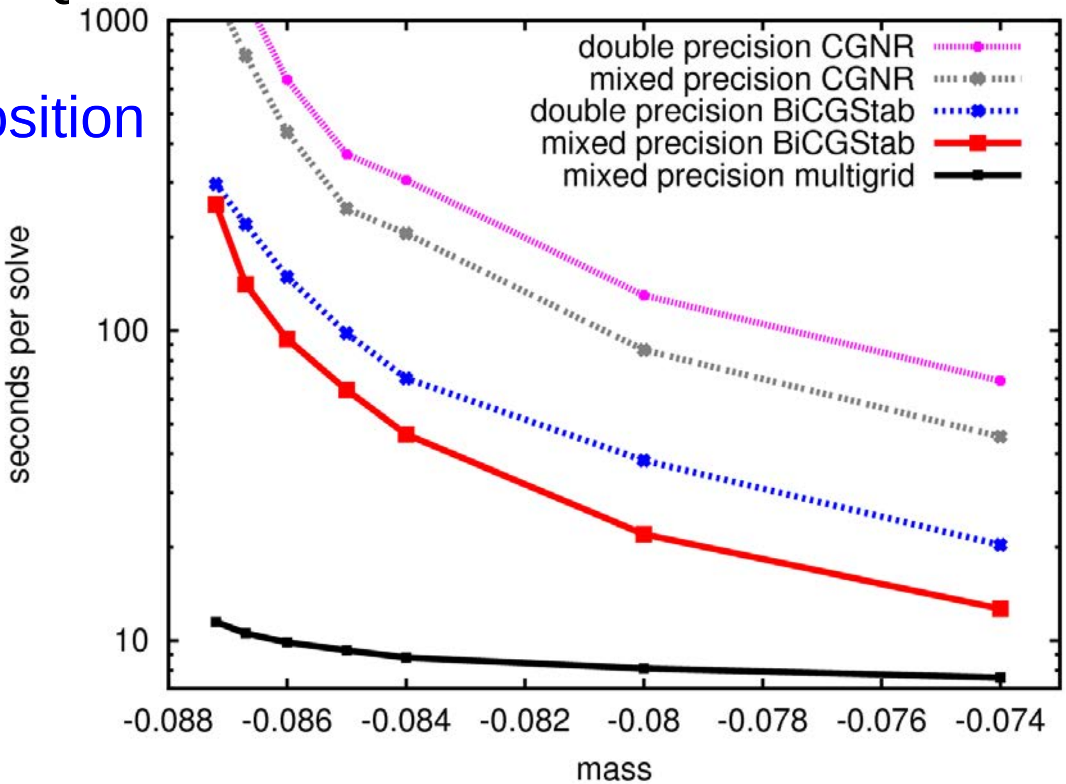
Inverting the fermion matrix
A computational challenge

Developing efficient numerical algorithms to invert the sparse QCD fermion matrix,

tuned for the particular features of a given discretization scheme,

remains to be the major challenge in QCD simulations

– multi-grid solver, domain decomposition implementation and tuning on new hardware for clover/Wilson, improved staggered and DWF



J. Osborn et al., PoS LATTICE 2010, 037 (2010) – Clover
S.D. Cohen, et al. PoS LATTICE 2011, 030 (2011) – DWF

Inverting the fermion matrix
A computational challenge

USQCD Nuclear Physics

– analysis software in Nuclear Physics lattice QCD applications requires multiple (10-th of thousands) inversions (= quark propagators) in quite different context

hadron spectroscopy: large basis of operators required to project onto excited states

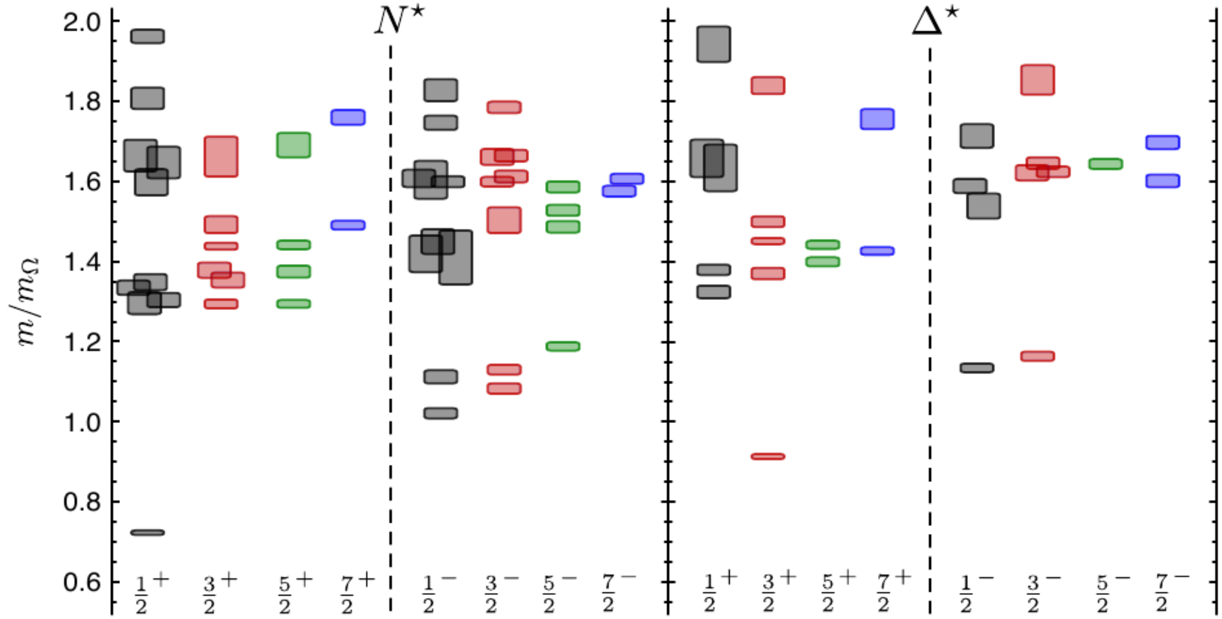
nucleon structure: disconnected diagrams require large statistics for impact on experiment; large spatial volumes, large time extent,

nuclei, hyper-nuclei: many-body problem results in many possible contractions of quark propagators; calculations in finite volume can make contact to dense QCD thermodynamics

dense hadronic matter: calculation of higher order cumulants of charge fluctuations requires large number of inversion on random sources; thermal hadron mass calculations become comparable to T=0 hadron spectroscopy

Hadron Spectrum – Excited states

Spin-identified spectrum of nucleons and deltas from the lattices at $m_\pi = 396\mathrm{MeV}$



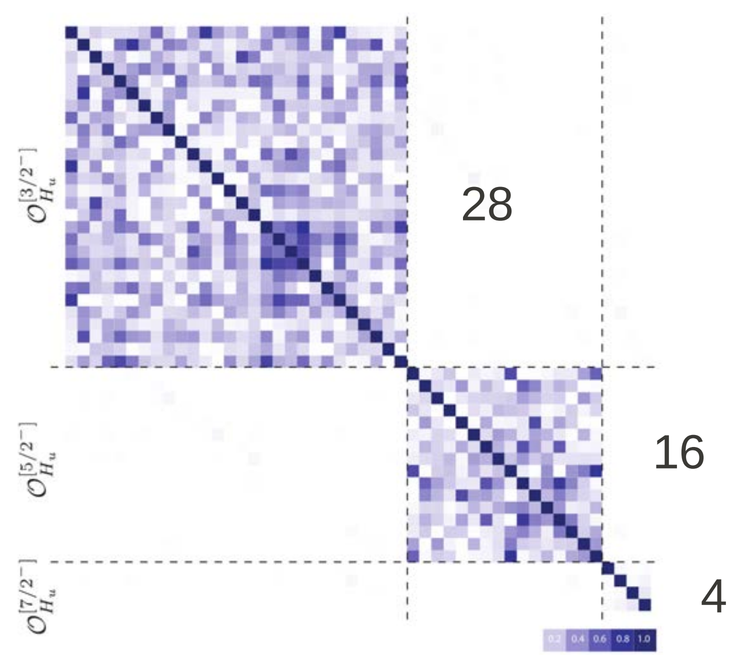
R.G. Edwards et al., arXiv:1104.5152

consistent with qqq constituent quark model
– seems to rule out quark-diquark picture

$$C_{ij}(t) = \sum_{\mathfrak{n}} \frac{1}{2E_{\mathfrak{n}}} \langle 0|\mathcal{O}_i|\mathfrak{n}\rangle\langle \mathfrak{n}|\mathcal{O}_j^\dagger|0\rangle\, e^{-E_{\mathfrak{n}} t}$$

The calculation of excited states with well defined quantum numbers requires to set up a large basis of operators

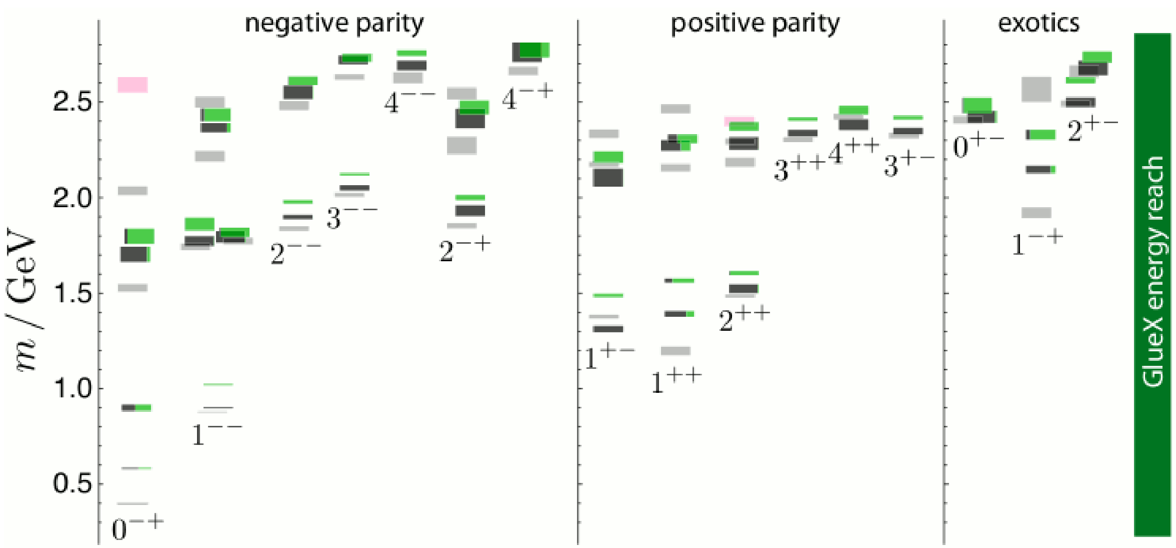
$$C_{ij}(t) = \langle 0|\mathcal{O}_i(t)\mathcal{O}_j^\dagger(0)|0\rangle$$



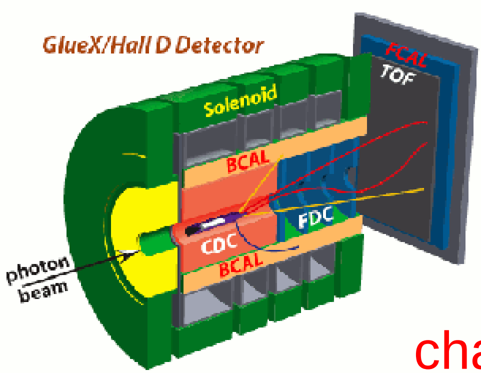
Hadron Spectrum – Exotic States

USQCD
Nuclear Physics

- Hadron Spectrum: Precision studies, missing resonances
- Excited states: include decay channels, calculate momentum dependent phase shifts
- Exotic states: flavor singlet spectrum, glueballs



GlueX,
JLab@12GeV



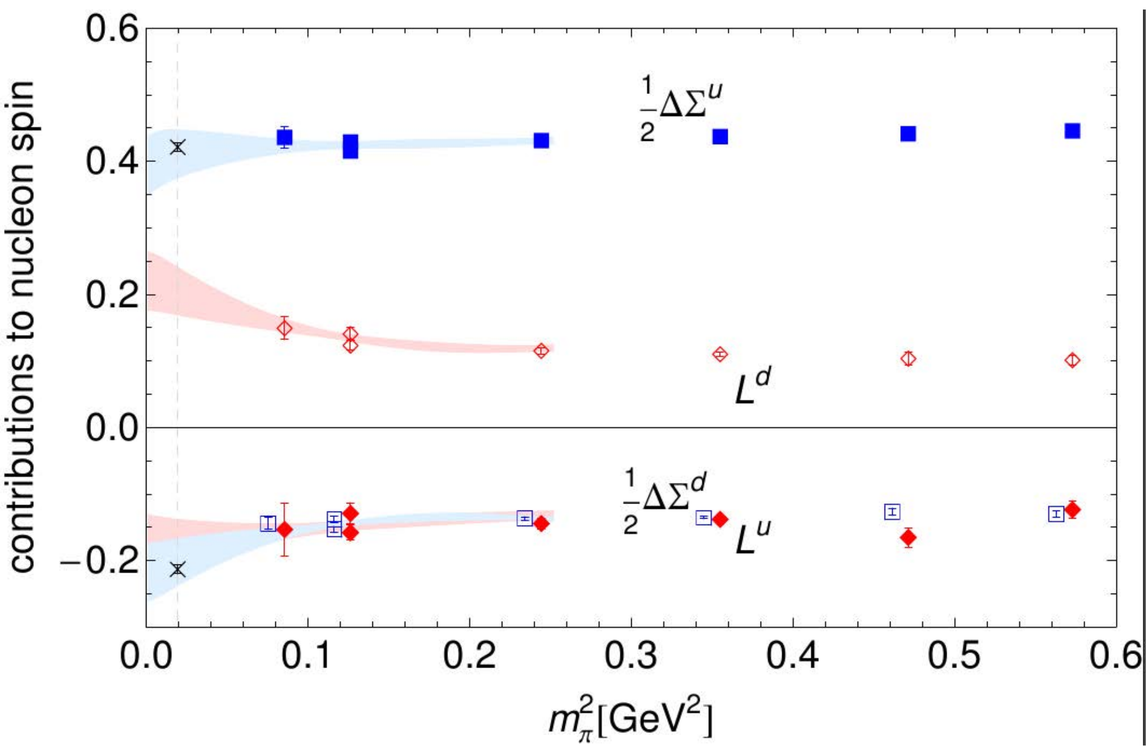
challenge:
get to physical
pion mass values

The spectrum of states for exotic quantum numbers for isovectors (grey) and isoscalars (black/green) for light quark masses corresponding to those of a pion of mass 396 MeV. The light/strange quark content is indicated by the fraction of black/green in the rectangle. The pink is the calculation of the pure Yang-Mills glueball. These results suggest the presence of many exotics in a region accessible to the future GlueX experiment.}

Hadron Structure

USQCD Nuclear Physics

- Precision calculations of form factors, moments of quark and gluon distribution functions as well as generalized parton distribution functions at the physical pion mass value:
  - controlling contributions from disconnected diagrams;
  - eliminating contributions from excited states and thermal excitations



Contributions of u,d quark spin (blue) and orbital angular momentum (red) to the spin 1/2 of the proton. Chiral extrapolations (shaded error bands) agree with HERMES data (crosses).

- angular momentum contributions $(L^u,\ L^d)$ cancel
- quark spins contribute only about (20-30)%
- gluon spin must contribute about 70%

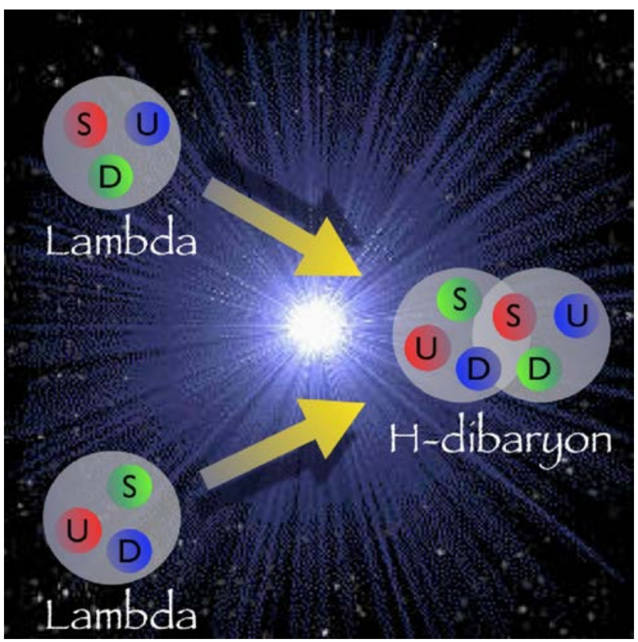
J.C. Bratt et al (LHPC Coll.) Phys. Rev. D82 (2010) 094502

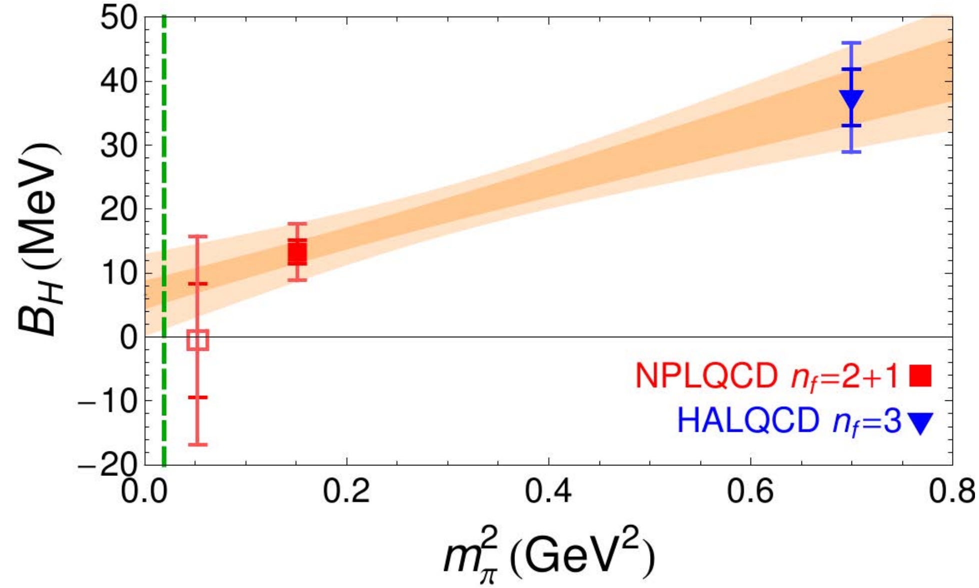
experimental impact: JLab, RHIC-spin, EIC

Nuclei

- Multi-hadron systems and hyper-nuclei:
  - establish their connection to fundamental parameters of QCD;
  - derive properties of the nuclear force from first principle calculations and basic QCD interactions of quarks and gluons

Evidence for a bound H-dibaryon ?



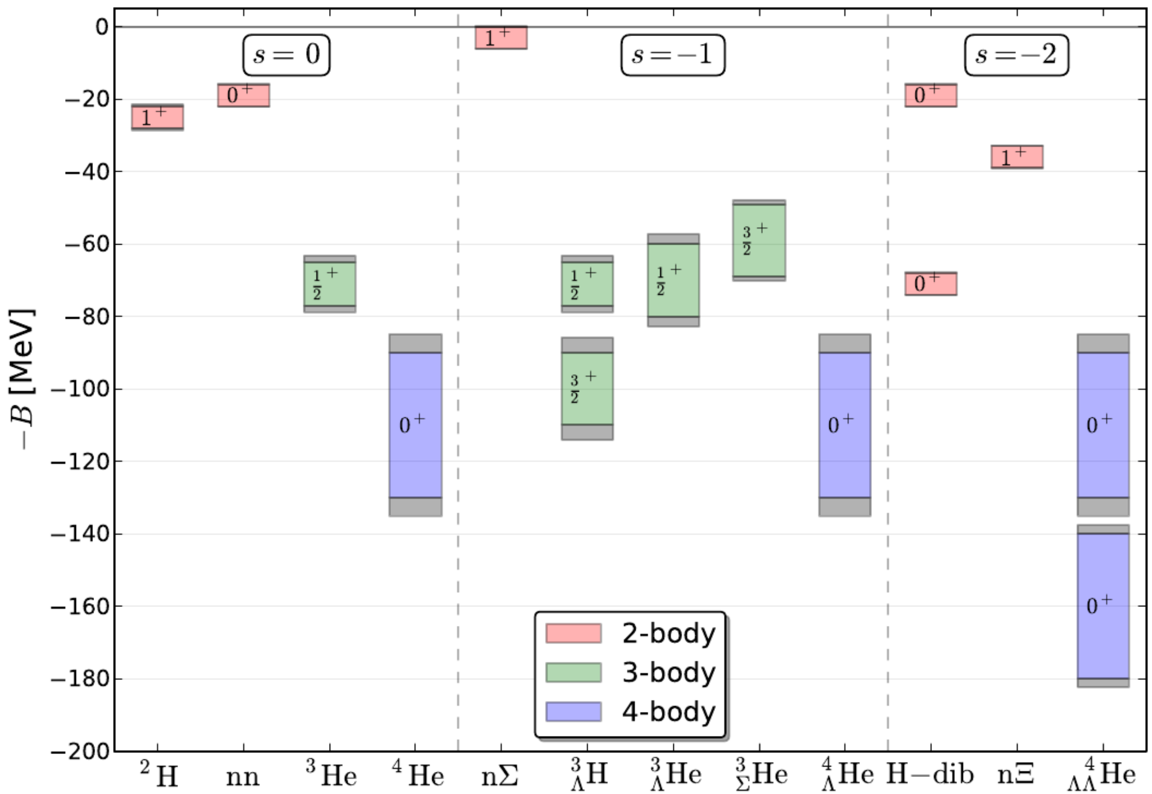


S.R. Beane et al, (NPLQCD), Phys.Rev.Lett. 106 (2011) 162001

Lattice calculations of the H-dibaryon mass. The green line corresponds to the physical pion mass. Sensitvity to quark mass needs to be better controlled.

Hyper-Nuclei

Spectrum of nuclei and hyper-nuclei in strangeness sectors S=0, -1, -2; consisting of A=2, 3 and 4 nucleons



S.R. Beane et al, (NPLQCD), arXiv:1206.5219

calculations on isotropic lattices in the SU(3) symmetric limit using clover fermions:

$$m_\pi \simeq 800\ MeV$$

$$a \simeq 0.18\text{fm}$$

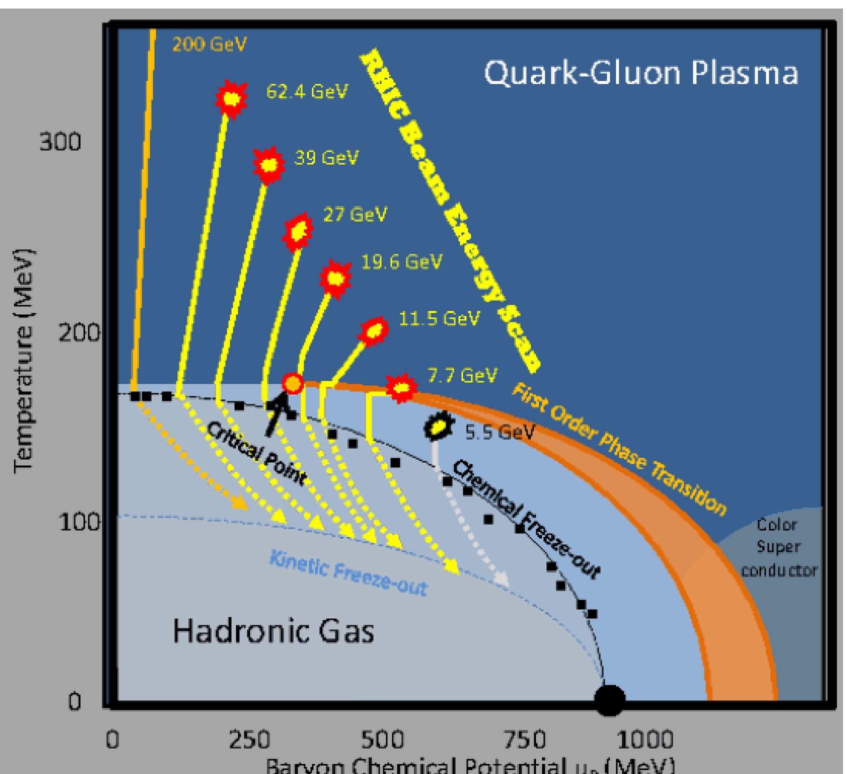
$$N_\sigma = 24,\ 32,\ 48$$

newly developed software for performing contractions of quark propagators allows to include up to 5 nucleons

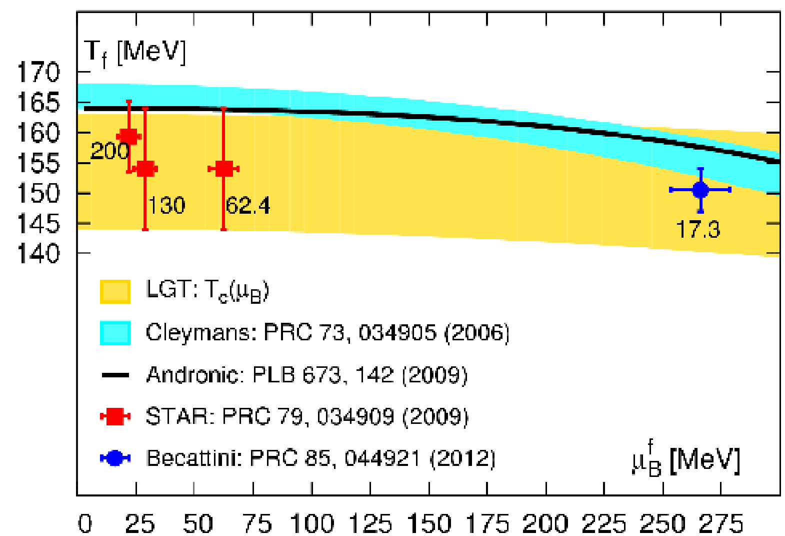
Matter under extreme conditions

USQCD Nuclear Physics

- QCD phase transition: chiral limit, role of axial anomaly
- Transport properties: (shear) viscosity, electrical conductivity, heavy quark diffusion,....
- Experimental probes: Di-lepton/Photon rates, Heavy Quark spectroscopy,
- Finite density QCD: Fluctuation of conserved charges, freeze-out and beam energy scan at RHIC



LGT transition and experimental freeze-out temperatures

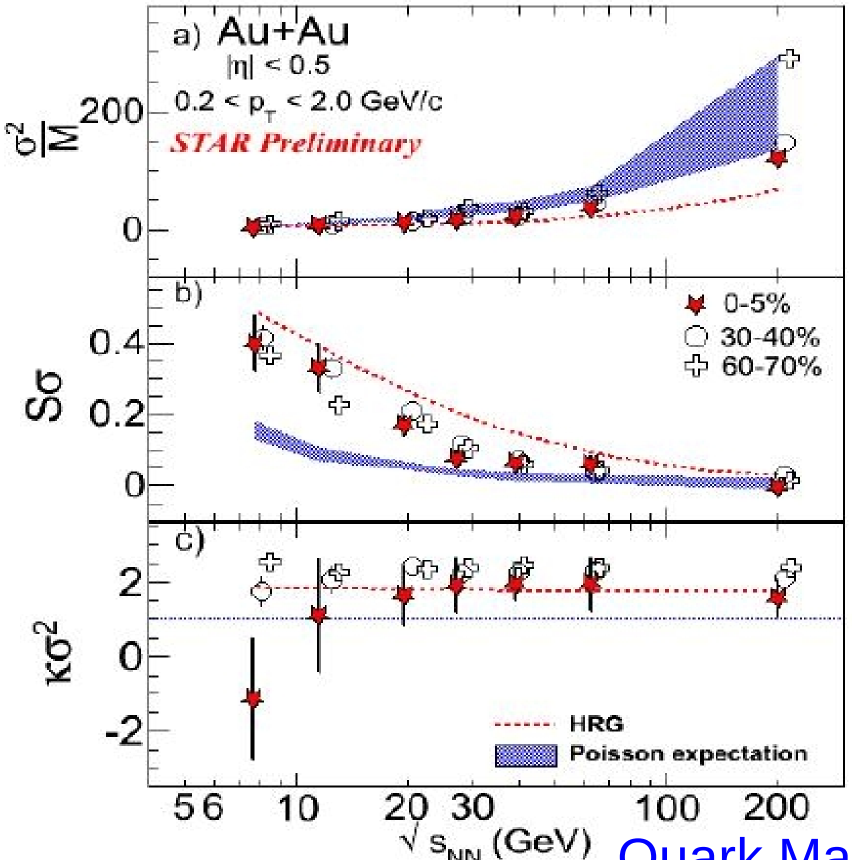


$T_c(\mu_B = 0)$: HotQCD, Phys. Rev. D85, 054503 (2012)

curvature: BNL-Bielefeld, Phys. Rev. D83, 014504 (2011)

Matter under extreme conditions

ratios of cumulants of net electric charge fluctuations: BES@RHIC



$$\frac{\sigma^2}{M} = \frac{\chi_2^Q}{\chi_1^Q}$$

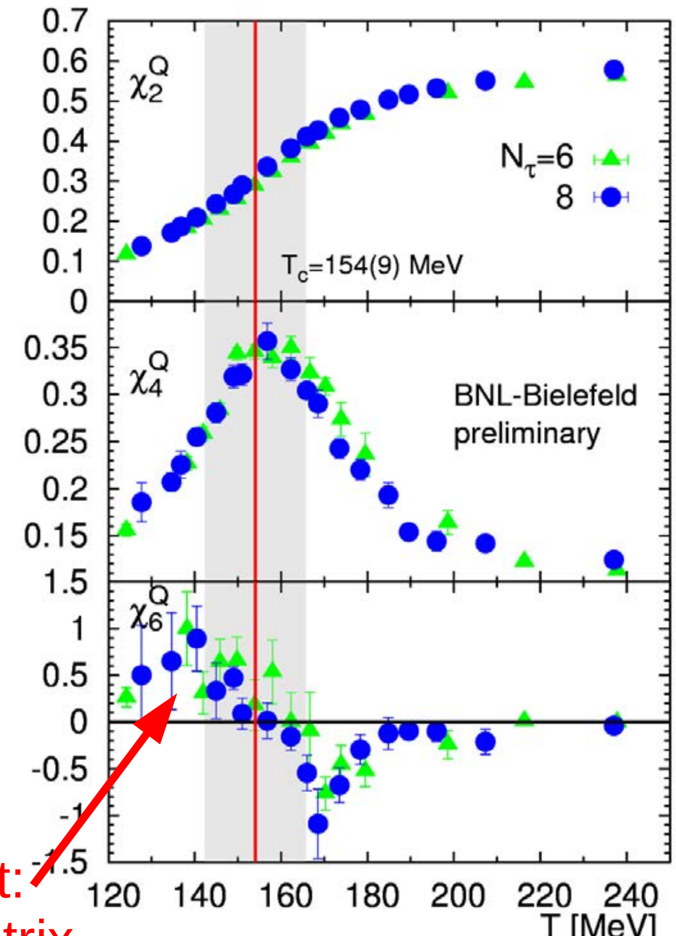
$$S\sigma = \frac{\chi_3^Q}{\chi_2^Q}$$

$$\kappa\sigma^2 = \frac{\chi_4^Q}{\chi_2^Q}$$

Quark Matter 2012

mean value (M), skewness (S) and kurtosis (κ) in appropriate units of the variance (σ^2)

lattice QCD calculation of some cumulants of electric charge fluctuations



each point:
~ 50M matrix inversions

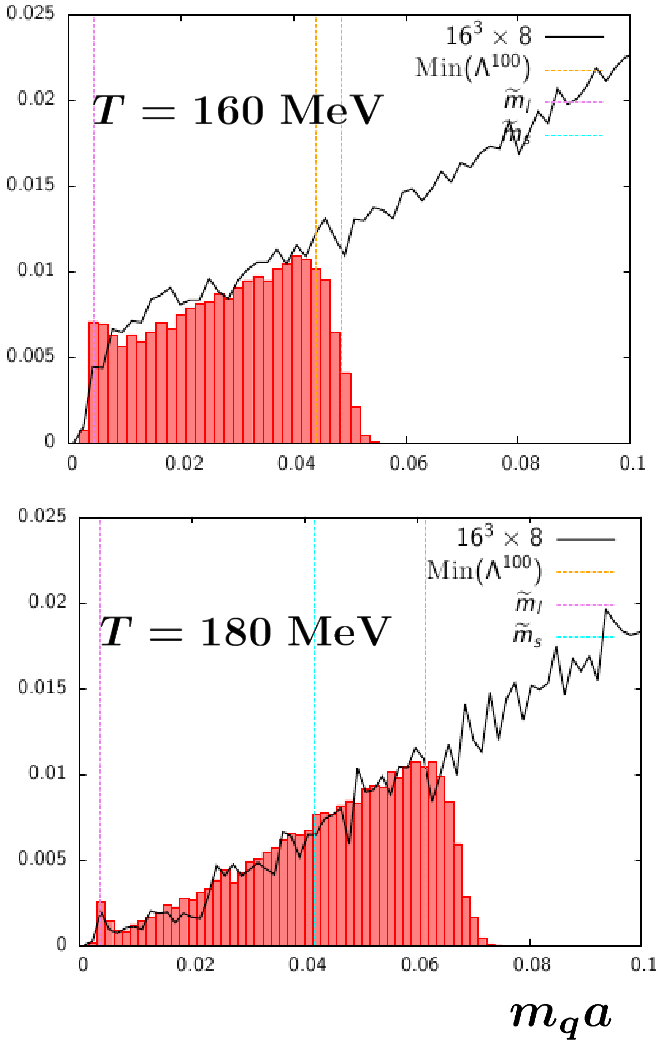
Quark Matter 2012

Matter under extreme conditions

USQCD Nuclear Physics

Domain Wall Fermions: a 5-dimensional discretization scheme;
advantage – exact chiral symmetry already for non-zero lattice spacing

$$N_\sigma^3 \times N_\tau \times L_s$$



eigenvalue distributions close to the QCD transition temperature on lattices of size $32^3 \times 8 \times 32$

$N_\sigma = 16$:

HotQCD Collaboration, arXiv:1205.3535

$N_\sigma = 32$:

gauge field configurations now generated by hotQCD on Sequoia

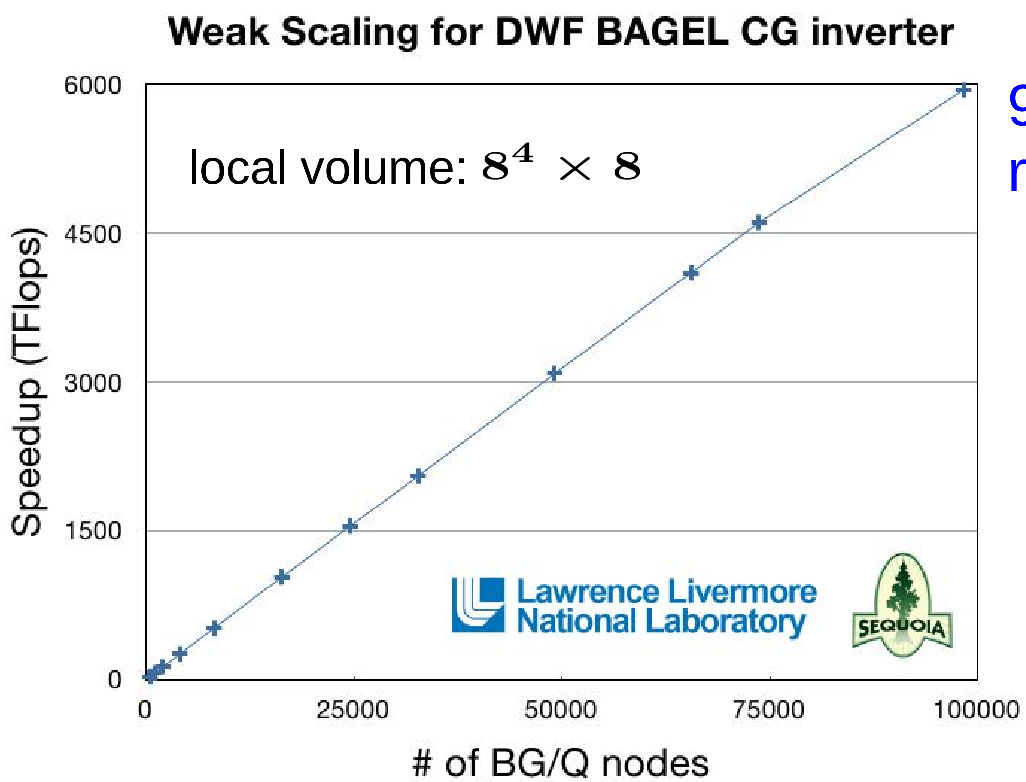
Computational Challenges

top priorities in Year 1:

- optimize gauge configuration generation code for BlueGene/Q
- tune inverter for all discretization schemes to get prepared for analysis projects; implement multi-grid on BG/Q; develop strategies for a staggered fermion multi-grid inverter

Domain Wall Fermions on BlueGene/Q

USQCD
Nuclear Physics



96 racks

Sequoia @ LLNL

early science time:
hotQCD Collaboration,
thermodynamics with DWF
on lattices of size up to
$64^3 \times 8 \times 24$

Code developed by Peter Boyle at the STFC funded DiRAC facility at Edinburgh

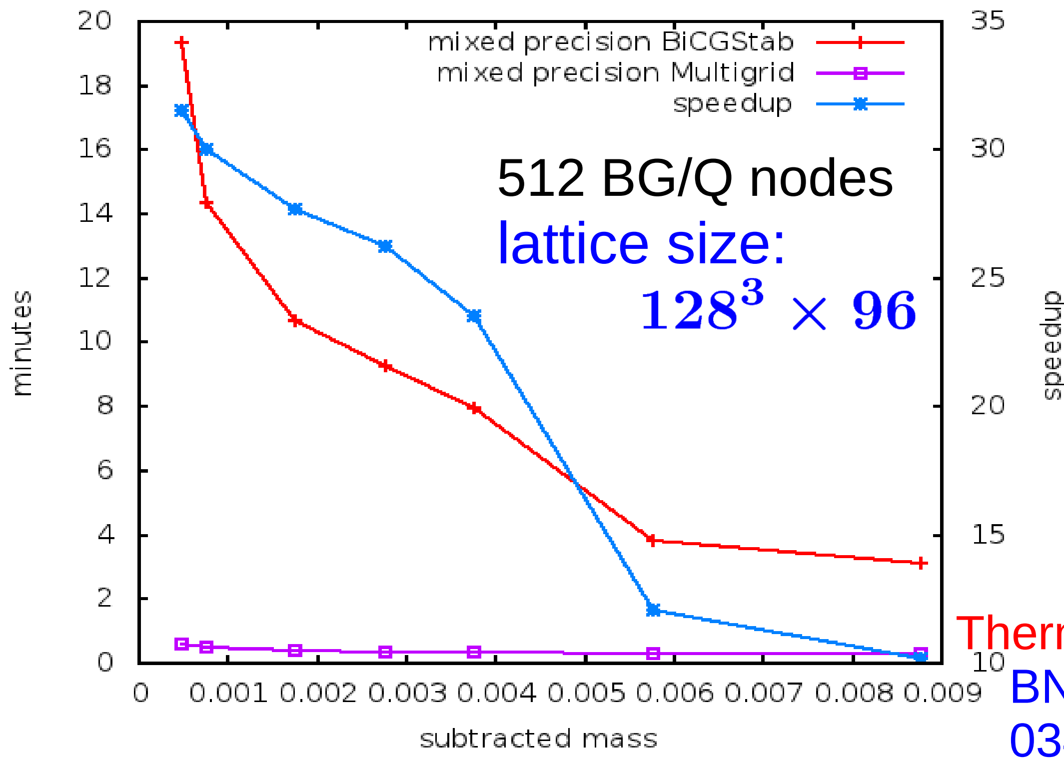
software suite: Columbia Physics System (CPS)

code development in collab. with UKQCD
(crucial parts are assembler coded):
C. Jung *et.al.*, SciDAC-2/3, USQCD

largest lattice $\sim 96^4 \times 96 \times 32$

(Thermal) Hadron spectra on BlueGene/Q

USQCD Nuclear Physics



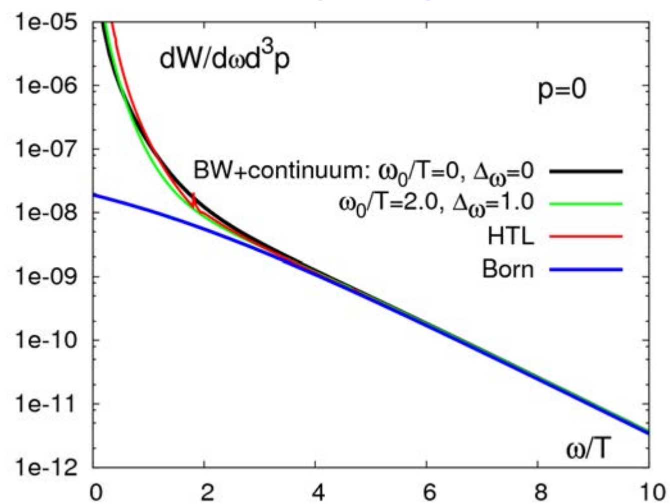
R. Brower (BU),
J. Osborn (ALCF),
BNL lattice group

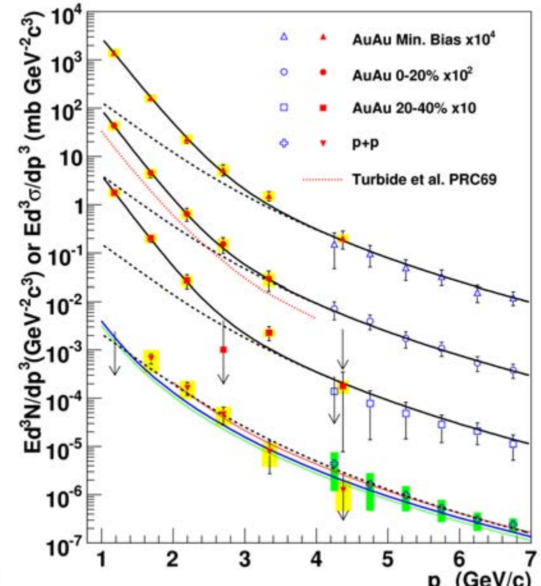
Mira @ ANL

Thermal photons@RHIC
PHENIX Collaboration,
PRL 104, 132301 (2010)

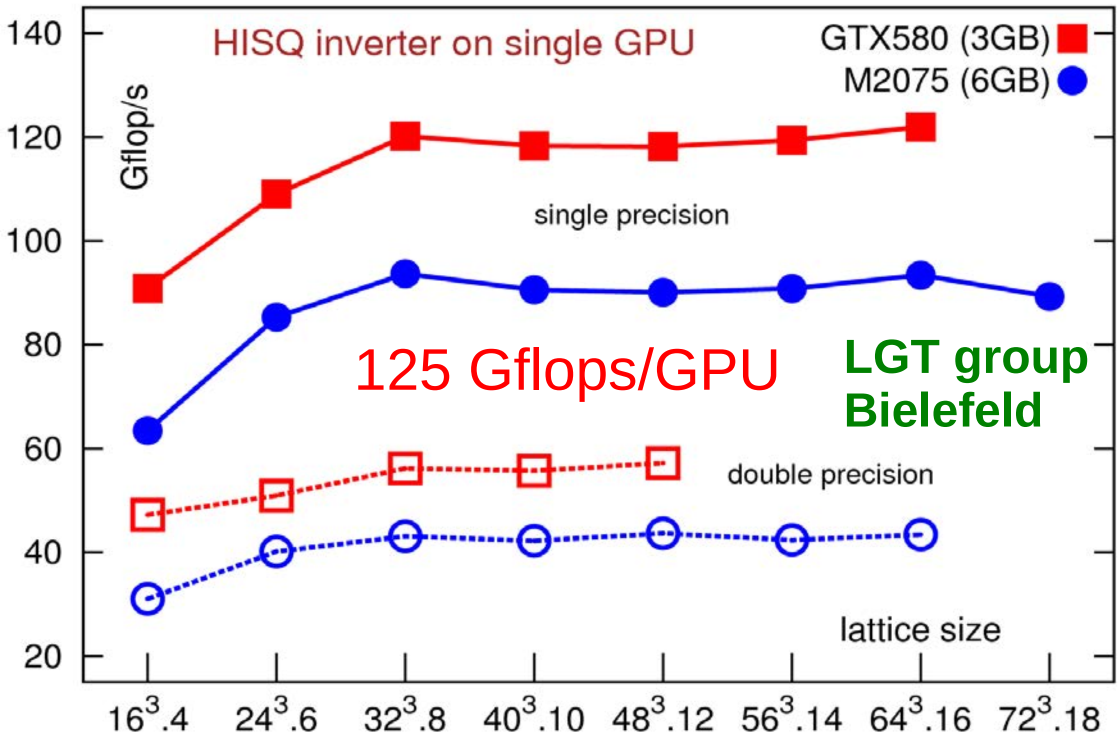
Thermal Dileptons in LGT,
BNL-Bielefeld, PRD83
034504 (2011)

optimization of Wilson-clover multi-grid inverter for thermal QCD, hadron spectroscopy and hadron structure studies





Dense QCD on graphics cards



USQCD GPU-cluster

10g @ Jlab

massive parallelizations possible
without sacrificing performance

- computations completely dominated by fermion matrix inversions
- at present, even the ultra-fine lattices fit into single GPU
- requires ~15K inversions on each gauge field configuration
- ideally suited for large scale GPU based architectures

HOT QCD on graphics cards

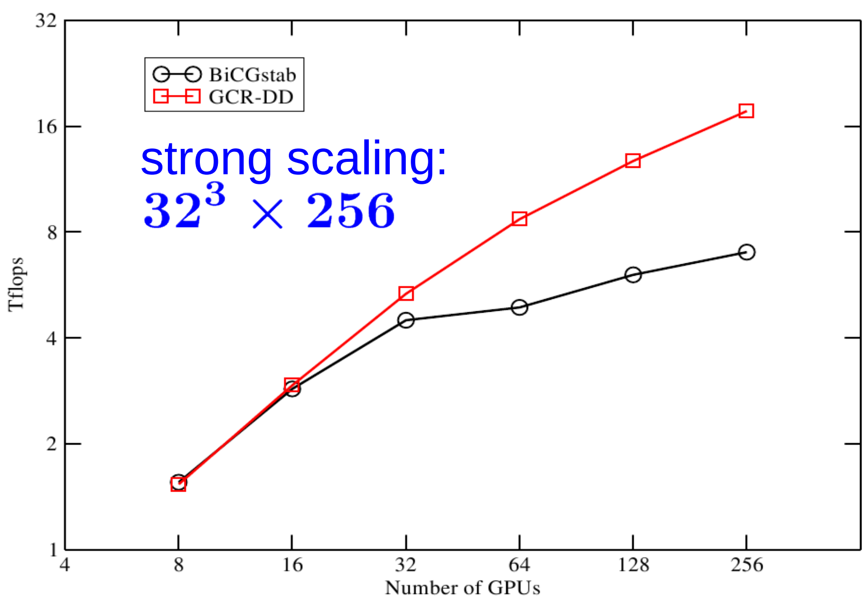
USQCD
Nuclear Physics

MILC, HEP USQCD SciDAC-3 project

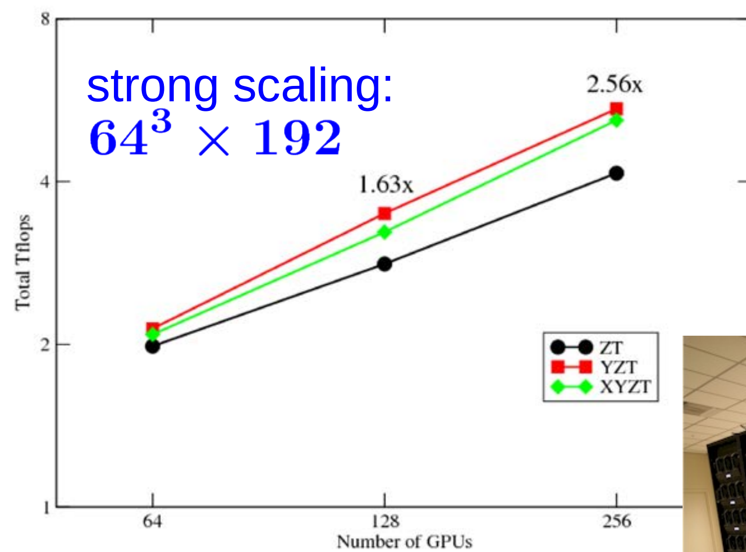
- generation and analysis of large lattices on GPUs requires the development of multi-GPU code
- inverter for HISQ (asqtad) and clover fermions

R. Babich et al., PoS LATTICE 2011, 033 (2011)

Wilson/clover inverter



HISQ (asqtad) CG inverter



hotQCD: equation of state

Edge @ LLNL

excellent scaling up to several hundred GPUs

Poster

I) Understanding the structure and interactions of matter in QCD
Robert Edwards (JLab)

II) Computing Properties of Hot and Dense Nuclear Matter from Quantum Chromodynamics, Frithjof Karsch (BNL)