Report from the computational nuclear physics town hall meeting I (Hot QCD)

Péter Petreczky

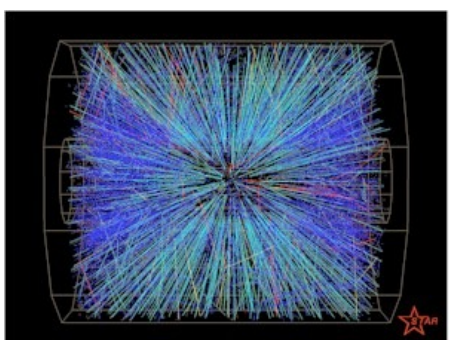
BROOKHAVEN NATIONAL LABORATORY

Computational nuclear physics (CNP) meeting, SURA, Washington D.C, July 14-15, 2014
http://www.jlab.org/conferences/cnp2014

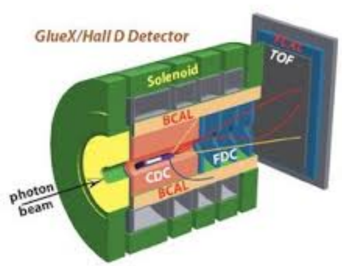
Organizers: A. Burrows, J. Carlson, R. Edwards, R. Hicks, F. Karsch, W. Nazarewicz, P. Petreczky, D. Richards, M.J. Savage
Writing committee: above + W. Detmold and R. Furnstahl

40 attendees

Hot QCD

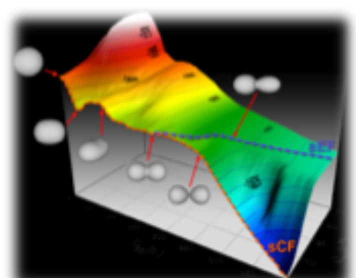


Cold QCD

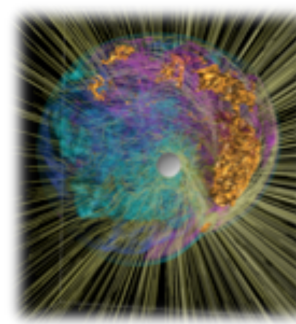


Talk by M. Savage

Nuclear structure



Nuclear astro



Goal of the CNP '14 meeting

Goal : to review the status of computational nuclear physics and identify hardware and personnel needs to accomplish DOE mission in NP,
i.e. providing support for the experimental NP program

Previous reports:

2009 : Exascale meeting – report,
http://science.energy.gov/ascr/news-and-resources/program-documents

2012 : CNP meeting in D.C. – whitepaper,
http://wwwold.jlab.org/conferences/cnp2012/

2013 : National Academy Report, "Nuclear Physics: Exploring the Heart of Matter"
http://www.nap.edu/catalog.php?record_id=13438
⇒ computations is the 3rd pillar of nuclear physics research

2013: Tribble Committee Report on implementing the 2007 Long Range Plan
http://science.energy.gov/np/nsac/reports/

2013: Whitepaper of USQCD:
http://www.usqcd.org/documents/13thermo.pdf,
http://www.usqcd.org/documents13nuclear.pdf

Here: the case in context of RHIC (based on inputs from S. Bass, U. Heinz, D. Molnar, B. Schenke, S. Schlitling, R. Venugopalan, thanks !)

Computational needs for RHIC physics

- Thermalization and initial conditions:

Early time dynamics is characterized by large occupation number of gluons

$\Rightarrow$ classical-statistical simulations

- Equilibrium properties of QCD matter:

$\Rightarrow$ Lattice QCD calculations of transition temperature, equation of state, in-medium hadron properties (spectral functions), transport coefficients

- Fireball evolution:

Local thermal equilibrium + expansion

$\Rightarrow$ initial conditions + hydrodynamics matched to hadron transport at later stages

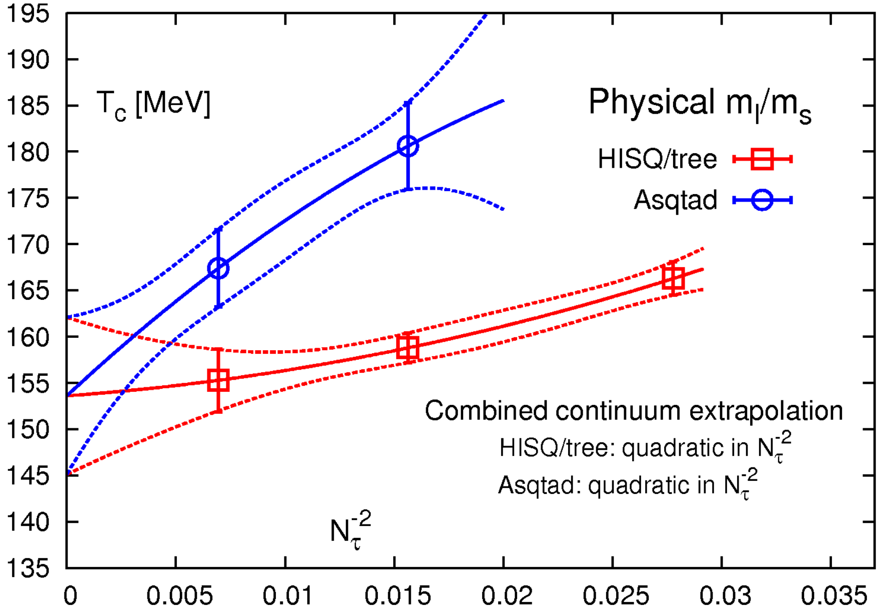
$\Rightarrow$ 3+1 dimensional hydrodynamic calculations with fluctuating initial conditions + transport match to experimental results on event-by-event basis

Accomplishments: LQCD

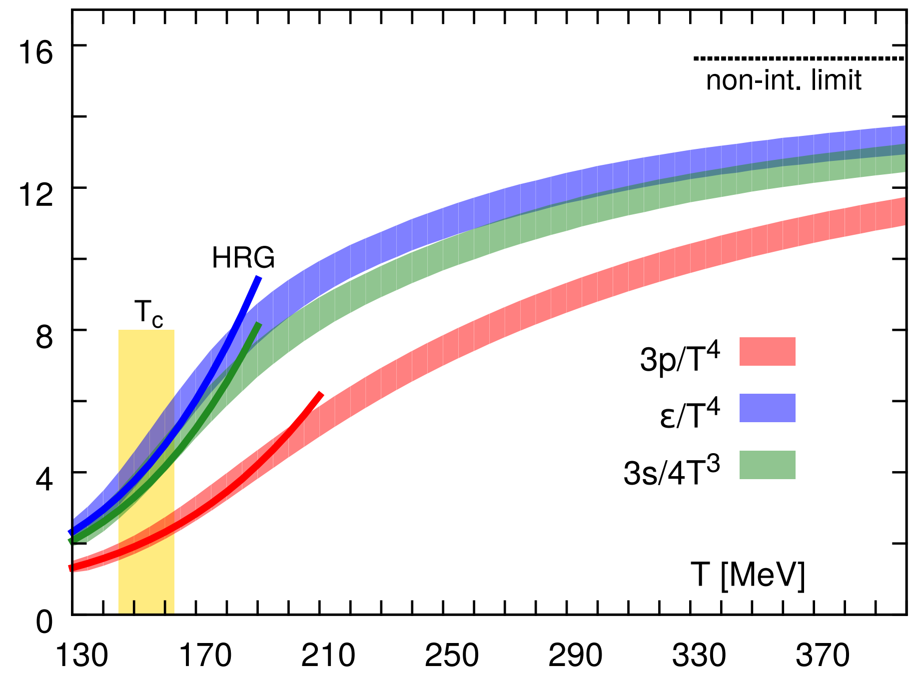
The QCD transition temperature and equation of state have been calculated for physical quark masses in the continuum limit

Bazavov et al, PRD85 (2012) 054503

$T_c = (154 \pm 8 \pm 1(scale))\text{MeV}$



Bazavov et al, arXiv:1407:6387



Input for hydro at RHIC model and matching hydro with hadron transport

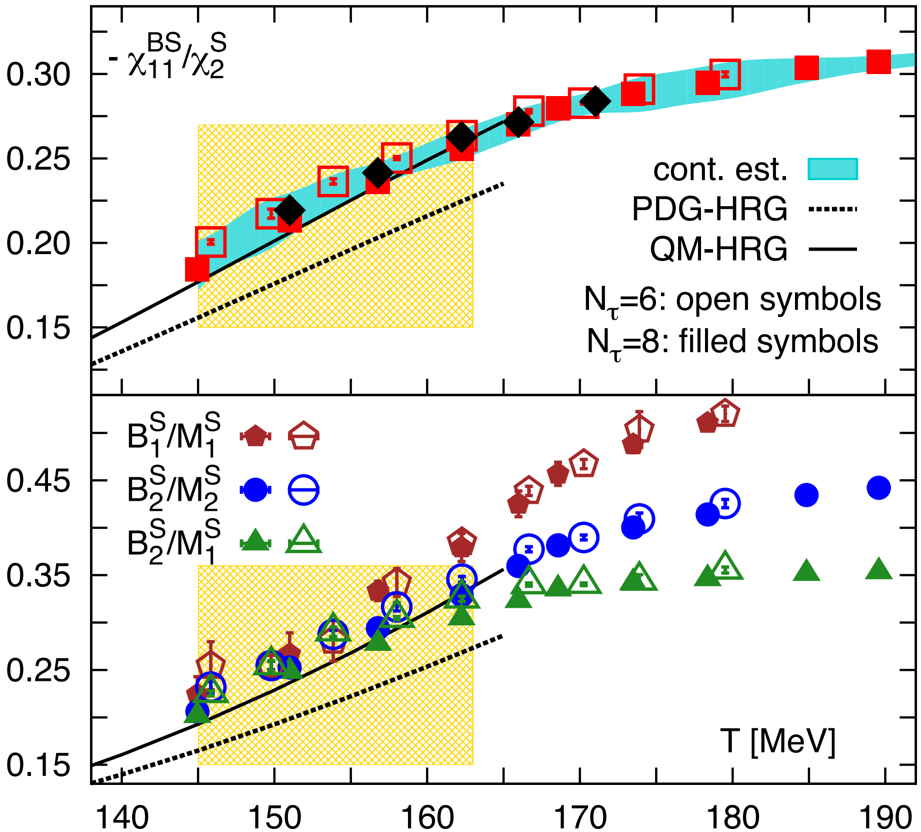
Computational costs: ~ 150 M core hours

Accomplishments: LQCD (cont'd)

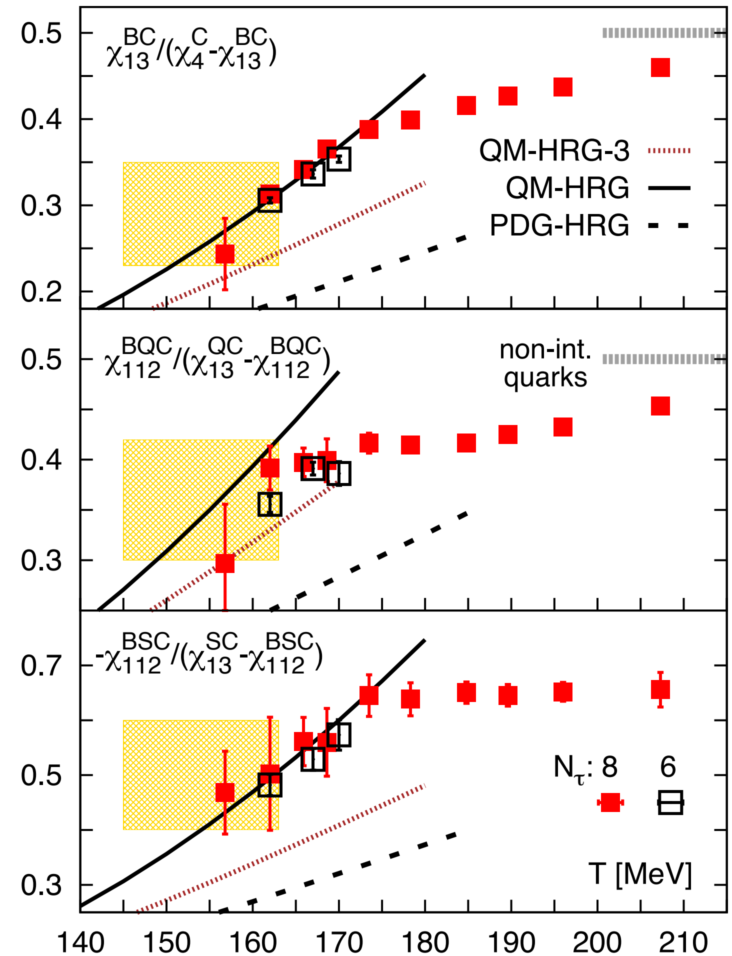
Fluctuations of conserved charges: even-by-event fluctuations at RHIC and freeze-out

Bazavov et al, PRL113 (2014) 072001; PLB737 (2014) 210; see talk by Mukherjee, Sep. 13, am

Strange baryon to meson pressure



Charm baryon to meson pressure

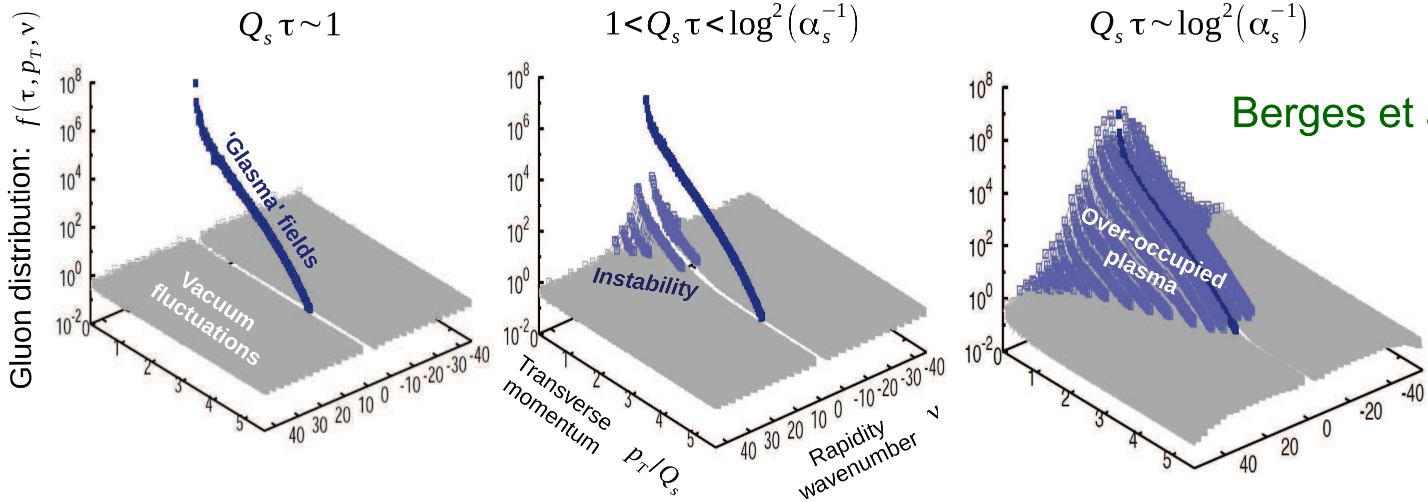


Evidence for "missing" strange baryons
⇒ Lower freeze-out temperature for strange particles at RHIC and LHC

Computational costs: ~ 250 M core h

Accomplishments: initial dynamics and phenomenology

Classical-statistical calculations of gluon distribution at early times



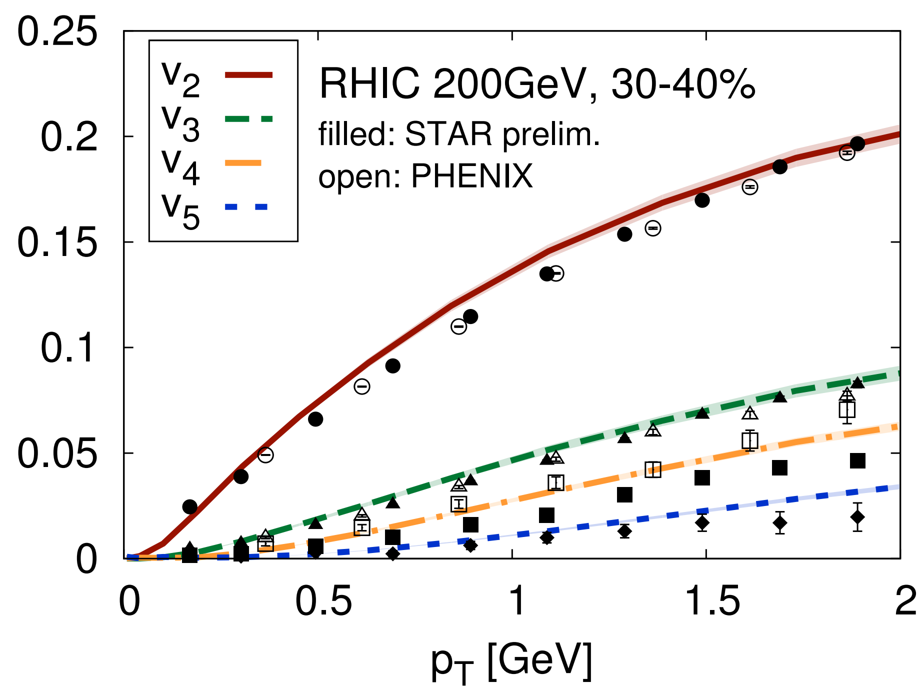
Berges et al, arXiv:1409.1638

New since 2007 is the need to include event-by-event fluctuations

Event-by-event 3+1 D hydro
(no hadron transport, *T*-independent *η/s* or only with simplified *T*-dependence)

Gale et al, PRL 110 (2013) 012302
(see also talk by Schenke, Sep. 13, am)

< 3 M core hours



Computational challenges (cont'd)

- Classical-statistical simulations of early time dynamics:

Current calculations are done in pure glue theory (~ 2M core h),
including fermions in simulations x100
⇒ 200 M core h
also need more realistic nuclear wave functions from JIMWLK

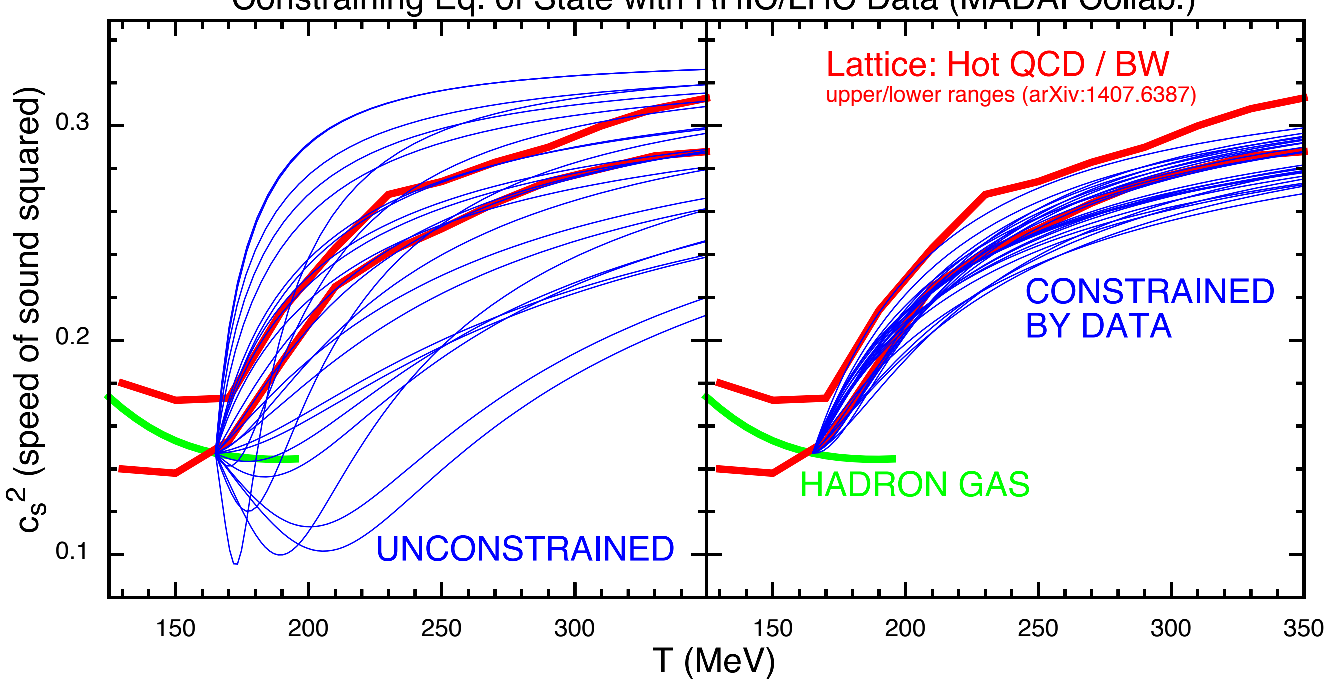
- Model to data comparison: 3D hydro + hadron transport with many initial conditions and set of physical parameters (e.g. *η/s, EoS, ς/s*)

⇒ 50 M core h

Talk by Pratt, Sep. 13, pm

More limited by manpower than computer power

Can be done using capacity computing



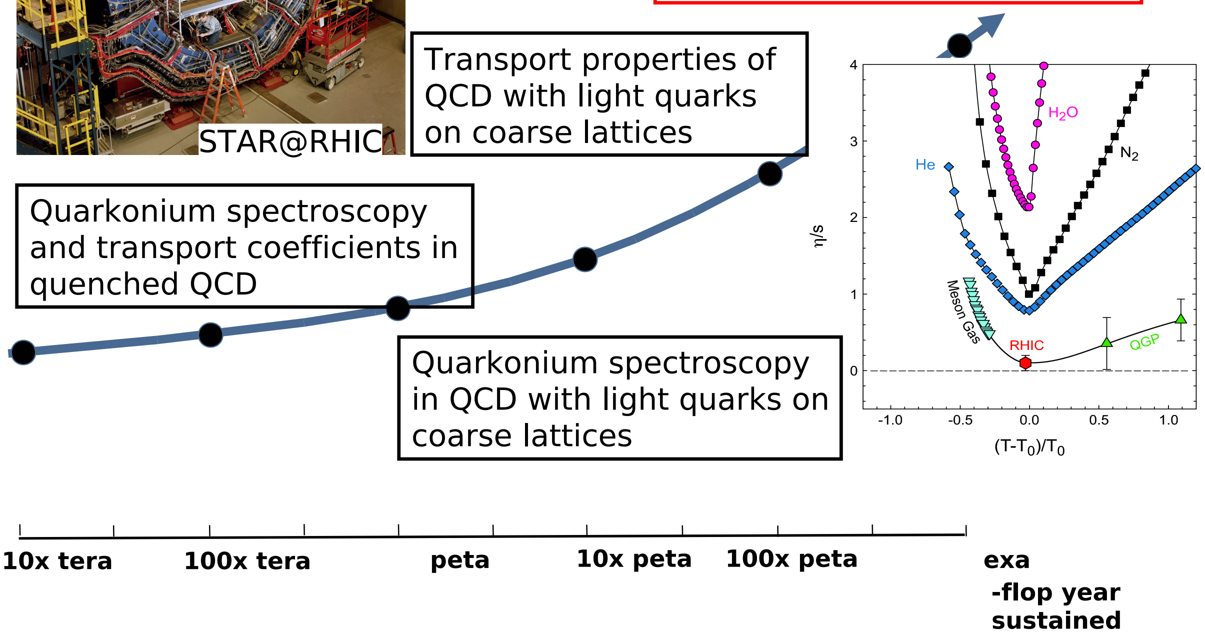
Computational challenges

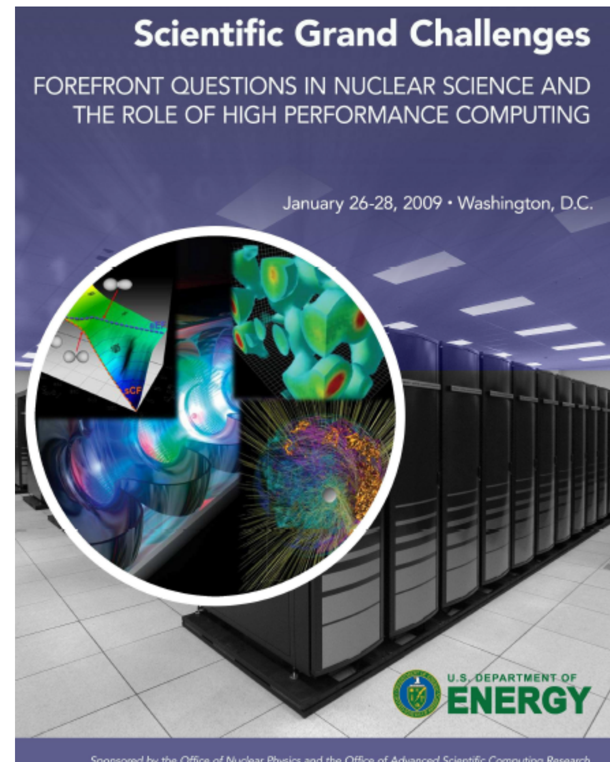
- Lattice QCD: equation of state and fluctuations of conserved charges at non-zero baryon density (BES program at RHIC) in continuum limit, study of meson spectral functions (quarkonia, photons/dileptons), transport coefficients

⇒ 3 Pflops*years (≈13,000 M core h) in short term

http://www.usqcd.org/documents/13thermo.pdf

- Melting temperatures and broadening of heavy quark bound states in QCD
- Transport properties of hot, strongly interacting matter





Findings of the CNP '14 meeting

Hardware Requirements for accomplishing DOE mission:

- Continued access to Leadership-Class computing
- ASCR , INCITE and ALCC awards
- constant fraction of US facilities (with Moore's Law growth)

- Significantly increased Capacity computing resources
- not ASCR, e.g. USQCD hardware, NSF centers
- in addition to NERSC awards

Personnel Requirements for accomplishing DOE mission:

- Enhanced HPC-trained workforce is required to execute the NP mission
- Enhanced collaborations with Computer Scientists, mathematiciar and between Nuclear Physicists, are critical, e.g. SciDAC projects"

"computers do not become faster only wider" (B. Messer)

e.g., development of efficient code for Intel Xeon Phi KL chip

NERSC Cori : 30Pflops in 2016 and NESAP code readiness program:

QCD thermo is one of the 20 approved projects of NESAP

Outcome of the CNP '14 meeting

- Recommendation: Realizing the scientific potential of current and future experiments demands large-scale computations in nuclear theory that exploit the US leadership in high-performance computing. Capitalizing on the pre-exascale systems of 2017 and beyond requires significant new investments in people, advanced software, and complementary capacity computing directed toward nuclear theory.

- Request: To this end, we ask the Long-Range Plan to endorse the creation of an NSAC subcommittee to to develop a strategic plan for a diverse program of new investments in computational nuclear theory. We expect this program to include:

  1) new investments in SciDAC and complementary efforts needed to maximize the impact of the experimental program;
  2) development of a multi-disciplinary workforce in computational nuclear theory
  3) deployment of the necessary capacity computing to fully exploit the nation's leadership-class computers;

with support ramping up over five years towards a level of around $10M per annum.

Unanimously endorsed by the CNP'14 meetings participants

For more details see:
http://www.jlab.org/conferences/cnp2014/compnuc2014.pdf