The program of USQCD

Lattice gauge theory briefing for OASCR, OHEP, and ONP

USQCD Collaboration

http://www.usqcd.org

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Germantown
March 15, 2011
The USQCD Collaboration

- Represents almost all of the lattice gauge theorists in the US; ~ 145 people.

- Was formed in 1999 at the request of the DOE to organize computing hardware and software infrastructure for lattice QCD in the US.

- Physics calculations are done by smaller component collaborations within USQCD:
  - Fermilab, HPQCD, JLab, LHPC, LSD, MILC, NPLQCD, RBC, ...
Major areas of physics research

• Standard model (Fermilab, SLAC, KEK, LHC-b)
  • Hadron spectrum; leptonic and semileptonic weak decay; meson-anti-meson mixing; the parameters of the standard model: the CKM matrix, the quark masses, and the strong coupling constant, ...

• Beyond the standard model (LHC)
  • Technicolor; dynamical SUSY breaking, ...

• High-temperature QCD (RHIC)
  • De-confinement temperature; QCD plasma equation of state; viscosity coefficients...

• Nuclear physics (JLab)
  • Resonance and exotics spectra, scattering lengths; and phases shifts; hadronic structure, ...
Science drivers: Fermilab

BBbar mixing was Fermilab’s most important discovery of the last ten years. Lattice QCD calculations enabled this measurement to constrain the standard model’s CP violating parameters \( \rho \) and \( \eta \) more tightly than ever before. (\( \rho \) and \( \eta \) govern the mixing of matter with antimatter in the SM.) The experiment has been done to 0.5% precision, so lattice calculations that match that precision are urgently needed. This is one of many such experiments.

Statement from Pier Oddone: Lattice QCD calculations will make the data we obtain from quark factories (both electron-positron colliders as well as the Tevatron and LHC) far more useful in determining the fundamental parameters of the standard model and revealing any model inconsistencies indicative of new physics. For example, the existence of good lattice calculations allowed Fermilab's discovery of BsBs-bar mixing to make an important bound on the CP violating elements of the CKM matrix. Much more accurate calculations of this and other quantities are now needed to make full use of the data from the Fermilab's program

HEPAP has made several strong endorsements of the importance of lattice calculations (most recent in 2008).
Science drivers: BNL

The lattice equation of state for the hot QCD plasma is fitted to an analytic ansatz, which at low-T turns into the analytic results for a hadron resonance gas and at high T is consistent with perturbation theory. This parametrization is used in 3d-hydro codes which model the expansion/cooling of matter formed in a RHIC heavy ion collision. This allows to calculate various observables, e.g. particle rates, or flow properties, that arise from emission at every stage of the expansion.

Statement from Tom Ludlam: The lattice QCD calculations performed at BNL have direct relevance for the experimental program at RHIC, where an accurate determination of the equation of state of dense QCD matter with lattice gauge calculations is of central importance to the understanding of hydrodynamic properties from experimental data. In addition, we are counting on the USQCD research program to provide guidance in the search for a QCD critical point in heavy ion collisions, and an understanding of the properties of strongly interacting matter near this landmark point on the QCD phase diagram.
**Science drivers: JLab**

GlueX at Jlab@12 GeV will seek mesons with exotic quantum number: This calculation suggests the presence of exotic mesons in an energy range accessible to GlueX. A more ambitious program including coupling to decay channels is underway.

**Statement from Hugh Montgomery:** The national efforts of the USQCD collaboration are key to the success of the lattice program at Jefferson Lab... A continued strong national program will ensure both the algorithmic developments, and the software infrastructure, to further exploit both frontier leadership-class and special-purpose computers, and thus provide the calculations that will capitalize on the DOE investment in the Jefferson Lab experimental program.

**NSAC, 2007 Long-Range Plan:** We recommend completion of the 12 GeV CeBAF Upgrade at Jefferson Lab... It will... ...test definitively the existence of exotic hadrons, long- predicted by QCD as arising from quark confinement.
USQCD organization

USQCD oversees on behalf of the US lattice community:

- SciDAC software grant (OHEP, ONP, OASCR).
  - ~$2.3 M/year since 2001.
  - Creates community libraries, optimized production programs, research on new approaches (GPUs are hot now), ...

- Community Incite grants on ASCR Leadership Computing Facilities.
  - Last year, used 187 M core-hours at ALCF, 40 M core-hours at ORLCF.

- Design and deployment at national labs of cost-efficient capacity hardware funded by LQCD-ext (OHEP and ONP).
  - ~ $4 M/year.
  - Infiniband clusters, now adding GPUs.
USQCD Executive Committee

The Executive Committee is responsible for writing USQCD’s proposals and for appointing the members of the other committees.

Executive committee:
Paul Mackenzie (chair), Rich Brower, Norman Christ, Frithjof Karsch, Julius Kuti, John Negele, David Richards, Steve Sharpe, Bob Sugar

In Germantown today. New to the EC.

Software committee:
Rich Brower (chair)

Scientific program committee:
Frithjof Karsch (chair)
USQCD Software Committee

Software Committee:
Richard Brower (chair), Boston University, Carleton DeTar, University of Utah, Robert Edwards, JLab, Rob Fowler, UNC, Donald Holmgren, Fermilab, Robert Mawhinney, Columbia University, Pavlos Vranas, LLNL, Chip Watson, JLab

• Organizes software work done under our SciDAC grant.
• Weekly conferences calls with 12-20 people, 40 people on mailing list.
• SciDAC grant pays for less than half of our software work.
  • $2.3 M/year, ~10 FTEs.
  • Much of work is done by people on their regular salaries working to accomplish the goals of their physics collaborations.
USQCD Scientific Program Committee

Frithjof Karsch, BNL (chair), Simon Catterall, Syracuse, Robert Edwards (Jlab), Taku Izubuchi, BNL, Martin Savage, Washington, Junko Shigemitsu, Ohio, Doug Toussaint, Arizona.

- Allocates time annually on USQCD’s hardware resources.
  - Highest capability computing through community Incite grant at Leadership Computing Facilities: ALCF and ORLAF.
  - Dedicated high capacity, cost-efficient resources at science labs.

- Advises the Executive Committee on scientific priorities.

- Charged with optimizing the scientific program consistent with the scientific goals stated in USQCD’s proposals.

- Allocated time for 41 separate physics projects in 2010.
USQCD timeline

USQCD Executive Committee formed.

Software grants
First two five-year SciDAC grants for lattice computing R&D.

SciDAC extension
SciDAC-3?
Absolutely essential for making effective use of Leadership Computing Facilities and our dedicated hardware, and for accomplishing our physics objectives.

Hardware grants
Construction of the QCDOC.
Funding from HEP and NP for hardware through LQCD and LQCD-ext projects.
The lattice QCD computing problem

Approximates the continuum theory by defining the fields on a four dimensional space-time lattice.

Quarks (*complex three vectors*) are defined on the sites of the lattice, and the gauge field *gluons* (*complex 3x3 matrices*) on the links.

Monte Carlo methods are used to generate a representative ensemble of gauge fields. Relaxation methods for sparse matrices are used to calculate the propagation of quarks through the gauge field.

Continuum quantum field theory is obtained in the zero lattice spacing limit. This limit is computationally very expensive.
Algorithms and methods

An ensemble of gauge configurations is created with Monte Carlo methods. A chain of configurations is made, one from the previous.

Once created, each configuration can be analyzed in parallel.

The main component of both jobs is solving a sparse matrix equation $MV = S$, with, for example, the bicongradstab algorithm.
Two main components of a typical lattice calculation

Generate $O(1,000)$ gauge configurations on a leadership facility or supercomputer center. Tens of millions of BG/P core-hours.

Transfer to labs for analysis on clusters. Comparable CPU requirements.

Gauge configuration generation:
a single highly optimized program,
very long single tasks,
moderate I/O and data storage.

Hadron analysis:
Large, heterogeneous analysis code base,
10,000s of small, highly parallel tasks,
heavy I/O and data storage.

TB file sizes

Two comparably sized jobs with quite different hardware requirements.
Current hardware resources

- Last year, used 187 M core-hours at ALCF, 40 M core-hours at ORLCF.
  - Expect about the same this year.
- The SPC is allocating on USQCD’s dedicated hardware
  - 262.3 M Jpsi-core hours on clusters at JLAB and FNAL
  - 4.2 M GPU-hours on GPU clusters at JLAB and FNAL
SciDAC software effort

• Organized the USQCD Software Committee

• SciDAC software program is essential for using hardware resources efficiently and accomplishing our physics goals.
  • leadership Incite and LQCD-ext

• Includes community libraries for QCD programming, called the QCD API, optimized high-level QCD codes, porting to new platforms, work with SciDAC centers and Institutes and with computer scientists.
The QCD API

Application Layer

Chroma    CPS    MILC

MDWF      QOP

Dirac Operators

QDP/C     QDP++   QIO

QLA       QMT Threads

QMP Message Passing

Tools

QA0, GCC-BGL, Workflow, Viz.

+ tools from collaborations with other SciDAC projects e.g. PERI
The QCD API

Active area of development now.

+ tools from collaborations with other SciDAC projects e.g. PERI
Community software

E.g., Chroma

• E.g., chroma
The USQCD SciDAC program has enabled us to make optimal use of the hardware resources available.

In 2008, Chulwoo Jung and James Osborn had QCD software for the BG/P ready to go when it became available at the ALCF. Chulwoo’s codes were able to identify a hardware error in the machine when it was delivered.

When Blue Gene/P use began at the ALCF in 2008, USQCD was one of only a few projects that had highly optimized software in place, and was the only one of these with a large-scale, three-year program mapped out. As a result, we able to make full use of the machine when it was relatively empty.
The USQCD SciDAC program has enabled young people to perform important physics projects on their own without investing a lot of their own time writing software.

The bounds in the $\rho$-$\eta$ plane arising from $KK$bar mixing come from the well-established RBC Collaboration and separately from Aubin, Laiho, and Van de Water, who were post-docs when they began.

Aubin et al. used Chroma community code developed at JLab, received advice form Balint Joo on running it and using the QCD API for additional programming, got help from Don Holmgren and colleagues at Fermilab using the Fermilab clusters, and advice from Chulwoo Jung on using the BG/P.
Collaboration with SciDAC Centers and Institutes: TOPS

- 1990: MG for QCD was attempted with limited success for weak coupling.

- 2005-2011: Large research Applied Math/Physics collaboration for Multigrid QCD. (TOPS, NSF ITR and PetaApps support; David Keys et al. + BU lattice group).


- 2009: 20x speed up in production code at small mass for 4-d Wilson-clover solver, after overhead.
Collaboration with SciDAC Centers and Institutes: PERI
Other activities

- Workshops with experimentalists
- Workshops with applied mathematicians
- Summer schools

See list in Reference Material at the end of the slides.
Coming hardware resources

Discuss clusters & GPUs, BG/Q, Blue Waters, Cray
## The next ten years of hardware

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<th>2010</th>
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Lattice calculations in 2020
The next ten years of hardware

Today’s 12-core chips are expected to evolve into 1,000-core or 10,000-core chips.

Memory per chip will grow by 100x.
Each core will communicate quickly only with nearby memory on chip.
~Six levels of (user-controlled?) cache.

We are taking the first steps toward dealing with these problems by solving the first signs of them on today’s computers.
Infiniband Clusters and GPUs

3 or 4 slides
GPUs

- Massively parallel
  - 480 cores on the Nvidia GTX 480 (or “Fermi”).
- x10 peak price/performance vs. clusters
- But ... very low memory/core, bandwidth/core
  - E.g., GTX 480 has 6 MB (!)/core, 370 MB/sec/core.
  - Problem will grow worse on all computers throughout this decade. Lessons learned now are important.
  - “Cores are like children: cheap to produce, expensive to feed.” (Bill Dally)
- Big coding investment needed.
GPUs: current issues

- Lattices up to around $32^4$ can fit into a single GPU.
  - Communications for QCD code in one direction have been implemented, with scaling up to 32 GPUs.
  - Multidimensional scaling underway.
- Optimization must reduce data movement, floating point not as important.
  - Easily reconstruct 8 or 12 of 18 SU(3) matrix components. Transfer only half.
  - Calculate desired double precision solution of $MV=S$ in single or half precision, use erroneous double precision residual of result $r=MV-S$ as a source to “polish” the result to double precision.
GPUs: computing achievements

- Sustained 4 teraflops on a 32 GPU cluster in weak scaling tests.
- Bigger challenge: strong scaling.

![Graph showing strong scaling results](image_url)
GPUs: physics achievements

- The JLab resonance and exotics calculations indicate exotics in the region of interest to GlueX.

- Next step in JLab program is inclusion of disconnected diagrams and coupling to decay channels.

- Requires great advances in both computing efficiency (GPUs) and methodology (“distillation”) to be tractable.

- Project is ideal for GPUs because it is almost entirely propagator calculation.

- On GPUs, over an order of magnitude gain in computation/$ compared with Infiniband clusters.
GPUs: future

- Will a standard software environment emerge?
  - At present, big coding investment is required. Our programming is done in CUDA; will OpenCL become a standard?

- Can USQCD lower level libraries be made to work with GPUs?
  - E.g., can QDP be implemented? How?

- Can fixed-size problems be made to work on large numbers of GPUs?

- Will GPUs be the wave of the future?
  - Next Oak Ridge machine may be Cray XE6 with Nvidia GPUs, will dwarf Jaguar.
  - GPUs are one possible path to the exascale.
The Blue Gene family arose from computers purpose-built for lattice QCD by Norman Christ’s group at Columbia.
The BG/Q

- A 10-petaflops (peak) will open for early science at the ALCF in 2012

- The Columbia group participated in the design of the BG/Q. They designed and implemented:
  - The interface between the processor core and the level-2 cache.
  - The look-ahead algorithms used to prefetch data from level-2 cache and main memory, anticipating misses in the level-1 cache.

- The cache management problem on current computers will become nightmarish on exascale computers. (6 levels of cache?)

- These BG/Q prefetching methods may serve as an approach to the exascale cache problem. (Pete Beckman.)
• Lattice QCD code of Columbia's UK collaborator Peter Boyle was first production code to run on prototype BG/Q hardware:
  • Was used to optimize the design.
  • Now being used to identify bugs in early hardware.
  • Currently determining Kπ3 amplitudes at the physical pion mass on BG/Q prototype hardware at Watson.

• Chulwoo Jung is creating production high-T QCD code that will also be running at Watson in a week or two.

• Lessons learned and likely segments of code will form the basis of the port of QLA, QDP, etc. to the BG/Q.

• USQCD expects to have optimized code ready by the beginning of Early Science.
Blue Waters

- 10 petaflops peak, to arrive at NCSA in 2012.

- USQCD **is sure** to have optimized production code ready to go when Blue Waters is accepted because MILC code is one of its acceptance tests. IBM doesn’t get paid until MILC runs at a sustained petaflop.

- MILC and Chroma running on prototype hardware (Joo, Gottlieb).
The Cray

- **Current machine at ORNL: Cray XT5 (Jaguar).**
  - Utilizing mixed precision solvers to improve performance
  - Employing a hybrid threaded-MPI model to exploit the multi-core Cray nodes

- **Coming machine: Cray XE6 in 2012?**
  - Likely with GPUs.
  - 20 petaflop peak. (Current 2.3 PF peak on Jaguar.)
  - Gemini interconnect (like the current XE6 at NERSC).
Achievements: computing

- A mission-critical software infrastructure:
  - QCD API libraries
    - QMP, QLA, QDP, QIO, level 3 subroutines, work with ILDG...
  - Community codes
    - MILC, Chroma, CPS ...
  - Program of porting, optimization, and algorithms

- Highly efficient use of Incite resources for capability computing.

- Creation and deployment of highly cost-efficient Infiniband clusters and GPU clusters for capacity computing.

Exit interview of 2009 LQCD review: "This is a large, integrated effort in hardware, algorithms, software, and science that is an exemplar of best practices, not only in lattice gauge theory, but across computational science.” Richard Kenway.
Achievements: physics

• RHIC: equation of state and Tc to sufficient accuracy to firmly constrain heavy-ion collision models for the first time (HotQCD, RBC)


• JLab: Single particle excited state and exotics spectrum; determination of orbital angular momentum in nucleon; $KK$, $K\pi$ scattering lengths.

• Fermilab: Many of the fundamental parameters of the Standard Model have been determined more accurately than ever before by USQCD collaborations.

  • Light quark masses, charm quark mass, strong coupling constant, $V_{cb}$ from $B\to D^* l\nu$, $V_{ub}$ from $B\to\pi l\nu$, constraints on $\rho$ and $\eta$ from $BB$bar and $KK$bar mixing ...
Physics challenges of the coming decade

- Tevatron, KEK, LHC-b: the standard model
  - Increase precision of weak matrix elements by an order of magnitude. (Experiments already completed require this.)

- CMS, Atlas: Beyond the standard model
  - Extend lattice techniques to new gauge theories.

- RHIC: heavy ion physics
  - Precision calculation of QGP transport coefficients for heavy-ion phenomenology.
    - (NSAC Milestone 2014 DM9: Perform calculations including viscous hydrodynamics to quantify, or place an upper limit on, the viscosity of the nearly perfect fluid discovered at RHIC.)
Physics challenges of the coming decade

- **JLab: nuclear physics**
  - Decays and EM properties of resonance and exotic mesons and baryons.
  - Flavor singlet and gluon contributions to hadronic structure.
    - NSAC milestone HP-9: Perform lattice calculations in full QCD of nucleon form factors, low moments of nucleon structure functions and low moments of generalized parton distributions including flavor and spin dependence.
  - Precision calculation of nucleon-nucleon interaction.
    - NSAC milestone HP10: Carry out ... lattice QCD calculations of hadron interaction mechanisms relevant to the origin of the nucleon-nucleon interaction.
Conclusions

• The Office of Science’s experimental programs will continue to have urgent needs for improved lattice calculations throughout the coming decade.

• USQCD’s software, hardware, and physics programs form a tightly integrated, coherent whole.

• OHEP and ONP experimental programs and OASCR leadership computing have directly profited from lattice QCD SciDAC work funded by one of the other offices.

• Strong participating from each office benefits all three offices.
March 6, 2011

Dr. Amber Boehnlein
U.S. Department of Energy
Germantown, MD  20874-1290

Dr. Tim Hallman
U.S. Department of Energy
Germantown, MD  20874-1290

Dear Amber and Tim,

I am writing to express BNL’s support for the SciDAC funded software development program of the USQCD collaboration and its lattice QCD based research program.

As you know, Brookhaven has strong lattice groups in both its high energy and nuclear physics programs. These groups are participants in the USQCD collaboration, and rely heavily on the dedicated QCDOC computing facility at BNL as well as other hardware operated by USQCD at JLab and FNAL. The lattice QCD calculations performed at BNL have direct relevance for the experimental program at RHIC, where an accurate determination of the equation of state of dense QCD matter with lattice gauge calculations is of central importance to the understanding of hydrodynamic properties from experimental data. In addition, we are counting on the USQCD research program to provide guidance in the search for a QCD critical point in heavy ion collisions, and an understanding of the properties of strongly interacting matter near this landmark point on the QCD phase diagram.

In close collaboration with Columbia University and the RIKEN-BNL research center the lattice groups at BNL are heavily involved in the development of new computing platforms. The QCDOC, which had been operated at BNL for the last five years, was the prototype of IBM’s successful BlueGene L and P computers. An efficient exploitation of these supercomputers would not have been possible without the software development performed by SciDAC funded personnel at BNL and in the other USQCD groups. Currently these groups contribute significantly to the development of the next generation of BlueGene computers at IBM. BNL will host prototypes of this new computer which are expected to arrive in the fall of 2011. Naturally, a large amount of new software development is needed to exploit these machines efficiently.
The collaborative effort of USQCD in software development for state-of-the-art computing platforms has proved to be very effective in supporting the extremely rapid progress that has been made in the lattice QCD community. It is an important collaboration for BNL, and I can assure you that Brookhaven’s interests and plans are accurately represented in these activities.

With best regards,

Thomas W. Ludlam
Chair, Physics Department

cc: P. Mackenzie, S. Vigdor
Dear Dr. MacKenzie,

I wish to articulate the critical importance of Lattice QCD calculations to the scientific program of Jefferson Lab.

Using Lattice QCD techniques, calculation of the consequences of QCD in the confinement regime can be made. The calculation of observables of direct relevance to the TJNAF experimental program ranges from the spectroscopy of baryons and mesons, to form factors and generalized parton distributions, to the origins of the nuclear force. Recently, a calculation of the masses of "exotic" mesons, states forbidden in the simple quark model, has been completed. The existence of such states could shed light on the mechanism of confinement. The search for these exotic states is the goal of the flagship GlueX experiment which will run when the 12 GeV Upgrade Project has been completed. The calculation suggests that such states will indeed exist in the energy regime accessible to GlueX. The continued development of these calculations will inform the expected production rates, providing the vital theoretical underpinnings for the experiment.

The national efforts of the USQCD collaboration are key to the success of the lattice program at Jefferson Lab. Notably, the calculations cited above were dependent on the advancement of new algorithmic techniques, the integration of those advances, and the design and construction of the software infrastructure to exploit emerging architectures. The shining example of the latter was the General-Purpose GPU facility.

A continued strong national program will ensure both the algorithmic developments, and the software infrastructure, to further exploit both frontier leadership-class and special-purpose computers, and thus provide the calculations that will capitalize on the DOE investment in the Jefferson Lab experimental program.

Sincerely,

Hugh E. Montgomery
Laboratory Director
Workshops with experimentalists
Workshops with applied mathematicians
Summer schools
Extra slides
Illustration of the relationship between lattice QCD and the experimental programs of the Offices of High Energy and Nuclear Physics.
Text