LQCD-ext and LQCD-ARRA Projects
2011 Annual Review

Overview and USQCD Collaboration Management

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http://www.usqcd.org

LQCD-ext and LQCD-ARRA Projects
2011 Annual Review
Fermilab
May 10-11, 2011

Synopsis

- Annual review of the LQCD-ext lattice computing hardware project, 2010-14. and the annual review of LQCD-ARRA hardware project, 2009-13.
  - Hardware is located at BNL, JLab, Fermilab.
  - Projects funded jointly by DoE's offices of HEP and NP.
- The LQCD Project is one of several hardware and software efforts overseen by the USQCD Collaboration.
- USQCD is a collaboration consisting of most US lattice gauge theorists. Its purpose is to develop the software and hardware infrastructure required for lattice gauge theory calculations.

Plan of talks

(Detailed schedule at http://projects.fnal.gov/lqcd/reviews/May2011Review/index.shtml/ .)

May 10

08:30 Executive session (45 min)
09:15 Welcome (10 min) – *Vicky White*
09:25 Logistics and Introductions (5 min) – *Bill Boroski*
09:30 LQCD Overview (45 min) - *Paul Mackenzie*
10:15 Break (15 min)
10:30 Science Talk 1: Lattice QCD and the Search for New Physics (30 min) - *Andreas Kronfeld*
11:00 Science Talk 2: Beyond the Standard Model Physics (40 min) – *Julius Kuti*
11:40 Science Talk 3: Hadron Spectroscopy, Structure and Interactions (40 min) – *David Richards*
12:20 Lunch / Executive Session
1:10 Science Talk 4: High Temperature/Density QCD (30 min) – *Frithjof Karsch*
1:40 LQCD-Ext Project: Management and Performance (30 min) - *Bill Boroski*
2:10 LQCD-ARRA Project: Management and Performance (20 min) – *Chip Watson*
2:30 LQCD-ARRA Technical Performance (30 min) – *Chip Watson*
3:00 Combined Break and Compute Facility Tour (45 min)
3:45 LQCD-Ext Technical Performance & Remaining Plans for FY2010/2011 Deployments (30 min) - *Don Holmgren*
4:15 LQCD-EXT Proposed Selection Strategy for FY2012 Deployment (45 min) – *Don Holmgren*
5:00 Executive Session (60 min)
6:00 Committee request for additional information - *Committee/Project Leadership*
6:30 Adjourn
7:00 Dinner

Overview

Scientific achievements

LQCD Project management and technology

Plan of this talk

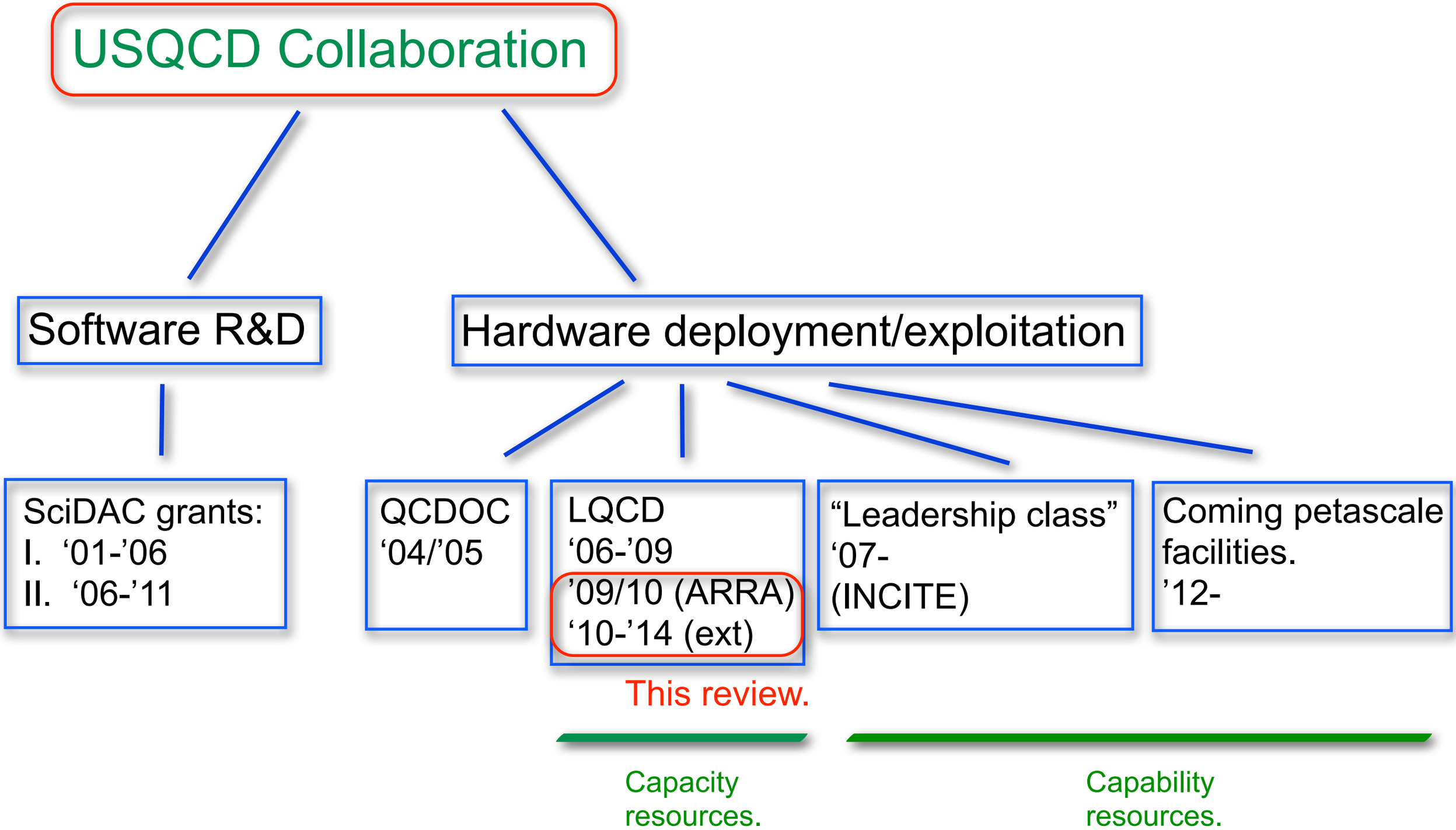
- Organization
  - The USQCD Collaboration
- Science
  - Lattice QCD
  - USQCD scientific goals.

I. The USQCD Collaboration

The importance of lattice QCD calculations to fully capitalize on the enormous investments in the HEP and NP experimental programs led DoE to ask the US lattice gauge theory community to organize itself to create software and hardware infrastructure for lattice calculations.

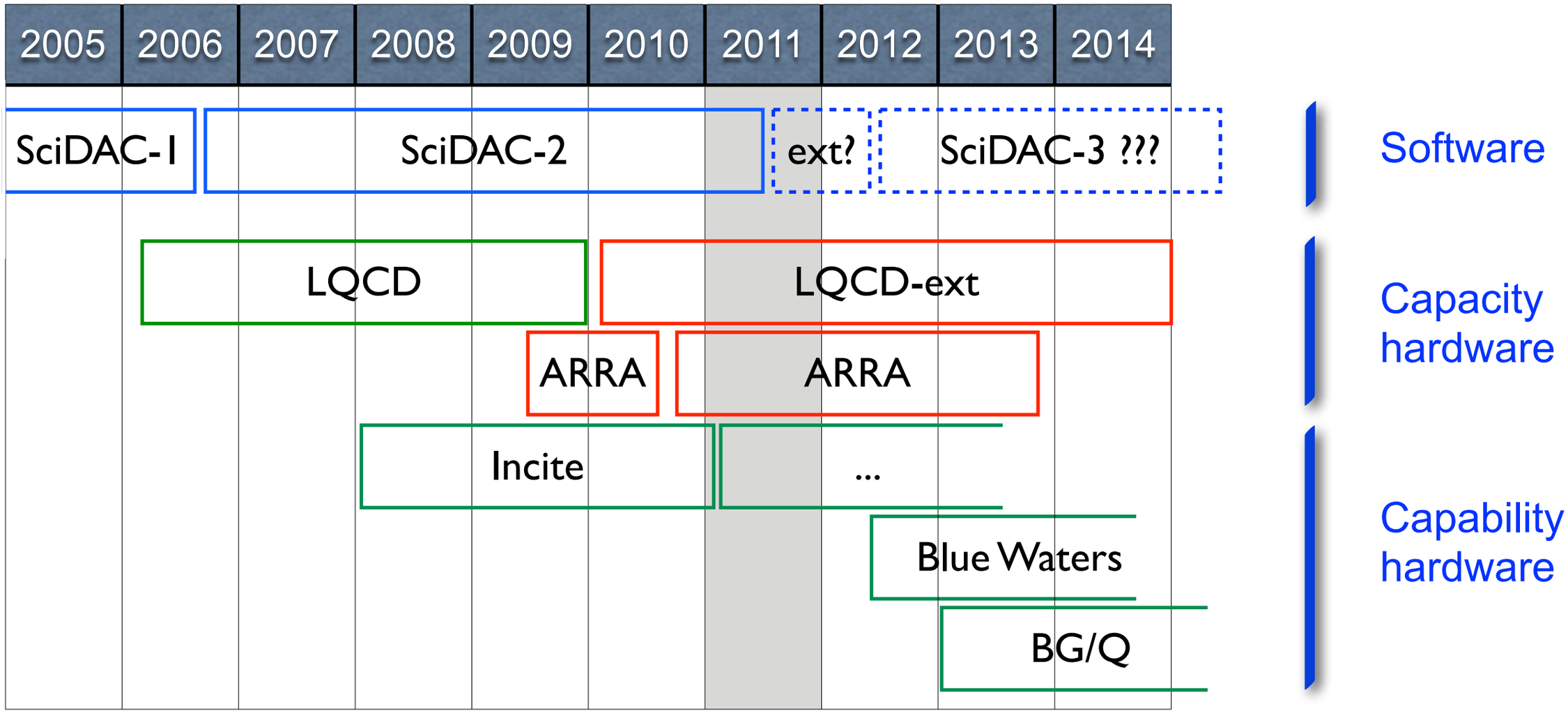
The USQCD Collaboration was the result.

Consists of almost all US lattice gauge theorists, ~160 members.
Purpose: develop hardware and software infrastructure for the US lattice community. (Physics projects are done by individual groups within USQCD.)



USQCD has grants for
- R&D for software development through the SciDAC program.
- Hardware deployment and use from several sources, including the current LQCD-ARRA and LQCD-ext projects.

Activities of USQCD



Being reviewed today.

USQCD Collaboration

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

New this year.

Scientific Program Committee:
Frithjof Karsch (chair)

Software Committee:
Rich Brower (chair)

LQCD-ext Project

Federal project director:
John Kogut (HEP)
Federal project monitor:
Helmut Marsiske (NP)

Contract project manager:
Bill Boroski
Assistant project manager:
Bakul Banerjee

Change control board:
Paul Mackenzie (chair), Bill Boroski, Steve Gottlieb, Tom Schlagel, Vicky White, Roy Whitney

LQCD-ARRA Project

DoE program manager:
Helmut Marsiske (NP)

Contract project manager:
Chip Watson

Change control board:
Paul Mackenzie, Chip Watson, Steve Gottlieb, Roy Whitney

The USQCD collaboration is funded through SciDAC, through the LQCD project, and through base HEP and NP funds at BNL, Fermilab, and JLab.

USQCD collaboration web page: http://www.usqcd.org

These two projects being reviewed today are managed cooperatively and operated as a coherent whole.

USQCD hardware resources

			Cores	M core-hours	GPUs
LQCD cluster resources	Fermilab	JPsi	6,912	50	
		Ds-1	7,840	75	
		Ds-2 (planned)	5,632	54	
		GPUs (planned)			128
	JLab	7n	2,720	15	
		9q	2,560	41	
		10q	1,536	25	
		9g+10g			500
	Total		27,200	260	
USQCD Incite resources 2010					
		Argonne allocated		67	
		Argonne low priority		120	
		Oak Ridge		40	

Current resources
Core-hours not normalized.

New: GPUs for lattice gauge theory

A dramatic speed up has been achieved in some of our projects with GPUs.
A major effort is underway to understand what fraction of our program can be accomplished with GPUs and to create the necessary codes.

USQCD GPU history

- 2008, Kuti. Lattice gauge theory on GPUs.
- 2008. USQCD SciDAC software starts GPU coding effort.
- Oct. 2008, Fermilab meeting. NVIDIA, Fermilab, BU, NCSA, ...
- Feb. 2009, Fermilab purchase with LQCD funds. 16 GPUs.
  - BU Disco project production.
- Aug. 2009, JLab workshop. USQCD+NVIDIA.
- 2009/10, ARRA 9g and 10g clusters,
  - 8 projects now running.
- 2011, GPU clusters planned at Fermilab. (Don Holmgren's talk.)

In-progress and future GPU work

- Coding!
- Measure speed-up of current projects by wall clock hours (not by inverter).
- We're improving our understanding of
  - The fraction of GPU-enabled hardware contained in new purchases.
    - Must take into account fraction of program that can use GPUs, GPU cost, ...
  - How to allocate GPU-enabled systems.
    - A possibility is service units that equate a core-hour on a new conventional clusters with a cost-equivalent amount of hardware on a new GPU-enabled system.
  - How to report the CPU power of a system including GPUs to the DoE.
    - One measure is the amount of CPU based computers that GPUs replace.
- We're dependent on SciDAC-3 to fully realize the dramatic improvement that GPUs have the potential to deliver.
  - Extension year of SciDAC-2 is proceeding and SciDAC-3 is expected to proceed at some level.

SciDAC lattice QCD computing R&D

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, Lawrence Livermore Lab, Chip Watson, JLab

USQCD has a SciDAC-2 grant of ~$2.2M/year for creating lattice QCD software infrastructure: community libraries, community codes, optimization and porting to new architectures, implementation of up-to-the-minute algorithm advances...
This has enabled optimally efficient operation on the USQCD hardware.

Increasing effort to understand and code GPUs.

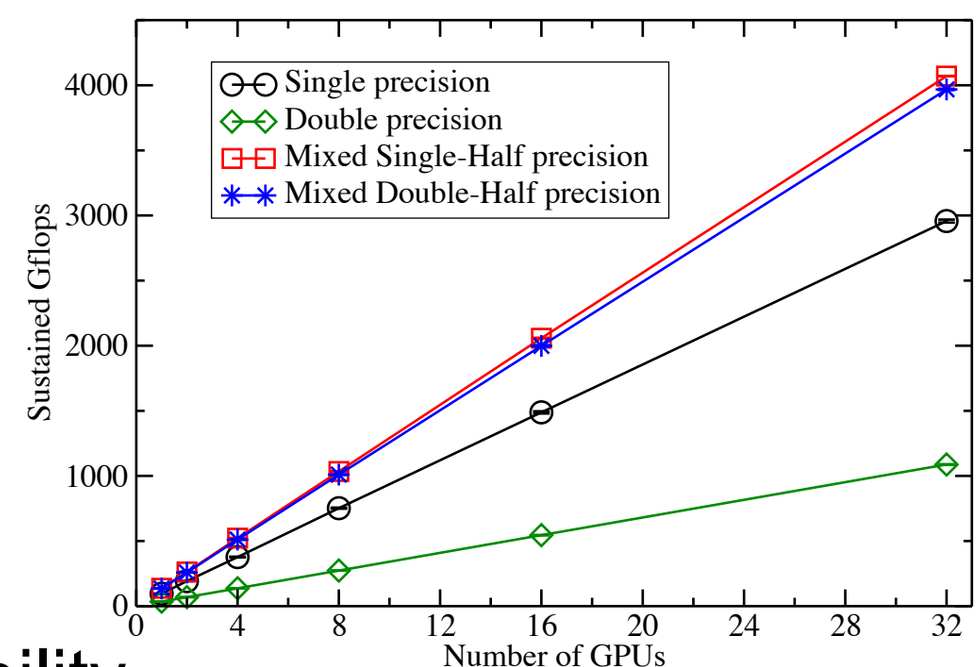
Regular Thursday phone conferences for people working on USQCD software.

Software achievements

- The QCD API and community libraries
  - Lower entrance barriers to lattice QCD.
  - Enable postdocs to run major projects without being part of major collaborations.
- Porting and optimizations for new platforms
  - In 2008, USQCD was the only project with a multiyear program ready to run on the Argonne BG/P from the start. Used ~1/3 of cycles in 2008, accomplished a three-year program of configuration generation in one year.
  - Now undertaking serious programs

    getting ready for new platforms:
    - GPUs (now!), Blue Waters (2011?),

      BG/Q (2012?).
- Projects in workflow, visualization, performance analysis, cluster reliability, ...



Babich, Clark, and Joo, arXiv:1011.0024v1

Hardware choices for 2012 capacity computing

- The LQCD-ext Project will have an unusually rich set of hardware possibilities for our capacity computing needs to choose from in 2012:
  - Infiniband clusters,
  - GPU-accelerated clusters,
  - Blue Gene/Q.
- With GPU clusters especially, cost efficiency varies greatly physics project to physics project, and is not well predicted by inverter performance.
  - The project plans to have a somewhat wider set of benchmarks including some analysis projects to help evaluate the choice.

Incite resources

for capability computing.

- The DOE allocates time on its leadership class supercomputers, the Cray XT4/XT5 at ORNL and the BlueGene/P at ANL, through its Incite Program.
  - These are very well suited to that part of our program requiring high capability computing, such as generation of large gauge configuration ensembles.
- USQCD currently has a three year grant running from calendar year 2011 though calendar year 2013.
- Resources are allocated one year at a time. The USQCD allocation for 2011 is one of the three largest in the program. It consists of:
  - 30 M core-hours on the Cray XT4/XT5 allocated . Used 23 M core-hours in ’09 and 54 M in ’10.
  - 50 M core-hours on the BlueGene/P allocated, one of three largest. Total time used was 359 M core-hours in 2008, 279 M in 2009, and 187 M in 2010.

Scientific Program Committee

Scientific Program Committee:
Frithjof Karsch (chair), BNL, Simon Catterall, Syracuse, Robert Edwards, JLab, Taku Izubuchi, BNL, Martin Savage, U. Washington, Junko Shigemitsu, Ohio State, Doug Toussaint, Arizona

Each year, the many smaller physics collaborations within USQCD submit proposals to the Scientific Program Committee for allocations of time on USQCD's LQCD and Incite resources.

The SPC creates a program to accomplish the goals set forth in the USQCD Collaboration's proposals.

The Executive Committee seeks the advice of the SPC on physics priorities when writing new proposals for DoE computing resources.

Chair rotates every two years. Members rotate every four years. Current committee contains none of the original members.

Allocation process

- Each year, the SPC issues a call for proposals for use of LQCD resources and DoE leadership class (Incite) resources.
- Three types of proposals.
  - Type A. Large projects expected to benefit the whole collaboration by producing data, such as gauge configurations, for general use, or by producing physics results listed among USQCD's strategic goals.
  - Type B. Need not share data or work toward USQCD's goals (although if they do, it's a plus). <2.5 M JPsi core-hours or 10 K GPU hours. Goal is 10-15% of total allocation.
  - Type C. Exploratory calculations such as for developing or benchmarking code. <100 K JPsi core-hours.
- The SPC reviews proposals, then organizes an all-hands meeting of USQCD. Plans of proposals are discussed by their proponents and by the collaboration as a whole.

Executive Committee

- Provides overall leadership for the collaboration and point of contact for the DoE.
- Writes the proposals for hardware and software and chooses the members of the other committees.
- Last year's review panel recommended increased rotations of the Executive Committee.
  - Two rotations this year.
  - Claudio Rebbi and Mike Creutz → Frithjof Karsch and Julius Kuti.
- Full rotation over ~ 10 years is planned.
  - We plan to rotate in a way that preserves rough balance between physics interests, HEP and NP, collaborations, etc.

2011 USQCD all-hands meeting

- Took place May 6-7, 2011 at JLab. ~55 members attended. (http://www.usqcd.org/meetings/allHands2011/ .)
- Reports from most physics projects requesting time on USQCD resources.
- Reports from the Executive Committee, the LQCD-ext and LQCD-ARRA Project Managers, the SPC, and the site managers.
- Round table discussions with
  - The Software Committee and with the Executive Committee.
- Report from D0 member and g-2 proponent Brendan Casey on the workshop Lattice QCD Meets Experiment, which was held at Fermilab in 2010.

2011/12 allocation requests

Proposals 11/12

- 22 type-A; 15 type-B proposals
- type-A proposals: 9 INCITE
  17 cluster
  6 GPU
- type-B proposals: 12 cluster
  3 GPU
- type-B: request 10.1%
  of available time

CPU time request

- cluster: 140% of available time
- GPUs: 140% of available time
- INCITE: (127+218)% of (not) available time

Report from the SPC at the 2011 All-Hands Meeting.

Lattice QCD meets experiment meetings

To increase the interaction between lattice gauge theory and experiment and phenomenology, members of USQCD have organized a series of workshops with experimenters and phenomenologists.

- SLAC, Sept. 16, 2006, Standard Model physics. With BaBar.
- Fermilab, December 10-11, 2007, Standard Model physics.
- Livermore, May 2-3, 2008, “Lattice Gauge Theory for LHC Physics”,
  - Beyond the Standard Model physics. No experimenters yet, but some BSM phenomenologists.
- JLab, Nov. 21-22, 2008, “Revealing the Structure of Hadrons”, Nuclear.
- BNL, June 8-9, 2009, “Critical Point and Onset of Deconfinement”, QCD thermodynamics.
- BU, Nov. 6-7, 2009, “Lattice Gauge Theory for LHC Physics”. BSM.
- Fermilab, April 26-27, 2010, “Lattice Meets Experiment” in flavor physics.
- BU, 8-10 September 2010, “Sixth Workshop on QCD Numerical Analysis, Boston.
- JLab, February 23-25, 2011, “Excited Hadronic States and the Deconfinement Transition”.

Each year, a member of the experimental or phenomenology communities at one of the meetings is invited to address the All-hands Meeting to assess the interaction between lattice and experiment at the meeting.

International collaboration

- Lattice QCD is an international field with very strong programs in Germany, Italy, Japan and the United Kingdom, and elsewhere. Groups within USQCD have formed a number of international collaborations:
  - The USQCD effort using DWF quarks is an international effort between the United States based RBC and LHPC Collaborations, the Edinburgh, Southampton and Swansea members of the UKQCD Collaboration, and RIKEN.
  - The Fermilab Lattice, HPQCD and MILC Collaborations have worked together in various combinations to study heavy quark physics using improved staggered quarks. HPQCD includes physicists in both USQCD and UKQCD.
  - Members of the RBC Collaboration studying QCD thermodynamics using improved staggered quark actions have a long term collaboration with physicists at the University of Bielefeld, Germany.
  - Members of USQCD working on the hadron spectrum using Clover quarks on anisotropic lattices have close ties with colleagues in Trinity College, Dublin.

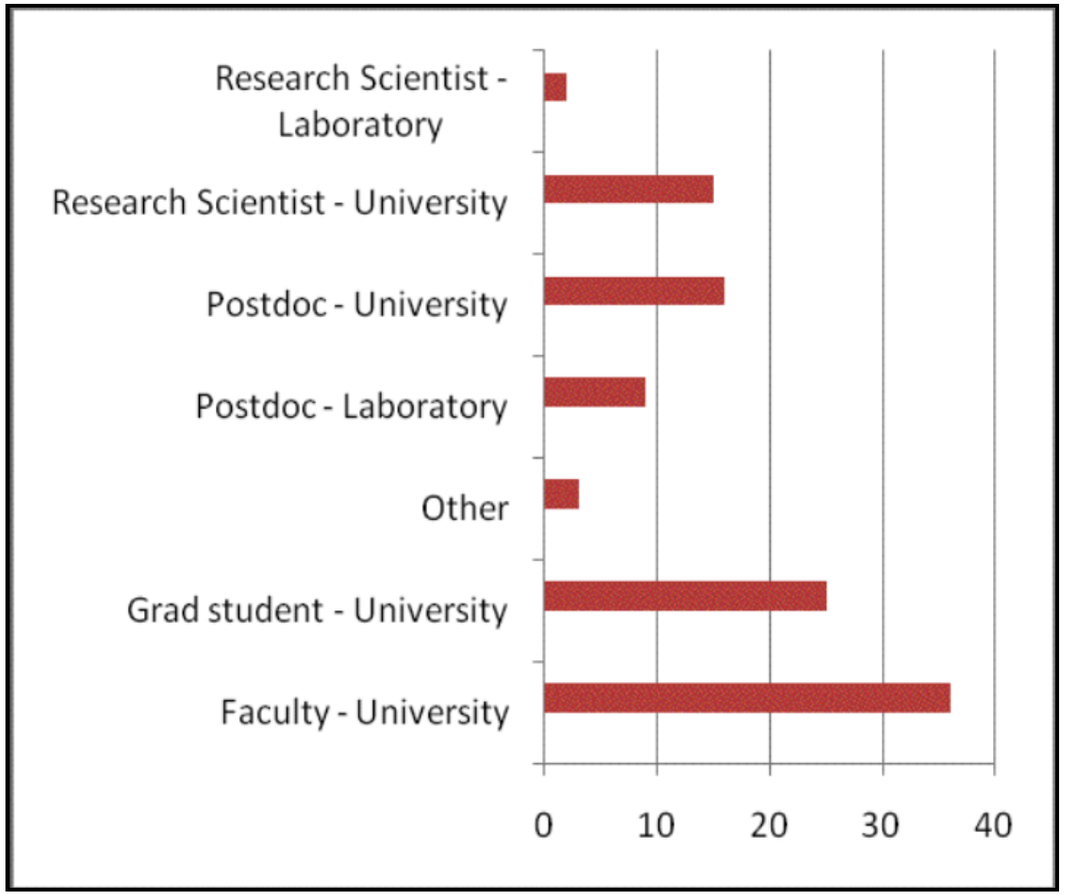
International cooperation

- USQCD has played an active role in the formation and work of the International Lattice Data Grid (ILDG) which is organizing the sharing of large data sets (gauge configurations and quark propagators) on the international level.
- The ILDG has developed standards for file format and content, and the middleware needed to archive and retrieve files.
- Groups in Europe, Japan and the United Kingdom, as well as those in the United States, are all making data sets available through the ILDG.

Membership survey and demographic information

- We are starting to collect membership and demographic information in a more organized way.
- Bakul Banerjee has conducted several surveys in the past year.
  - New membership list.
    - Currently, ~ 165 members.
  - Demographic survey.

Current USQCD demography.



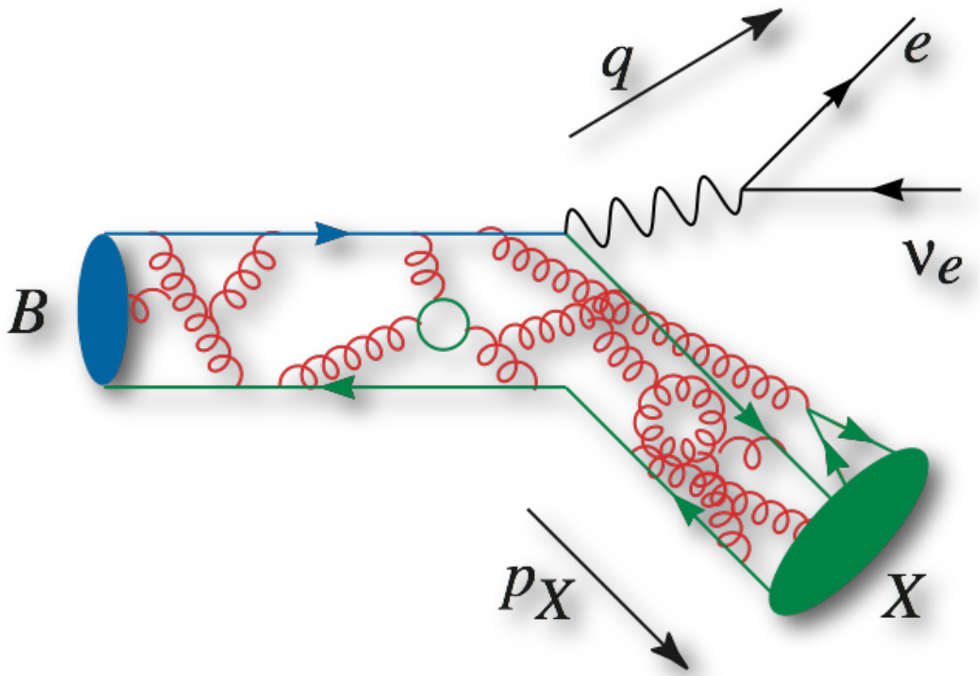
II. Lattice QCD

QCD is the theory of quarks and gluons. Quarks and gluons cannot be directly observed because the forces of QCD are strongly interacting.

Quarks are permanently confined inside hadrons, even though they behave as almost free particles at asymptotically high energies.

"Asymptotic freedom", Gross, Politzer, and Wilczek, Nobel Prize, 2004.

Lattice QCD is used to relate the observed properties of hadrons from the properties of their quark and gluon constituents.



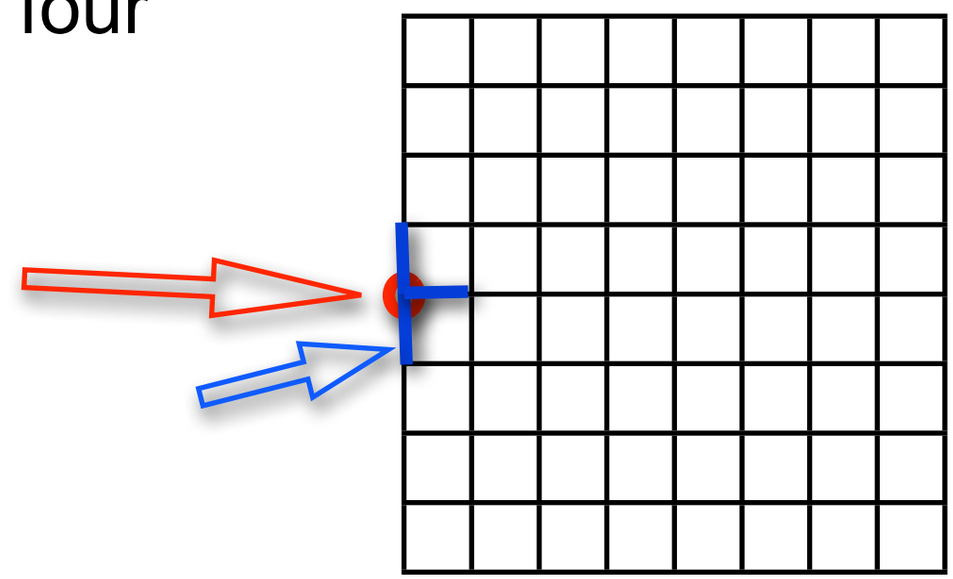
$B \to \pi l \nu$ semileptonic decay

Luke

Lattice quantum field theories

Approximate the path integral of quantum field theory by defining the fields on a four dimensional space-time lattice.

Quarks (ψ) are defined on the sites of the lattice, and gluons (U_μ) on the links.



Monte Carlo methods are used to generate a representative ensemble of gauge fields. Relaxation methods 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.

The Dirac, or “Dslash”, operator

The fundamental operation that consumes the bulk of our cycles is the solution of the Dirac equation on the lattice.

The fundamental component of the Dirac operator is the discrete difference approximation to the first derivative of the quark field on the lattice.

$$\partial_\mu \psi(x) \to \Delta_\mu \psi(x) \approx \frac{1}{2a}(\psi(x+\hat{\mu}a) - \psi(x-\hat{\mu}a)) + \mathcal{O}(a^2)$$

Quarks in QCD come in three colors and four spins.
The color covariant Dslash operator of lattice QCD is

$$D_\mu \gamma_\mu \psi(x) \equiv \frac{1}{2}\left(U_\mu(x)\gamma_\mu\psi(x+\hat{\mu}) - U_\mu^\dagger(x-\hat{\mu})\gamma_\mu\psi(x-\hat{\mu})\right)$$

γ operates on spin four-vector.

U operates on color three-vector of the quark.

The bulk of the flops envisioned in this project are consumed in multiplying complex 3-vectors by 3x3 complex matrices.

The computational challenge of lattice QCD

Lattice	Quark			Gauge	ensembles		Analysis propagators, correlators		
spacing *a* (fm)	mass *ml/ms*	Volume (sites)	Configu rations	Core-hours (M)	TB/ ensemble	Files/ ensemble	Core-hours (M)	TB/ ensemble	Files/ ensemble
0.15	1/5	16^3*48	1000	1	0.1	1,000	1	4	155,000
0.15	1/10	24^3*48	1000	2	0.2	1,000	2	12	“
0.12	1/5	24^3*64	1000	3	0.3	1,000	3	16	155,000
	1/10	32^3*64	1000	8	0.6	1,000	8	39	“
	1/27	48^3*64	1000	26	2.0	1,000	26	130	“
0.09	1/5	32^3*96	1000	10	0.9	1,000	10	58	155,000
	1/10	48^3*96	1000	35	3.1	1,000	35	196	“
	1/27	64^3*96	1000	46	7.2	1,000	46	464	“
0.06	1/5	48^3*144	1000	38	4.6	1,000	38	294	155,000
	1/10	64^3*144	1000	128	10.9	1,000	128	696	“
	1/27	96^3*144	1000	218	36.7	1,000	218	2,348	“
0.045	1/5	64^3*192	1000	135	14.5	1,000	135	928	155,000
	1/10	88^3*192	1000	352	37.7	1,000	352	2,412	“
	1/27	128^3*192	1000	1083	116.0	1,000	1,083	7,422	“
0.03	1/5	96^3*288	1000	685	73.4	1,000	685	4,697	155,000
				2,770					

Example gauge ensemble library.

CPU times normalized in JPsi core-hours.

Planned MILC HISQ ensembles of guage configurations. m_l=1/27m_s= m_{phys}

Operationally, lattice QCD computations consist of

1) Sampling a representative set of gauge configurations with Monte Carlo methods,

   E.g., the Metropolis method, the hybrid Monte Carlo algorithm, ...
   Consists of one long Markov chain. A capability task.

2) Calculating the propagation of quarks through the gauge configurations,

   Solve the Dirac equation on each configuration with relaxation methods, e.g., biconjugate gradient algorithm, etc. A capacity task.

3) Constructing hadron correlation functions from the quark propagators (smaller task).

Anatomy of a typical lattice calculation

TB file sizes

Generate gauge configurations on a leadership facility or supercomputer center.
Tens of millions of BG/P core-hours in a single job.

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

A single highly optimized program,
very long single tasks,
moderate I/O and data storage.
Needs high capability computing.

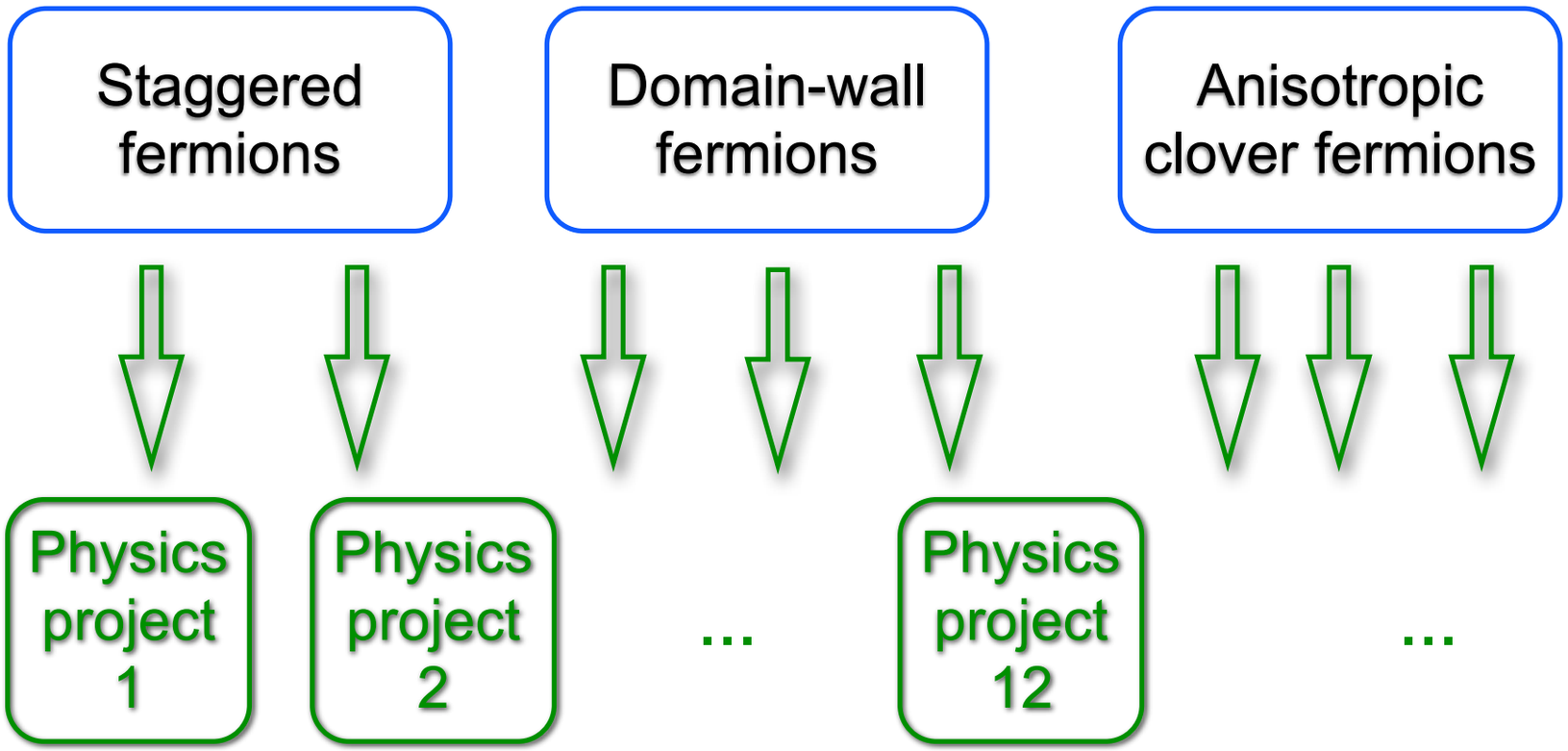
Large, heterogeneous analysis code base,
10,000s of small, highly parallel tasks,
heavy I/O and data storage.
Needs high capacity computing.

Two comparably sized jobs with quite different hardware requirements.

US lattice gauge theory work flow

Zero-temperature QCD:

Currently three main streams of QCD gauge configurations are being generated by USQCD:

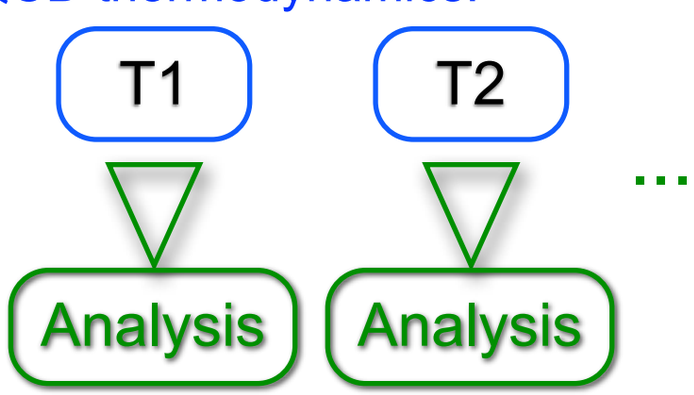


Shared among a couple of dozen groups, in both HEP and NP.

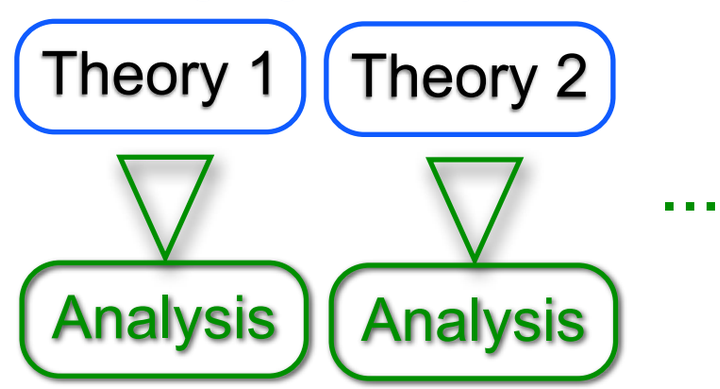
Physics projects are done on these configurations by smaller groups of 5-15 members within USQCD.

Around 90 of the 170 members of USQCD have submitted jobs to USQCD hardware.

QCD thermodynamics:



BSM gauge theory:



Purposes of ensembles

Currently three main streams of QCD gauge configurations for zero temperature QCD are being generated by USQCD:

Staggered fermions	Domain-wall fermions	Anisotropic clover fermions
Tuned toward small lattice spacings and light quark masses for precision on Standard Model parameters. Planned HISQ program: $a \sim 0.03 - 0.15$ fm, $m_l \geq 1/27\ m_s$, $V \sim (3\text{-}5\ \text{fm})^3$.	Clean chiral action. Physics aims are accurate nucleons and two-pion states. AuxDet action. $a \sim 0.081 - 0.114$ fm, $m_l > 0.05\ m_s$, $V \sim (2.7\ \text{fm})^3$.	Tuned toward very small temporal lattice spacings for investigation of excited states. $a_s \sim 0.122$ fm, $a_t \sim 0.035$ fm, $m_l \rightarrow 0.037\ m_s$ ($=m_{\text{phys}}$) $V \rightarrow (5\ \text{fm})^3$.

2010 USQCD physics projects

Projects for configuration generation

Projects initiated by post-docs or students

Beyond-the-Standard-Model projects

2010 Type A Proposals (more than 2,000,000 J/Psi core-hours)

PI	Project Web Page
Christopher Aubin	Hadronic contributions to the muon g–2 using Asqtad staggered fermions
Norman Christ	Simulations with Dynamical Domain-wall Fermions
Robert Edwards	Dynamical Anisotropic-clover Lattice Production for Hadronic Physics
George Fleming	Two-Color Gauge Theories for TeV Physics
Peter Lepage	Attoscale lattice QCD
Taku Izubuchi	Isospin breaking effects in hadrons
Julius Kuti	Nearly Conformal Gauge Theories and the Higgs Mechanism
Ruth Van de Water	$\Delta I = 1/2$, $K \rightarrow \pi\pi$ matrix elements with Domain-Wall Valence Quarks and Staggered Sea Quarks
Keh-Fei Liu	Hadron Spectroscopy and Nucleon Form Factors
Paul Mackenzie	B and D Meson Decays with Unquenched Improved Staggered Fermions
Robert Mawhinney	Pion and Kaon Physics from 2+1 Flavor DWF Lattices with m_π = 250 and 180 MeV, II
Doug Toussaint	QCD with Four Flavors of Highly Improved Staggered Quarks
Kostas Orginos	Baryon Form Factors on Dynamical Anisotropic-Clover Lattices
Peter Petreczky	QCD Phase Diagram with Highly Improved Staggered Quarks
David Richards	Excited Meson and Baryon States using Anisotropic Clover Lattices
Silas Beane	Lattice QCD Study of Hadronic Interactions (plus GPU Technical Proposal)
Stephen Sharpe	B_K and related matrix elements with unquenched, improved staggered fermions
Junko Shigemitsu	High-Precision Heavy-Quark Physics
Sergey Syritsyn	Nucleon Structure in the Chiral Regime with Domain Wall Fermions
Alexei Bazavov	HotQCD studies with the HISQ action
Andre Walker-Loud	Hadronic electromagnetic properties
Oliver Witzel	B-meson decay constants, B0-B0bar-mixing and B*Bπ coupling with domain-wall light quarks and relativistic heavy quarks

2010 Type B Proposals (less than 2,000,000 core-hours)

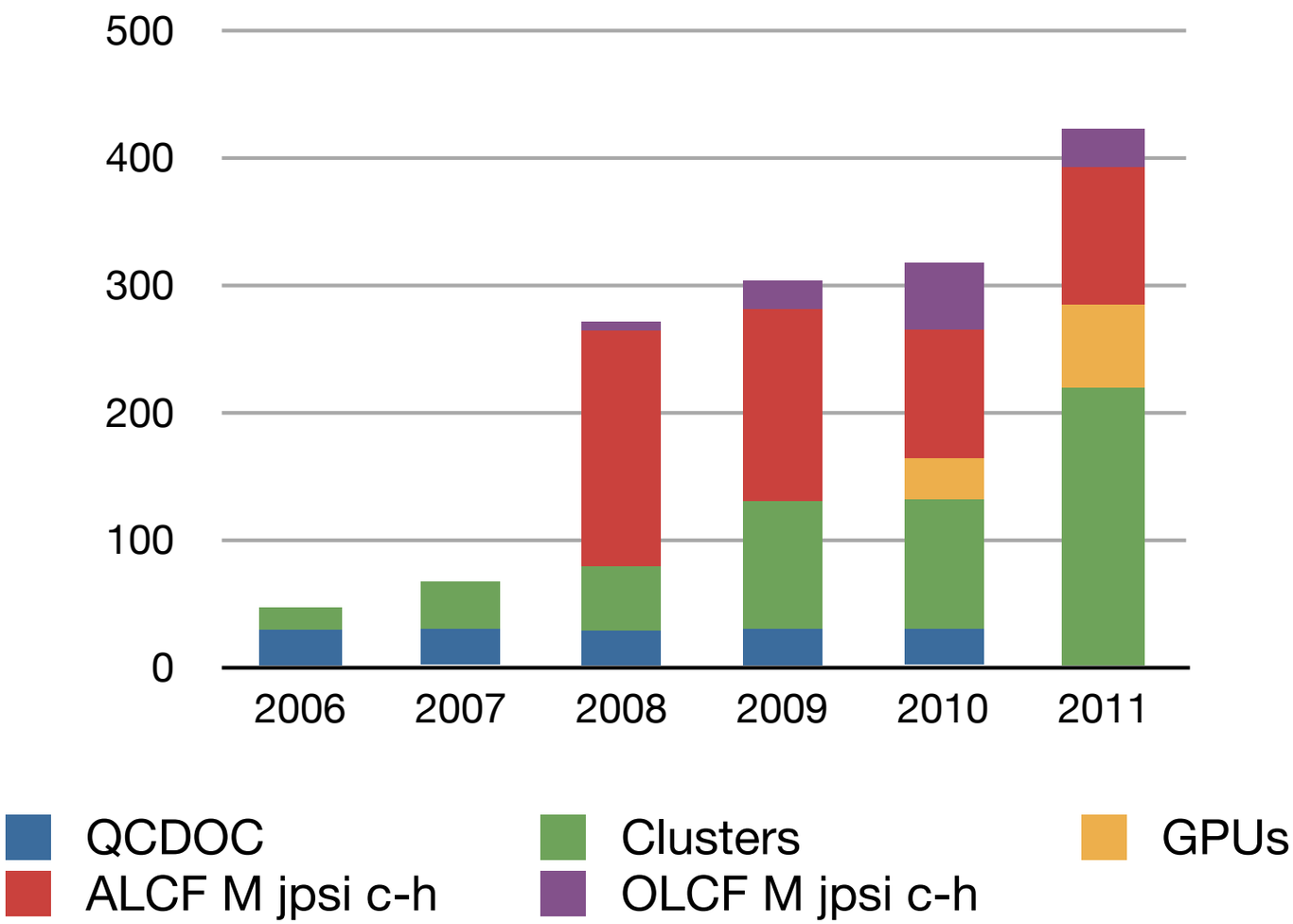
PI	Project Web Page
Andrei Alexandru	Hadron electric polarizability in the chiral limit
Simon Catterall	Simulations of $N = 4$ Super Yang-Mills
Joel Giedt	Monte Carlo Renormalization Group for Minimal Walking Technicolor
Anna Hasenfratz	Study of many flavor systems with Monte Carlo renormalization group
Swagato Mukherjee	Finite density QCD and critical behavior with improved staggered fermions on GPUs
Bernhard Musch	Transverse Momentum Dependent Parton Distribution Functions with Domain Wall Valence Fermions
James Osborn	Disconnected contributions to nucleon form factors
Meifeng Lin	Nucleon Form Factors with Partially Twisted Boundary Conditions
Stephen Sharpe	Non-perturbative renormalization with improved staggered fermions
Carleton DeTar	Quarkonium Physics with Unquenched Improved Staggered Fermions

Main scientific thrusts

- The fundamental parameters of the Standard Model and the search for new physics with Lattice QCD. Talk by Andreas Kronfeld.
  - Experiments impacted: BaBar (SLAC), Belle (KEK), CLEO-c (Cornell), CDF and D0 (FNAL) and LHC (CERN).
- Understanding the properties of new strongly interacting gauge theories that may be discovered at the LHC. Talk by Julius Kuti.
  - Experiments impacted: LHC (CERN).
- Understanding the structure and interactions of nucleons. Talk by David Richards.
  - Experiments impacted: CEBAF (JLab), RHIC (BNL), COMPASS and HERMES (DESY).
- Understanding the behavior of QCD in extreme conditions. Talk by Frithjof Karsch.
  - Experiments impacted: RHIC (BNL), FAIR (GSI) and LHC (CERN).

Extra slides

Extra slides



Resources history.