Overview of LQCD Computing Project

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May 14 Agenda

9:00	Overview Bob Sugar
10:00	Fundamental Parameters of the Standard Model Steve Sharpe
10:45	Break
11:00	Nucleon structure and spectroscopy, and hadronic interactions David Richards
11:45	High Temperature/Density QCD Frithjof Karsch
12:30	Lunch
1:30	Project Management Bill Boroski
2:00	USQCD Computing Resources and User Services Bill Boroski
2:25	Installation of the FY 2007 Cluster at JLab Chip Watson
2:50	Break
3:05	Hardware plans for FY 2008-2009 Don Holmgren
3:30	USQCD Allocation Process Andreas Kronfeld
4:00	SciDAC Software Rich Brower
4:30	User Experience Kostas Orginos
5:00	Executive Session

Synopsis

- The mission of the project is to acquire and operate dedicated hardware for the study of quantum chromodynamics (QCD).
- Hardware is located at BNL, FNAL and JLab.
- The project began in FY 2006 and runs through FY 2009.
- The project is funded jointly by the DOE's Offices of High Energy Physics and Nuclear Physics.

Year	FY2006	FY2007	FY2008	FY2009	Total
Hardware	$1,850	$1,592	$1,630	$798	$5,870
Operations	$650	$908	$870	$902	$3,330
Total	$2,500	$2,500	$2,500	$1,700	$9,200

The USQCD Collaboration

- The LQCD Computing Project is a key element in the efforts of the USQCD Collaboration to build the computational infrastructure needed for the study of QCD.
- The USQCD Collaboration consists of nearly all the high energy and nuclear physicists in the United States involved in the numerical study of QCD.
- The Collaboration was formed eight years ago with the goal of developing the computational infrastructure needed for these studies.
- Membership in USQCD is open to all scientists based in the United States, and the infrastructure is available to all.

Other USQCD Infrastructure Projects

- Construction of the QCDOC, a computer specially designed for the study of QCD. The USQCD's QCDOC was funded by the DOE's Offices of Advanced Scientific Computing Research, High Energy Physics and Nuclear Physics.
- The design and construction of commodity clusters optimized for the study of QCD under a grant from the DOE's SciDAC-1 Program with supplementary funding from FNAL, JLab, and the Office of High Energy Physics.
- The development of community software under the grants from the DOE's SciDAC-1 and SciDAC-2 Programs. Talk by Richard Brower

Other USQCD Infrastructure Projects

- The projects listed on the last slide are not part of the LQCD Computing Project, and are therefore not under review; however, they have a very positive impact on the Project.
  - Although the construction of the QCDOC and the SciDAC-1 Clusters was not part of the LQCD Computing Project, these computers are operated by it and make important contributions to its computing capability.
  - The SciDAC Software significantly enhances the productivity of the LQCD Computing Project hardware.

The Standard Model

- The Standard Model consists of two components:
  - The Weinberg–Salam theory of weak and electromagnetic interactions.
  - Quantum Chromodynamics, the theory of the strong interactions.
- The Standard Model has been enormously successful. However, it has proven very difficult to extract many of the predictions of QCD. To do so requires large scale numerical simulations within the framework of lattice gauge theory.
- The objectives of these simulations are to fully understand the physical phenomena encompassed by QCD, and to make precise calculations of the theory's predictions.

Major Scientific Objectives

- Calculate weak interaction matrix elements of strongly interacting particles to the accuracy needed to determine some of the least well known parameters of the Standard Model, and to make precise tests of it. Talk by Steve Sharpe.
- Calculate the masses of strongly interacting particles, and obtain a quantitative understanding of their internal structure and their interactions. Talk by David Richards.
- Determine the properties of strongly interacting matter at high temperatures and densities, such as those that existed immediately after the big bang, and are created today in relativistic heavy ion collision experiments. Talk by Frithjof Karsch.

Major Scientific Objectives

- Develop the tools needed to perform quantitative studies of strongly coupled theories that may be necessary to describe physical phenomena at shorter distance scales than have been explored to date.

Impact on Experimental Programs

- Weak Matrix Elements
  - BaBar (SLAC)
  - D0 and CDF (FNAL)
  - CLEO-c (Cornell)
- High Temperature/Density QCD
  - RHIC (BNL)
  - LHC (CERN)
- Hadron Structure
  - CEBAF (Jlab)
  - RHIC (BNL)
- Physics Beyond the Standard Model
  - LHC (CERN)

Office of Science Mission Statements

- HEP Mission: Explore the fundamental interactions of energy, matter, time and space
  - Explore unification of the forces and particles of nature
  - Understand the cosmos and the destiny of the universe
  - Develop the tools for scientific revolutions to come
- NP Mission: Explore nuclear matter – from quarks to stars
  - Studies of hot, dense nuclear matter
  - The quark structure of matter
  - Nuclear structure/astrophysics, fundamental symmetries, and neutrinos

Progress in LQCD Calculations

Enormous progress has been made in Lattice QCD calculations over the past five years thanks to:

- Dedicated computing facilities funded by the DOE.
- Improved formulations of QCD on the lattice, which reduce systematic errors due to finite lattice spacing artifacts and chiral symmetry breaking.
- The development of new algorithms, which reduce the number of floating point operations needed for some studies by factors as large as six
- The development of software under the DOE SciDAC Program, which enables effective use of a wide range of existing computers, and rapid porting of efficient code to new ones.

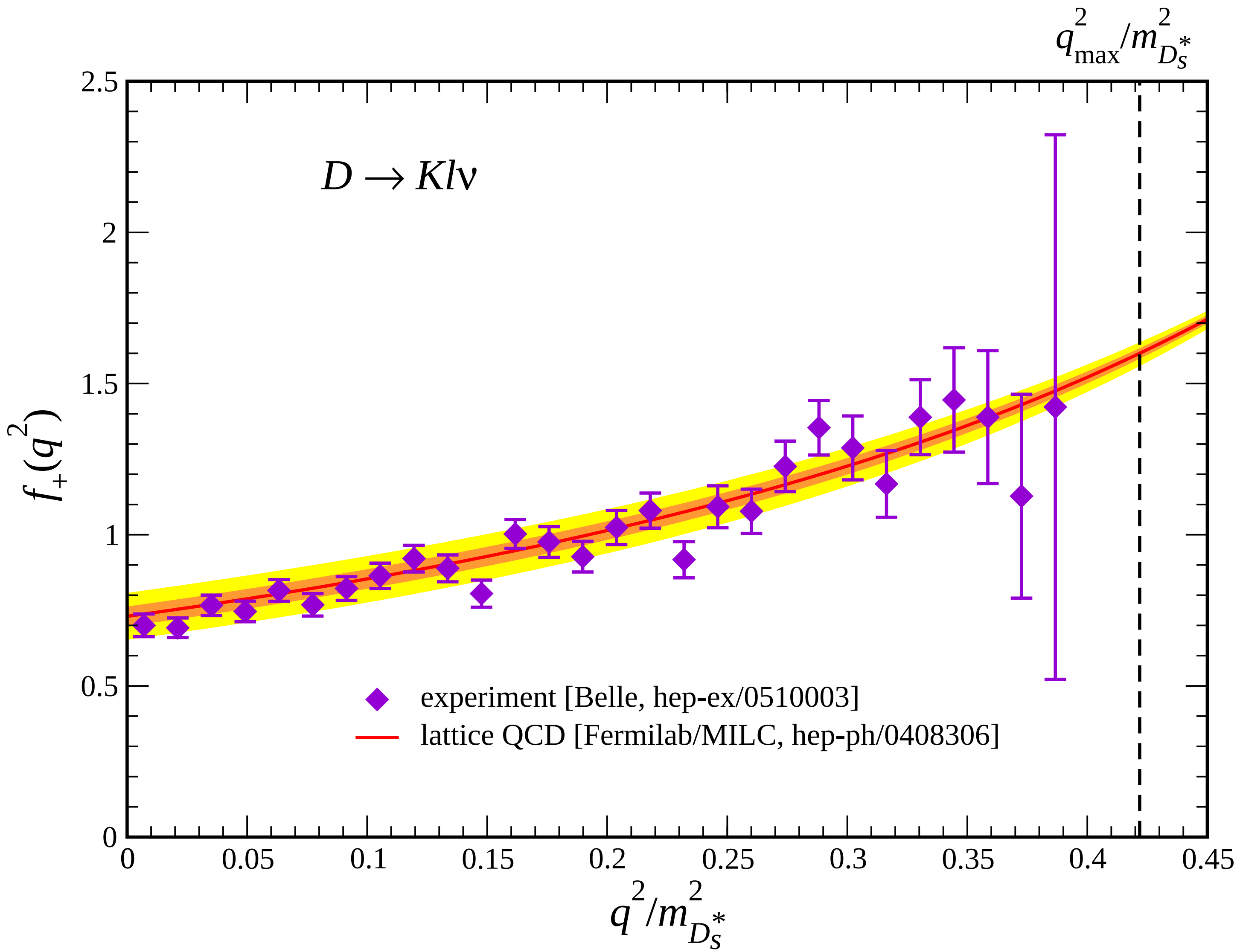
Validation of Methodology

Quantity	Lattice QCD	Experiment
$\alpha_S(M_Z)$	0.1170 ± 0.0012	0.1185 ± 0.0014
f_π	128.6 ± 3.0 MeV	130.7 ± 0.4 MeV
f_K/f_π	$1.208\,^{+0.007}_{-0.014}$	1.223 ± 0.012
V_{us}	$0.2223\,^{+0.0026}_{-0.0014}$	0.2257 ± 0.0021
m_{Ω^-}	1667 ± 52 MeV	1672 MeV
$\Delta E_\psi(1P - 1S)$	422 ± 16 MeV	428 MeV
$\Delta E_\Upsilon(1P - 1S)$	447 ± 9 MeV	440 MeV
$\hat{B}_K$	0.77 ± 0.08	0.75 ± 0.09
g_A	1.226 ± 0.084	1.270 ± 0.003

Predictions Verified by Experiment

Quantity	Lattice QCD	Experiment
f_D	$201 \pm 3 \pm 17$ MeV	$223 \pm 17 \pm 3$ MeV
f_{D_s}/f_D	$1.21 \pm 0.01 \pm 0.04$	$1.27 \pm 0.12 \pm 0.03$
m_{Bc}	6304 ± 22 MeV	6286 ± 5 MeV
f_B	216 ± 22 MeV	$229 \pm 36 \pm 34$ MeV

Semileptonic Form Factor of the D Meson



LQCD Computing Project Hardware

Computer	Site	Nodes	Performance (teraflop/s)
QCD	FNAL	127	0.15
3g	JLab	128	0.10
4g	JLab	384	0.54
Pion	FNAL	518	0.86
QCDOC	BNL	12,288	4.20
6n	JLab	256	0.55
Kaon	FNAL	600	2.56
7n	JLab	396	2.90*

The average of the performances of the inverters of the Dirac operator for domain wall (DWF) and improved staggered (Asqtad) quarks on typical production runs is used as the measure of performance of the computers.

* The performance of the 7n cluster is anticipated to be 2.9 teraflop/s or greater.

Acquisition Milestones

- The yearly acquisition milestones are:

Year	FY 2006	FY 2007	FY 2008	FY 2009
Performance in teraflop/s	2.0	2.9	4.2	3.0

- The components of the 6n and Kaon clusters purchased with FY 2006 Project funds have a total throughput of 2.6 teraflop/s.
- The FY 2007 acquisition is an Infiniband cluster, 7n, to be located at JLab. It is expected to meet or exceed the FY 2007 acquisition milestone, although full deployment will be delayed. Talk by Chip Watson.
- We propose to combine the FY 2008 and 2009 acquisitions to place a single large machine at FNAL. Talk by Don Holmgren.

Delivered Computing Resources Milestones

- Delivered computing resources are measured in TF-Years. One TF-Year is the number of floating point operations that a computer with a throughput of one teraflop/s will deliver in one 8000 hour year.
- The yearly milestones are:

Year	FY2006	FY2007	FY2008	FY2009
Delivered TF-Years	6.2	9.0	12.0	15.0

- A total of 6.21 TF-Years were delivered in FY 2006.
- The Project is on track to deliver 9.35 TF-Years in FY 2007 without any contribution from the new 7n cluster. Including the contribution of the 7n cluster, a total of 9.80 TF-Years is expected to be delivered.

Scientific Milestone Projects

- Generation of gauge configurations with improved staggered quarks.
- Generation of gauge configurations with domain wall quarks.
- Calculation of CKM matrix elements with improved staggered quarks (Leptonic decays of B and D mesons).
- Calculation of the properties of hot hadronic matter.
- Hybrid calculation of the quark structure of the nucleon.
- Pentaquark and N^* spectroscopy. (The pentaquark portion of this project was discontinued following further experimental study).

Progress on Scientific Milestones

- All FY 2006 milestones were met.
- All projects except that involving the internal structure of the nucleon are on track to meet their FY 2007 milestones, and it was not allocated sufficient USQCD resources to do so.
- In several cases, the groups carrying out the projects supplemented USQCD time with other resources.
- The scientific milestones in FY 2008 and 2009 are formulated as TF-Years delivered towards the completion of each year’s scientific program.

Project Managers

- Contract Project Manager: Bill Boroski (FNAL).
  - Responsible for the overall management of the Project. Talk by Bill Boroski.
  - Primary interface with the DOE for financial matters, reporting and reviews of the Project.
  - Bill became Contract Project Manager on January 1, 2007, replacing Don Holmgren who guided the Project throught its first fifteen months.
- Associate Contract Project Manager: Bakul Banerjee (FNAL).
  - Maintains the Project's work breakdown structure and other documents related to its management.
  - Tracks expenditures and progress in achieving milestones.

Site Managers

- Eric Blum (BNL)
- Don Holmgren and Amitoj Singh (FNAL)
- Chip Watson (JLab)
  - Responsible for hardware deployment and operations at their laboratories.
  - Responsible for developing and executing the components of the work breakdown structure relevant to their sites.

Change Control Board

- William Boroski (FNAL)
- Steven Gottlieb (Indiana U.)
- Thomas Schlagel (BNL)
- Robert Sugar (UCSB, Chair)
- Victoria White (FNAL)
- Roy Whitney (JLab)
  - The Change Control Board must approve all major changes in the Project's milestones.
  - It assures that changes to the Project are managed with the primary focus on the advancement of the scientific goals.

Lattice QCD Executive Committee

- Richard Brower (Boston U.)
- Norman Christ (Columbia U.)
- Michael Creutz (BNL)
- Paul Mackenzie (FNAL)
- John Negele (MIT)
- Claudio Rebbi (Boston U.)
- David Richards (JLab)
- Stephen Sharpe (U. Washington)
- Robert Sugar, (UCSB , Chair)

Lattice QCD Executive Committee

- The Executive Committee provides leadership for the USQCD Collaboration's efforts to develop computational infrastructure for the study of QCD.
- Its members are the principal investigators of the QCD SciDAC grants.
- The Executive Committee's role in this project is to set scientific goals and determine the computational resources needed to reach them.
- The Executive Committee appoints the Scientific Program Committee.

The Scientific Program Committee

- Thomas Blum (U. Connecticut)
- Andreas Kronfeld (FNAL, Chair)
- Colin Morningstar (Carnegie Mellon U.)
- John Negele (MIT)
- Stephen Sharpe (U. Washington)
- Junko Shigemitsu (Ohio State U.)
- Doug Toussaint (U. Arizona)
    - The Scientific Program Committee allocates the computational resources operated by the LQCD Computing Project. Talk by Andreas Kronfeld.
    - It organizes an annual All Hands meeting of the USQCD Collaboration.
    - It monitors the scientific progress of the effort, and provides leadership in setting scientific priorities.

International Efforts

Country	Sustained Teraflop/s
Germany	10–15
Italy	5
Japan	14–18
United Kingdom	4–5
Unites States	
LQCD Project	9
National Centers	2
US Total	11

Computing resources in sustained teraflop/s estimated to be available for the study of Lattice QCD in various countries, as of February, 2007.

International Efforts

- The estimates of computing resources available for the study of Lattice QCD in other countries were obtained from an informal survey of senior physicists in those countries.
- The United States resources do not include three computers which are located in the U.S., but not available to all members of the USQCD Collaboration:
  - A QCDOC funded by the Riken Institute of Japan and located at BNL. It is used by members of the Riken Brookhaven Research Center.
  - A large BlueGene/L located at LLNL, some time on which is available to a subset of the USQCD Collaboration for a study of high temperature QCD.
  - A one rack BlueGene/L located at MIT, which is used in part by MIT physicists for the study of Lattice QCD.

Conclusions

- Given sufficient computing power it is possible to use lattice QCD to perform accurate calculations of a wide range of quantities of importance to the experimental programs in high energy and nuclear physics.
- The Lattice QCD Computing Project is enabling physicists in the United States to play a leading role in an exciting area of science.