Overview of LQCD Computing Project

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Chair, LQCD Executive Committee

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

Funding of the LQCD Computing Project in thousands of dollars.

Outline

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II. Scientific Objectives
III. Some Recent Results
IV. Scientific Priorities and Allocations
V. The 2008 All Hands Meeting
VI. International Participation
VII. Conclusions

I. The USQCD Collaboration

The USQCD Collaboration

- The LQCD Computing Project is the key element in the efforts of the USQCD Collaboration to build the computational infrastructure needed for the study of Lattice QCD.
- USQCD consists of nearly all the high energy and nuclear physicists in the United States involved in the numerical study of QCD. It was formed nine 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. USQCD software is publicly available, and its hardware is available to all members on a peer reviewed basis.
- We build infrastructure as a community, but do science in groups or as individuals.

USQCD Infrastructure Projects

- SciDAC 1 grant (2001 – 2006)
  - Development of the QCD API which enables lattice gauge theorists to write highly efficient, portable code.
  - Development of prototype clusters optimized for lattice QCD (1.37 teraflop/s now in operation*).
- SciDAC 2 grant (2006 – 2011)
  - Optimization of the QCD API for BlueGene, Cray and clusters base on multi-core processors.
  - Physics toolbox containing sharable codes.

* Performance is measured as the average of that sustained by the sparse matrix inversion routines for Domain Wall and Improved Staggered quarks.

USQCD Infrastructure Projects

- Construction of the QCDOC (2004 – 2005)
  - Computer specially designed for lattice gauge theory by a group of physicists centered at Columbia U.
  - Sustains 4.20 teraflop/s.
- Lattice QCD Computing Project (2006 – 2009)
  - Clusters sustaining 6.16 teraflop/s have been acquired since the start of the Project.
  - The remaining SciDAC-1 clusters, the QCDOC, and the clusters acquired through the LQCD Computing Project are all operated by the Project. These computers sustain a total of 11.75 teraflop/s.
  - A cluster estimated to sustain 6.2 teraflop/s is planned for installation at FNAL in 2008-2009. Talk by Don Holmgren.

LQCD Computing Project Hardware

Computer	Site	Nodes	Performance (teraflop/s)
QCD	FNAL	127	0.15
4g	JLab	384	0.36
Pion	FNAL	518	0.86
QCDOC	BNL	12,288	4.20
6n	JLab	256	0.62
Kaon	FNAL	600	2.56
7n	JLab	396	2.98

Computers operated by the LQCD Computing Project. The first three are SciDAC-1 clusters, and the last three are clusters obtained during the LQCD Computing Project. As always, performance is measured as the average of that sustained by the sparse matrix inversion routines for Domain Wall and Improved Staggered quarks.

USQCD Incite Grant

- The DOE allocates time on its leadership class supercomputers, the Cray XT4 at ORNL and the BlueGene/P at ANL, through its Incite Program.
- USQCD currently has a three year grant running from calendar year 2008 though calendar year 2010.
- Resources are allocated one year at a time. The USQCD allocation for 2008 is the largest in the program. It consists of:
  - 19.6M core-hours on the BlueGene/P
  - 7.1M core-hours on the Cray XT4

USQCD Incite Grant

- The total allocation produces the same number of flops as a dedicated computer sustaining 2.8 teraflop/s, using our usual measure of performance. However, the leadership class computers are capable of bringing to bear very large number of processors on a single job, and are therefore particularly well suited for our most computationally intensive work.
- USQCD is one of eight groups selected to participate in the Early Science Program at ANL. We do not have a specific allocation, but have already obtained more time through this program than our 2008 Incite allocation.

II. Scientific Objectives

Objectives of Lattice QCD Calculations

- Our objective is to perform calculations of QCD in the strong coupling regime to the accuracy needed to support experimental programs in high energy and nuclear physics.
- Lattice QCD calculations have reached the point where some quantities have been calculated to an accuracy that equals or exceeds that of the corresponding experiments.
- The algorithms, formulations of QCD on the lattice, and community software developed in recent years will enable accurate determination of a wide range of important quantities in the near future provided sufficient computational resources become available.

Objectives of Lattice QCD Calculations

- Some quantities that are well known experimentally have been calculated to an accuracy of a few percent, providing checks between theory and experiment.
- Predictions have been made, which were later confirmed by experiment.

Areas of Focus

- The determination of fundamental parameters of the Standard Model, and precision tests of the Standard Model. Talk by Paul Mackenzie.
  - Experiments impacted: BaBar (SLAC), Belle (KEK), CLEO-c (Cornell), CDF and D0 (FNAL) and LHC (CERN).
- The spectrum, internal structure and interactions of hadrons. Talk by David Richards.
  - Experiments impacted: CEBAF (JLab), RHIC (BNL).

Areas of Focus

- QCD at nonzero temperature and density.
  Talk by Frithjof Karsch.
  - Experiments impacted: RHIC (BNL), FAIR (GSI) and LHC (CERN).
- Theories for Physics Beyond the Standard Model.
  - Experiments impacted: LHC (CERN).

White Papers

- Four white papers providing detailed discussions of recent progress and future opportunities in each of the areas listed on the last two slides can be found on the Review Web Page, and on the USQCD website www.usqcd.org.
- These documents consider the period 2007 to 2014. They therefore discuss some projects that will be carried out under the LQCD Computing Project, and others that will require significantly greater computer power than the Project provides.

Nature of the Calculations

- Zero temperature calculations are performed in two steps:
  - Monte Carlo methods are used to generate gauge configurations with a probability proportional to their weight in the Feynman path integrals that define QCD.
  - These configurations are stored, and use to calculate a wide variety of physical observables.
- High temperature calculations are typically carried out on smaller lattices than zero temperature ones, and fewer quantities are measured. However, large computational resources are needed because the calculations must be performed for many values of the temperature.

Controlling Systematic Errors

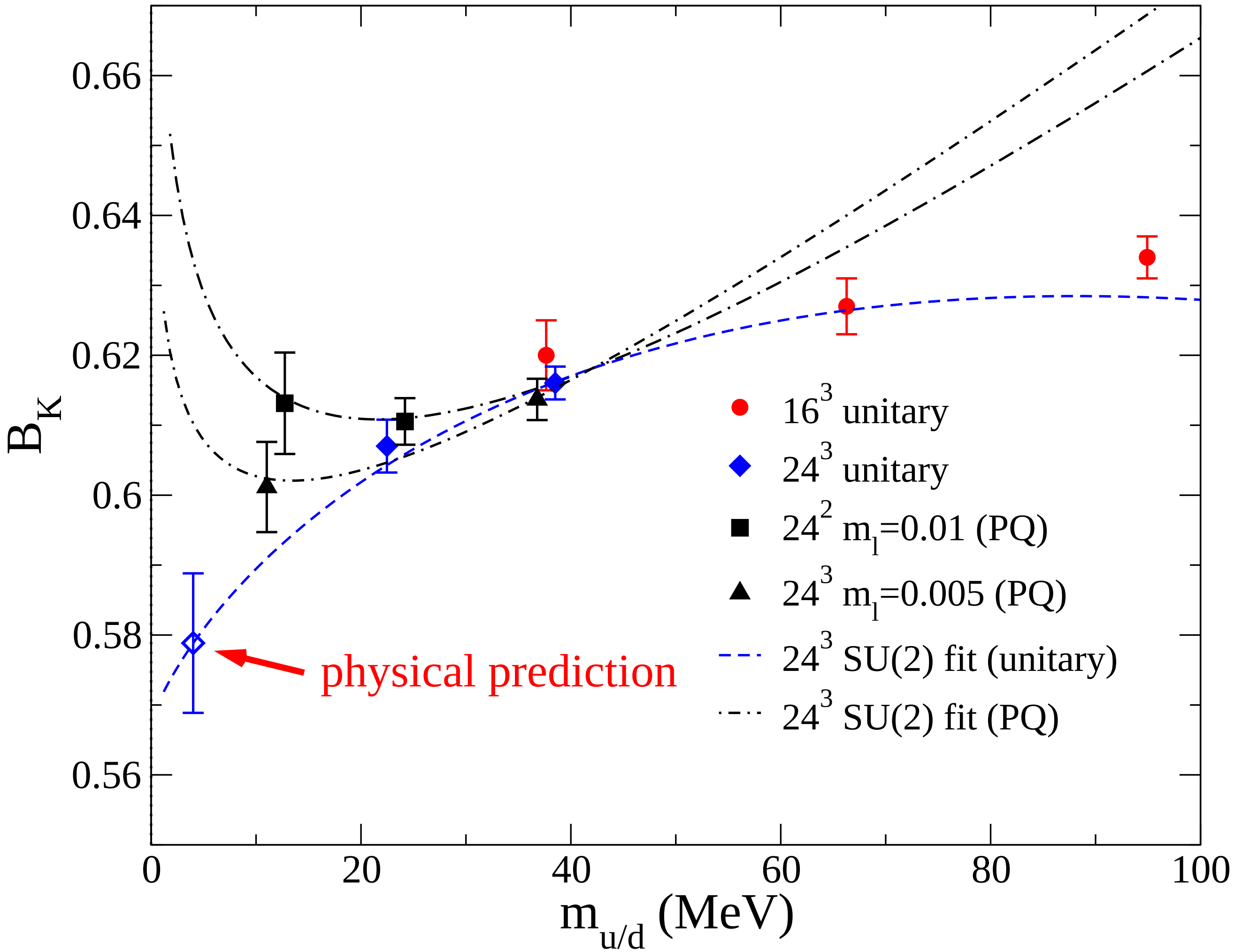
- Finite lattice spacing errors: Calculations must be performed at several small values of the lattice spacing in order to extrapolate to the continuum limit.
- Chiral extrapolation errors: Calculations must be performed at several small values of the up and down quark masses to extrapolate to their physical values using chiral perturbation theory.
- Improved actions: The use of actions (improved formulations of QCD on the lattice) greatly increases the accuracy of these extrapolations, and is essential for reaching our scientific goals.

III. Some Recent Results

The $K^0 - \overline{K}^0$ Mixing Parameter $\hat{B}_K$

- The RBC-UKQCD Collaboration has calculated the $\mathbf{K^0 - \overline{K}^0}$ mixing parameter $\mathrm{B_K}$, which is used to determine the CP violating phase in the CKM matrix from Kaon decay measurements. They find: $\hat{\mathbf{B}}_{\mathbf{K}} = \mathbf{0.72 \pm 0.04}$.
- The errors are a factor of two smaller than the world average from previous lattice results.
- The lattice result should be compared to that from the Unitary Triangle Analysis: $\hat{\mathbf{B}}_{\mathbf{K}} = \mathbf{0.78 \pm 0.09}$.
- The RBC/UKQCD calculation will improve significantly as results from configurations with a smaller lattice spacing become available over the next year or two.

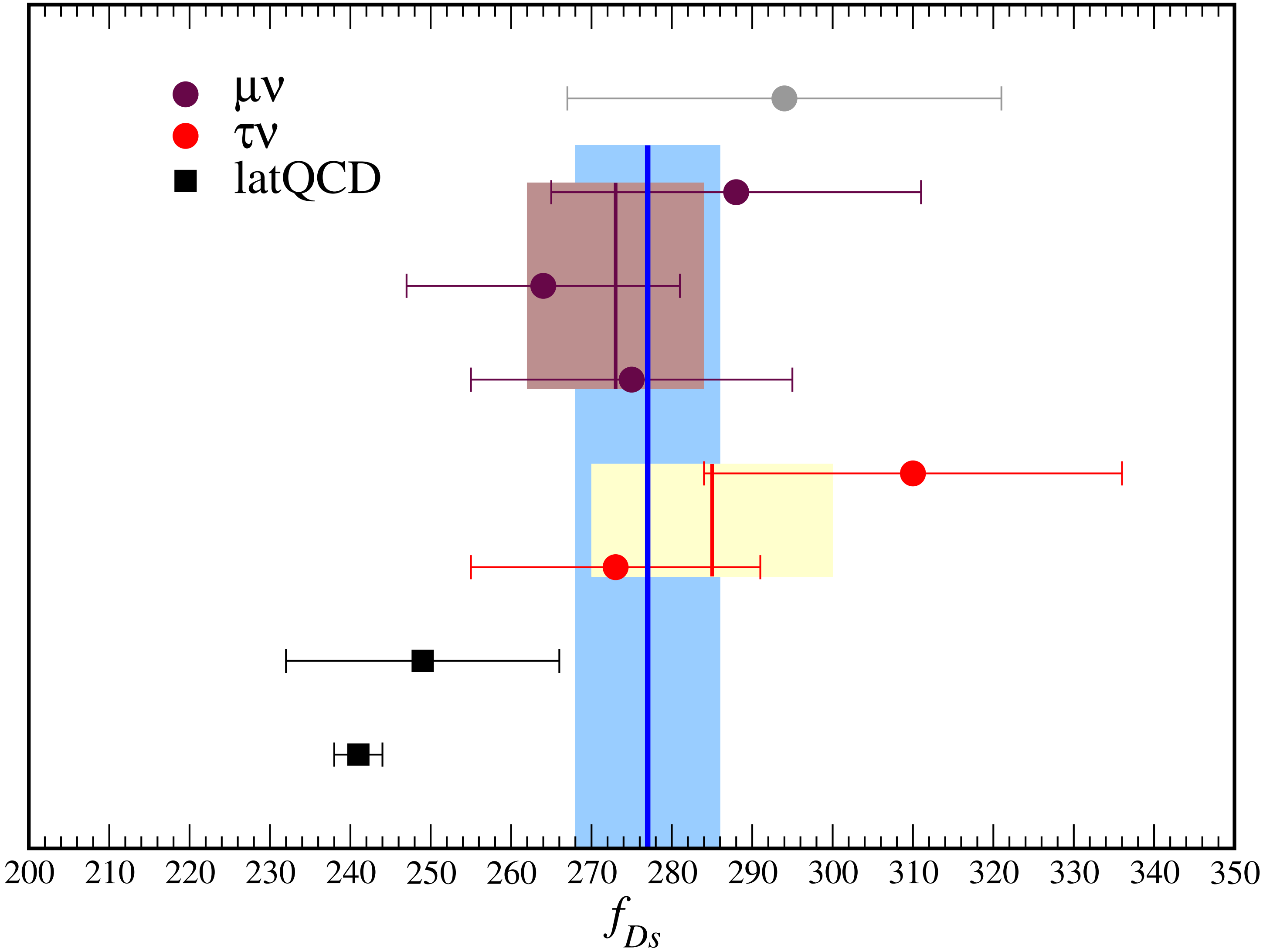
The $K^0 - \overline{K}^0$ Mixing Parameter $\hat{B}_K$



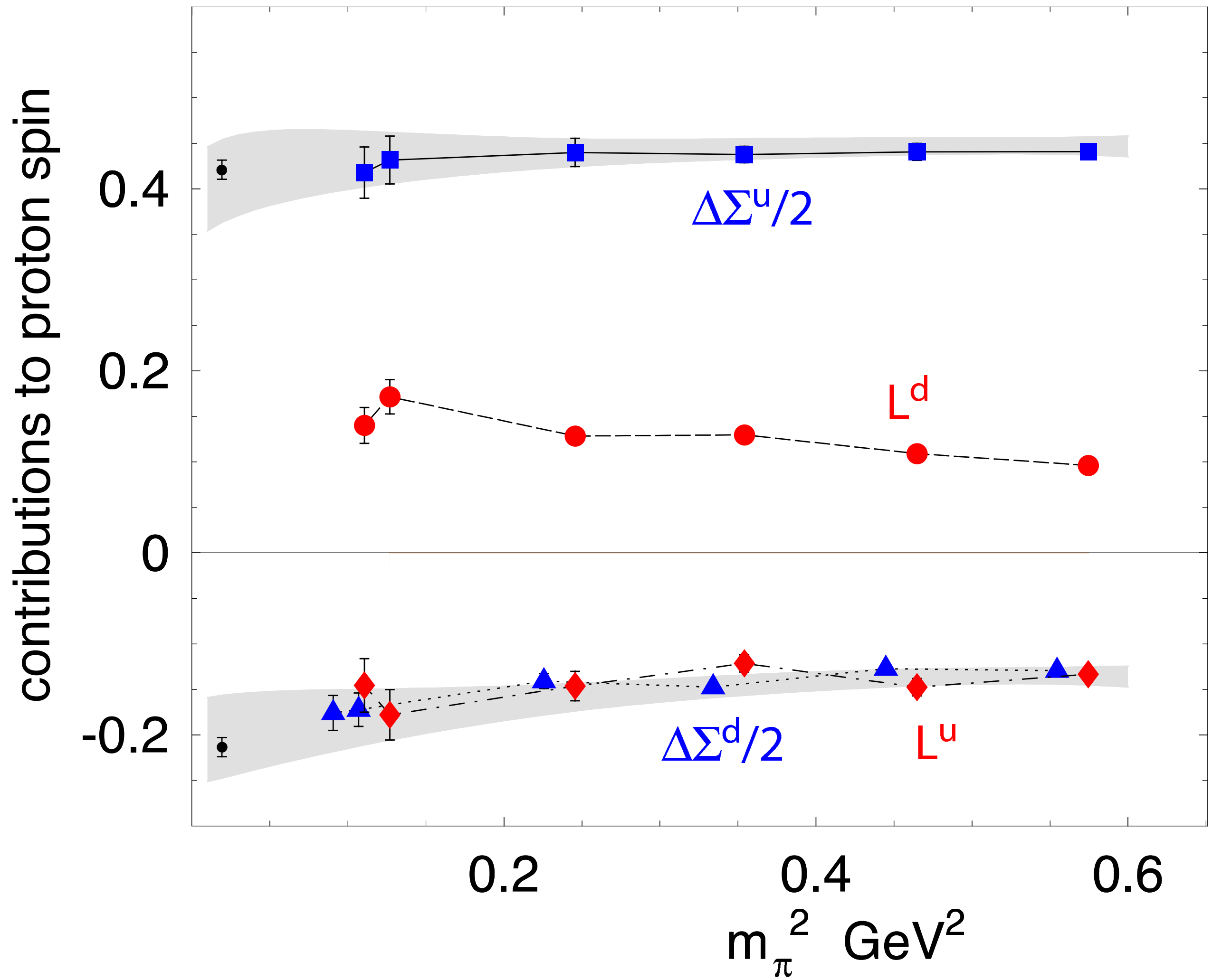
Leptonic Decay Constant of the $\mathrm{D_s}$ Meson

- This year the HPQCD Collaboration obtained: $\mathbf{f_{D_s} = 241 \pm 3}$ MeV.
- This was a major improvement over the earlier FNAL/MILC result: $\mathbf{f_{D_s} = 254 \pm 8 \pm 11}$ MeV.
- However, the HPQCD result differs from the average of experimental results from Belle and CLEO-c at the $3.8\,\sigma$ level: $\mathbf{f_{D_s} = 270.4 \pm 7.3 \pm 3.7}$ MeV.
- The HPQCD result for the leptonic decay constant of $\mathbf{D}^+$, $\mathbf{f_{D^+} = 207 \pm 4}$ MeV, is in agreement with the most recent CLEO-c result: $\mathbf{f_{D^+} = 206.7 \pm 8.5 \pm 2.5}$ MeV.
- HPQCD/UKQCD and FNAL/MILC use the same gauge configurations, but different formulations for the valence quarks. Both calculations should improve in accuracy during the coming year.

Leptonic Decay Constant of the D_s Meson



The Spin Content of the Proton

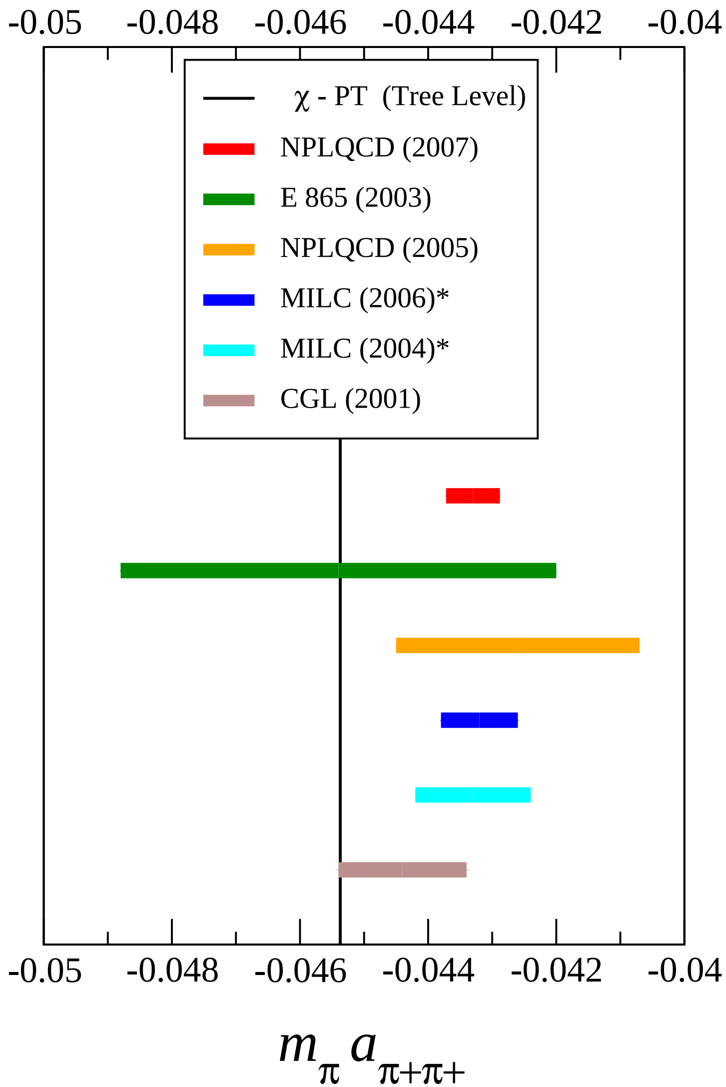


Contributions of the quark spins $\mathbf{\Delta\Sigma^{u,d}/2}$ and the orbital angular momentum $\mathbf{L^{u,d}}$ to the spin of the proton by the LHP Collaboration. The gray bands are chiral extrapolations of the quark spin contributions, the black symbols are the recent HERMES experimental results.

$\pi^+ - \pi^+$ Scattering Lengths

- The NPLQCD Collaboration has made significantly progress in its determination of the $\pi^+ - \pi^+$ scattering lengths.
- It has also made the first lattice calculation of the $K^+ - K^+$ scattering lengths and performed exploratory studies of the nucleon–nucleon and hyperon–nucleon scattering length.
- The accuracy of all of these calculations will improve markedly over the coming year as NPLQCD moves to smaller lattice spacings.

$\pi^+ - \pi^+$ Scattering Lengths



IV. Scientific Priorities and Allocations

The LQCD 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 USQCD SciDAC and Incite grants.
- The Executive Committee's role in The Lattice QCD Computing Project is to set scientific goals and determine the computational resources needed to reach them.
- The Executive Committee holds a conference call every other week to monitor progress and discuss major issues.

Members of the LQCD 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)

The Scientific Program Committee

- The LQCD Executive Committee has formed a Scientific Program Committee (SPC), which allocates USQCD computing resources.
- Members serve three year terms. The current ones are:

  Thomas Blum (U. Connecticut)

  Christopher Dawson (U. of Virginia)

  Frithjof Karsch (BNL)

  Andreas Kronfeld (FNAL, Chair)

  Colin Morningstar (Carnegie Mellon U.)

  John Negele (MIT)

  Junko Shigemitsu (Ohio State U.)

Scientific Priorities and Resource Allocations

- The SPC issues a call for proposals for the use of dedicated resources once a year. It also invites authors of the proposals to identify projects that would be appropriate for the DOE's leadership class computers. Proposals are grouped into three classes:
  - Type A proposals are for very large scale projects. They are expected to benefit the whole Collaboration by producing data, such as gauge configurations or quark propagators, that can be used by all, or by producing physics results listed among USQCD's strategic goals.
  - Type B proposals are for investigations of medium to large scale. They are not required to share data or to work towards stated USQCD goals, although if they do, it is a plus.

Scientific Priorities and Resource Allocations

- Type C proposals are for exploratory calculations, such as those needed to develop and/or benchmark code.

- The SPC reviews the proposals, and then organizes an All Hands meeting of the Collaboration. Authors of the proposals are invited to describe their plans at the All Hands meeting, and the plans are discussed by the Collaboration as a whole.
- With input from this discussion the SPC allocates USQCD's computational resources. It also transmits to the Lattice QCD Executive Committee the priorities of the Collaboration for use of leadership class computers to guide it in future proposals.
- This process sets the priorities of USQCD on a yearly basis.

Strengths of the Allocation Process

- USQCD research priorities are examined and, if necessary, reordered on a yearly basis with broad community input.
- The SPC consists of seven highly respected lattice gauge theorists who are balanced among the major research areas pursued by USQCD. With input from the Collaboration as a whole, it is in an excellent position to carry out its responsibilities.
- This process has a particularly positive impact on younger physicists who are likely to have difficulty obtaining the large allocations they need to advance their careers at national supercomputer centers. The SPC has made a concerted effort to solicit and fund proposals from younger members of the field.

V. The 2008 All Hands Meeting

The 2008 All Hands Meeting

- The 2008 All Hands Meeting took place at JLab on April 4–5. Fifty-nine members of USQCD attended.
- Reports from the Executive Committee, the Project Manager, the Scientific Program Committee, the Software Committee and the Site Managers brought attendees up to date on the infrastructure effort. They were followed by a round table discussion on computing and software.
- Presentations were made by representatives of each of the Type A proposals, and most of the Type B proposals. A round table discussion was held on each type of proposal.

Outcome of the Allocation Process

- The 15 Type A proposals were awarded 50.46 million 6n equivalent node hours on LQCD Computing Project and leadership class computers, which was 56% of the time requested.
- The 16 Type B proposals were awarded 7.42 million 6n equivalent node hours on LQCD Computing Project computers, which was 96% of the time requested.
- Approximately 35% of the cycles allocated were on leadership class computers, with the remaining 65% on LQCD Computing Project computers.
- The Scientific Program Committee noted an acceleration of the growth in requests for Beyond the Standard Model projects.

VI. International Participation

International Collaborations

- Lattice QCD is an international field with very strong programs in Germany, Italy, Japan and the United Kingdom, and excellent work being done in many other countries.
- Groups within USQCD have formed a number of international collaborations. Among the most noteworthy are:
    - The USQCD effort using DWF quarks is an international effort begun with equal participation by the United States based RBC Collaboration and Edinburgh, Southampton and Swansea members of the UKQCD Collaboration. During the past year this activity has expanded to include the LHPC group.

International Collaborations

- 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 the P4 staggered quark action 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 Collaborations

- Our international collaborators have made major contributions to the scientific effort, and to the development of algorithms and software. They have provided very significant computational resources for the joint work.

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.

Conclusions

- It is now possible to use lattice QCD to perform accurate calculations of a wide variety of quantities of importance to experimental programs in high energy and nuclear physics.
- The Lattice QCD Computing Project has enabled major progress in the numerical study of QCD, and much more important work is to be expected by the end of the Project.
- The DOE's support of dedicated hardware for the study of lattice gauge theory is enabling physicists in the United States to play a leading role in an exciting area of science.