National Computational Infrastructure for Lattice Gauge Theory: Final Report

Lattice QCD Executive Committee

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1 Introduction

In this document we describe work done under the SciDAC-1 Project *National Computational Infrastructure for Lattice Gauge Theory*. The objective of this project was to construct the computational infrastructure needed to study quantum chromodynamics (QCD). Nearly all high energy and nuclear physicists in the United States working on the numerical study of QCD are involved in the project, as are Brookhaven National Laboratory (BNL), Fermi National Accelerator Laboratory (FNAL), and Thomas Jefferson National Accelerator Facility (JLab). A list of the senior participants is given in Appendix A.2. The project includes the development of community software for the effective use of terascale computers, and the research and development of commodity clusters optimized for the study of QCD. The software developed as part of this effort is publicly available, and is being widely used by physicists in the United States and abroad. The prototype clusters built with SciDAC-1 funds have been used to test the software, and are available to lattice gauge theorists in the United States on a peer reviewed basis.

QCD is the component of the Standard Model of subatomic physics that describes the strong interactions. The Standard Model has been enormously successful; however, our knowledge of it is incomplete because it has proven extremely difficult to extract many of the most important predictions of QCD, those that depend on the strong coupling regime of the theory. To do so from first principles and with controlled systematic errors requires large scale numerical simulations within the framework of lattice gauge theory. Such simulations are needed to address problems that are at the heart of the DOE's large experimental programs in high energy and nuclear physics. Our immediate objectives are to 1) calculate weak interaction matrix elements of strongly interacting particles to the accuracy needed to make precise tests of the Standard Model; 2) determine the properties of strongly interacting matter under extreme conditions, such as those that existed in the very early development of the universe and are created today in relativistic heavy ion collisions; and 3) calculate the masses of strongly interacting particles and obtain a quantitative understanding of their internal structure. The infrastructure we have built under this grant is essential to achieving these objectives. Some examples of research carried out with the aid of this infrastructure can be found in Section 4, and a list of paper enabled by it is given in Appendix A.1.

2 SciDAC-1 Software

Under its SciDAC-1 grant, the U.S. lattice gauge theory community created a unified program environment that enables its members to achieve high efficiency on a wide variety of high performance computers. Among the design goals were to enable users to quickly adapt codes to new architectures, easily develop new applications and incorporate new algorithms, and preserve their large investment in existing codes. These goals were achieved through the development of the QCD Applications Programming Interface (QCD API), which is illustrated in Fig. 1.

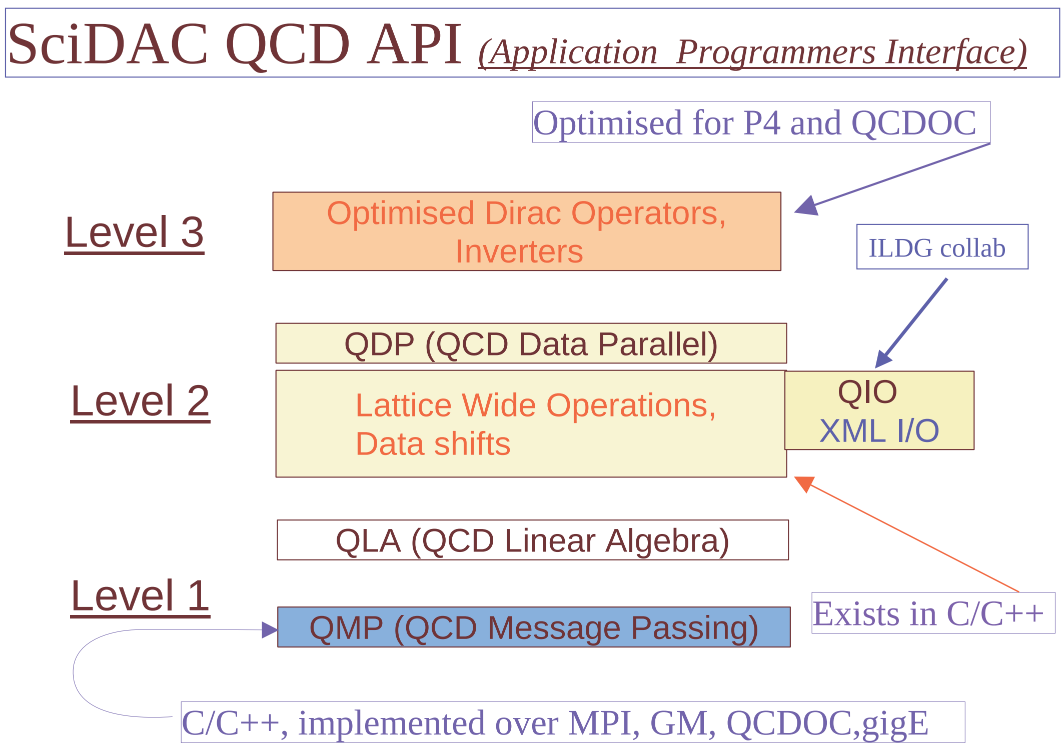

Figure 1: Structure of the QCD API developed under SciDAC-1.

All of the fundamental components of the QCD API have been implemented and are in use on the U.S. QCDOC hardware at BNL, on both the switched and mesh architecture Pentium 4 clusters at FNAL and JLab, and on a number of general purpose supercomputers. The QCD API is being used by a growing number of physicists in the U.S. and abroad. The software code and documentation can be found at the USQCD http://www.usqcd.org/usqcd-software. Here we briefly describe each of its components.

The QCD API has a layered structure which is implemented in a set of independent libraries. Level 1 provides the code that controls communications and the single core processor computations. To obtain high efficiency on terascale facilities, much of this layer may have to be written in hardware specific assembly language. However versions exist in C and C++ using MPI for transparent portability of all application codes.

Message Passing: QMP defines a uniform subset of MPI-like functions with extensions that (1) partition the QCD space–time lattice and map it onto the geometry of the hardware network, providing a convenient abstraction for the Level 2 data parallel API (QDP); (2) contain specialized routines designed to access the full hardware capabilities of the QCDOC network and to aid optimization of low level protocols on networks in use and under development on clusters. There is a basic test suite to verify each implementation.

Linear Algebra: All lattice QCD calculations make use of a set of linear algebra operations in which the basic elements are three–dimensional complex matrices, elements of the group SU(3). These operations are local to lattice sites or links and do not involve inter–processor communications. We have collected them into a single Level 1 library called QLA. The QLA routines can be used in combination with QMP to develop complex data parallel operations in QDP or in existing C or C++ code. The C implementation has about 19,000 functions generated in Perl, with a full suite of test scripts. The C++ implementation makes considerable use of templates, and so contains only a few dozen templated classes (the required specific classes are generated on demand by the compiler). For both C and C++ it is important to optimize the code for the most heavily used linear algebra modules.

Data Parallel Interface: Level 2 (QDP) contains data parallel operations that are built on QMP and QLA. The C implementation is being used to improve performance of the MILC code, a large, publicly available suite of applications. Despite the fact that the MILC code has been carefully optimized over its fifteen year lifetime, rewriting computationally intensive subroutines in QDP makes a significant improvement in its performance. Chroma, an entirely new application code base, has been written *di novo* in the C++ implementation of QDP. QDP allows extensive overlapping of communication and computation in a single line of code. By making use of the QMP and QLA layers, the details of communications buffers, synchronization barriers, vectorization over multiple sites on each node, etc. are hidden from the user.

Level 3 Subroutines: A very large fraction of the resources in any lattice QCD simulation go into a few computationally intensive subroutines, most notably the repeated inversion of the Dirac operator, a large sparse matrix. To obtain the level of efficiency at which we aim, it is necessary to optimize these subroutines for each architecture. For example, on the QCDOC, the assembly coded inverter for the Domain Wall and Asqtad quark actions, the two quark formulations that are being used in initial work, is as high as 42% and 45% of peak, respectively. (The precise performance depends on the number of lattice sites assigned to each processor). These percentages correspond to total sustained performances of 4.1 and 4.4 teraflop/s for the full 12,288 processor machine. Level 3 codes written with SSE2 instructions achieve up to 3.0 gigaflop/s per processor for the last cluster built at JLab with SciDAC-1 funds. It has 3.0 GHz dual core Pentium 4 processors.

Data Management: A very large fraction of the computing resources used in lattice QCD calculations go into Monte Carlo simulations that generate representative configurations of the QCD ground state. The same configurations can be used to calculate a wide variety of physical quantities. Because of the large resources needed to generate configurations, the U.S. lattice community has agreed to share all of those that are generated with DOE resources. To enable this sharing we have created standards for file formats, and written an I/O library (QIO) that adheres to them. We are charter members of the International Lattice Data Grid (ILDG), which is setting a basic set of meta-data and middleware standards to enable international sharing of data. The U.S. lattice gauge theory community is fully capable of archiving and retrieving data on the ILDG.

3 Prototype Commodity Clusters

The SciDAC-1 project undertook investigations of commodity hardware for lattice QCD. By selecting the most cost effective and appropriately balanced combinations of processor and network interconnect, as opposed to the products which individually had the best performance, and by taking advantage of the modest requirements for memory size and disk bandwidth, the SciDAC-1 project built large scale clusters dedicated to lattice QCD calculations with better price/performance than any existing general purpose parallel computing platform. The processors investigated during the project included Intel Pentium, Xeon, and Itanium, AMD Athlon and Opteron, DEC Alpha, and IBM PPC970. The project also investigated several high performance networks, including Myrinet, gigabit ethernet meshes, and Infiniband. Each year the most promising technologies were chosen to build prototype production clusters listed in Table 1.

Site	Cluster	Processor	Network
JLab	2m	Xeon (single)	Myrinet
JLab	3g	Xeon (single)	3D GigE
JLab	4g	Xeon (single)	5D GigE
JLab	6n	Pentium (dual core)	Infiniband
FNAL	w	Xeon (dual)	Myrinet
FNAL	qcd	Xeon (dual)	Myrinet
FNAL	pion	Pentium (single)	Infiniband

Table 1: Prototype production clusters built under SciDAC-1.

The DOE Lattice QCD Computing Project, which started October 2005, is building upon the experience of the SciDAC-1 cluster effort to procure and operate large scale systems. This project is planned for FY2006 through FY2009, with funding of $9.2 million from the High Energy and Nuclear Physics Programs of the DOE. Approximately $6 million of this funding will be used for commodity hardware, specifically clusters in the first year, and most likely clusters for the subsequent three years. The designs of the first clusters built by the project in 2006 were derived directly from the prototype clusters assembled during the SciDAC-1 project.

The prototype clusters from the SciDAC-1 project have proven to be very successful in delivering physics results. Operation for physics production of many of these clusters, specifically the 3g, 4g, and 6n clusters at JLab, and the qcd and pion clusters at FNAL, is now part of the facilities project. These clusters have an aggregate capacity of nearly two teraflop/s.

4 Research Achievements

In this section we describe a few examples of research achievements enabled in whole or in part by this grant.

The Role of Sea Quarks

The greatest challenge to performing accurate numerical calculations of quantum chromodynamics (QCD) is the inclusion of the full effects of sea quarks, quarks that are created and destroyed during the course of a process, rather than being part of the initial and final states. Only the *u*, *d* and *s* quarks are light enough so that their sea quarks need to be included. So, over the last five years the MILC Collaboration has generated an extensive set of gauge configurations, snap shots of the QCD ground state, that fully include the effects of these sea quarks [1]. The computational resources needed to generate configurations grows rapidly as the sea quark masses decrease. Although it is possible to work directly at the mass of the *s* quark, with current computers it is too expensive to do so for the much lighter *u* and *d* quarks. Instead one generates configurations for a range of *u* and *d* quark masses, and extrapolates to their physical values using chiral perturbation theory, which predicts the dependence of physical observables on the light quark masses. Of course the accuracy of the extrapolation increases as the masses of the *u* and *d* quarks decrease, as do the required computing resources. The MILC configurations have been made publicly available, and are being used to study a wide range of physical phenomena. Among the important achievements of the SciDAC Program has been to encourage sharing of resources and the formation of collaborations among existing groups.

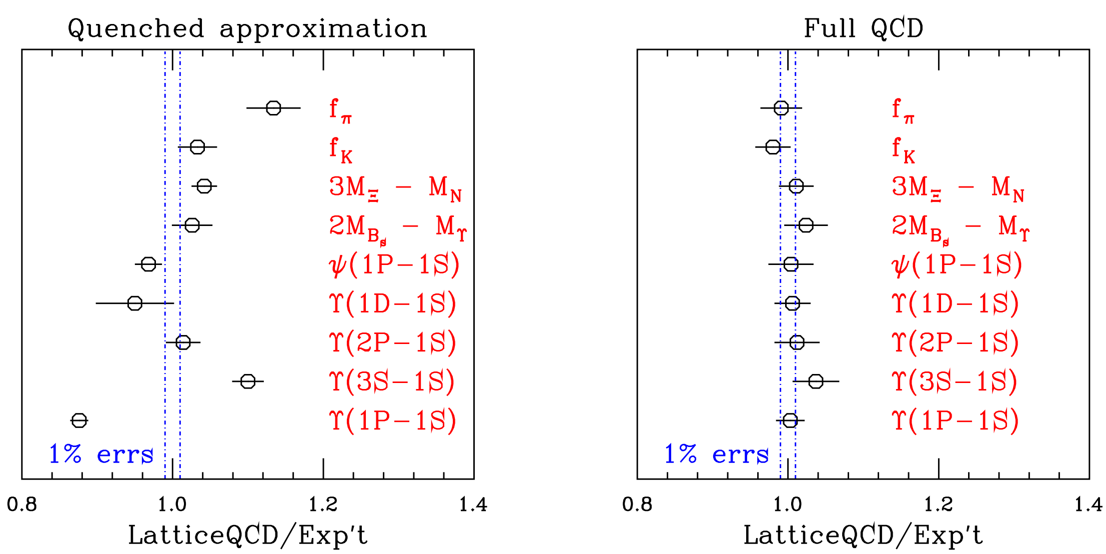

Figure 2: The ratio of several quantities calculated in lattice QCD to their experimental values. The panel on the left shows results from the quenched approximation, and that on the right from full QCD.

The Fermilab Lattice, HPQCD, MILC and UKQCD Collaborations have used the MILC configurations to calculate a number of quantities whose values have been precisely determined experimentally [2]. The quantities studied were among the easiest to calculate to high accuracy, so a failure to obtain agreement with experiment would have indicated a serious problem with the calculational approach. Results are shown in Fig. 2, and compared with ones from the quenched approximation in which the effects of sea quarks are neglected. Clearly, the inclusion of sea quarks is essential for obtaining high precision results. This work was described in a *News and Views* article in *Nature* [3], as well as in a *News Focus* article in *Science* [4]. Within the high energy community, it has been featured in *Fermi News Today* [5], *Physics Today* [6] and in a cover article in the *CERN Courier* [7].

The Strong Coupling Constant

The HPQCD and UKQCD Collaborations have used the MILC configurations to make the first determination of the strong coupling constant α_S that fully includes the effects of sea quarks in the chiral (physical value of the u and d quark masses) limit [8]. The value of α_S depends on the energy scale at which it is measured. At high energies, where the coupling is weak, the energy dependence of α_S can be calculated using perturbation theory, but the overall normalization must be determined by an experiment or a lattice calculation. Results of the HPQCD/UKQCD calculation are shown in Fig. 3.

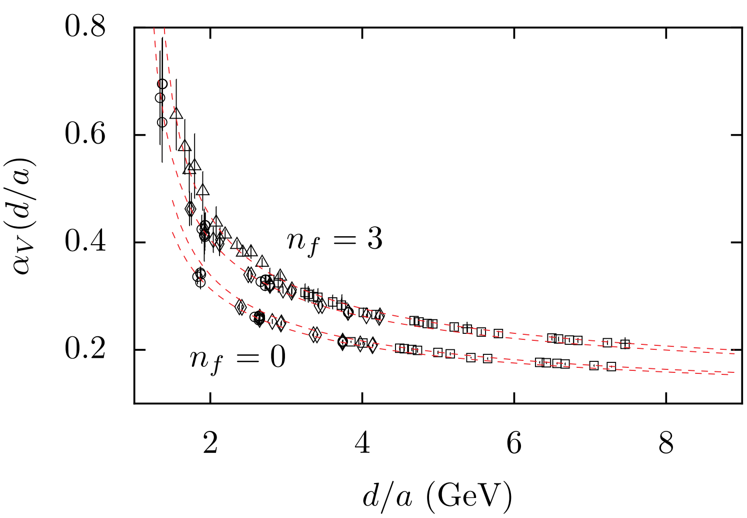

Figure 3: The strong coupling constant as a function of the energy d/a. The plotting symbols are the lattice data, and the red dashed lines are the perturbation theory results with the overall normalization one sigma above and one sigma below its central value. The data and curves marked $n_f = 3$ fully include the effects of the three light sea quarks, u, d and s. Those labeled $n_f = 0$ neglect the effects of sea quarks.

It is customary to compare different determinations of α_S at the mass of the Z meson. The lattice result is $\alpha_S(M_Z) = 0.1170 \pm 0.0012$. The previous world average, which is comprised of a number of different experimental determinations and an older lattice one, is $\alpha_S(M_Z) = 0.1176 \pm 0.0020$ [9].

Thus, the lattice calculation is consistent with the previous world average, but has somewhat smaller error bars.

Properties of π and K Mesons

The MILC Collaboration has made an extensive study of the properties of π and K mesons. This work provided an opportunity to check lattice methods to high (2% to 3%) precision, and to calculate phenomenologically important physical quantities that are difficult or impossible to obtain with controlled errors by other methods. One outcome was the determination of the leptonic decay constants of the π and K mesons to an accuracy of better than 3% [2, 10]. These calculations are illustrated in Fig. 4. The results for the decay constants in turn led to a new approach for determining the Cabibbo-Kobayashi-Maskawa (CKM) matrix element V_{us} [11]. (The CKM matrix describes how quarks couple to the weak interactions. Its elements are fundamental parameters of the Standard Model of subatomic physics). The current lattice value is $|V_{us}| = 0.2223^{+26}_{-14}$). The Particle Data Group (2006) gives $V_{us} = 0.2257(21)$ [9] from the $K \to \pi\mu\nu$ experimental rate and non-lattice theory. The lattice results are expected to improve significantly during the coming year.

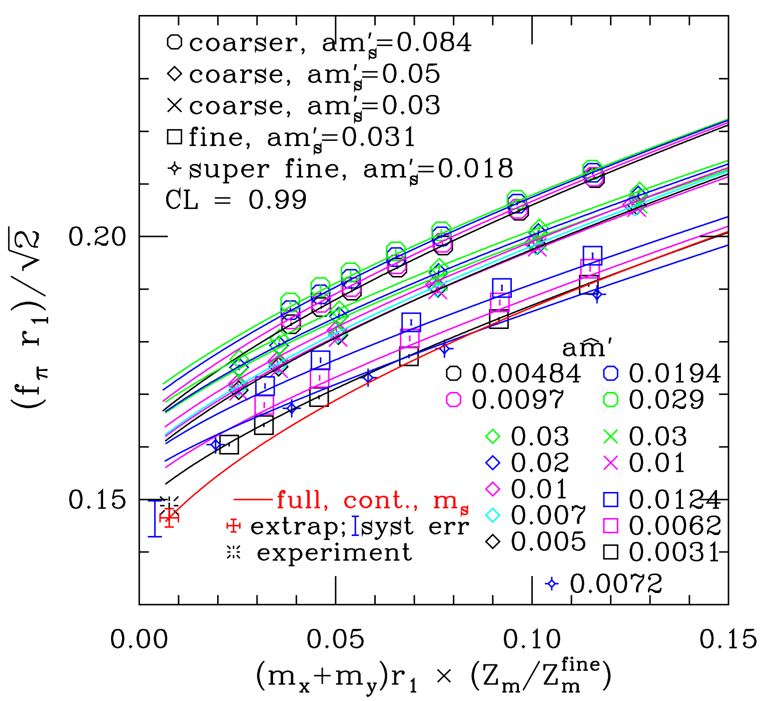

Figure 4: The pion decay constant *vs.* quark mass, in units of the scale r_1 which is determined from the static quark potential. Lines through the data points come from a staggered chiral perturbation theory fit to the entire data set for decay constants and masses. The red line represents the fit function in "full QCD" after extrapolation of parameters to the continuum, and with the mass of the strange sea quark fixed at its physical value. The red plus shows the extrapolated value of the decay constant f_π, in agreement with experiment (black burst) within systematic errors (blue bar).

This set of calculations also yielded the first evaluation of the masses of the u, d and s quarks fully taking into account the effects of light sea quarks[10, 12, 13]. These results are particularly significant because uncertainty in the strange quark mass has severely limited the theoretical precision of a variety of phenomenological studies, and determination of the up quark mass addresses the long standing proposal that this quantity vanishes.

The Axial Charge of the Nucleon

The nucleon axial charge g_A is a fundamental property of the nucleon, which governs the β decay of a free neutron into a proton, electron, and neutrino. It provides an important test of our ability to calculate nucleon properties from first principles. The computational challenge in calculating g_A has been to generate gauge configurations with small enough values of the *u* and *d* quark masses to reliably extrapolate to their physical values and to infinite volume using chiral perturbation theory.

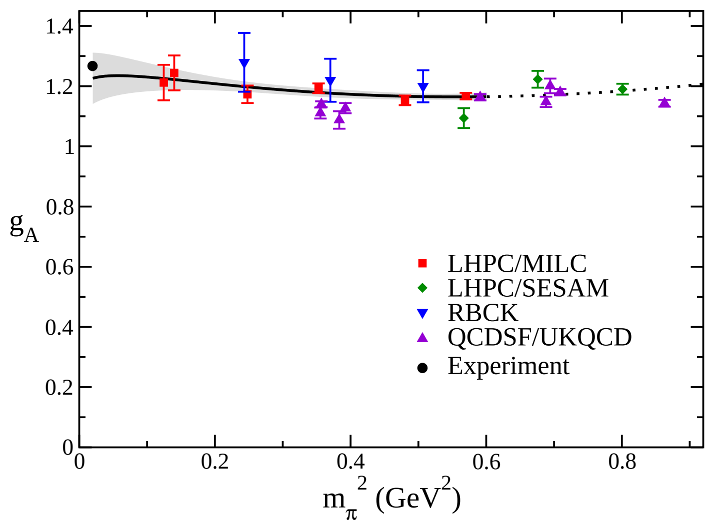

Figure 5: The axial charge of the nucleon g_A as a function of the square of the pion mass. The six red points are the LHPC's high statistic calculations using MILC gauge configurations, and the solid curve is a fit to the data using chiral perturbation theory. For comparison, the figure also shows three points by the RBCK collaboration [15] using dynamical domain wall fermions (blue), the most recent results by the QCDSF/UKQCD collaboration[16] using improved Wilson dynamical fermions (purple), and previous LHPC calculations using SESAM configurations[17] with dynamical Wilson quarks (green).

To address this exceedingly demanding regime of light quark masses and large volume the Lattice Hadron Physics Collaboration (LHPC) has recently calculated g_A using a hybrid approach in which they combine improved staggered sea quarks in gauge configurations generated by the MILC Collaboration with domain wall quarks in the initial and final states [14]. The improved staggered quark action has the advantage that it can be used to generate configurations with light sea quarks with current computers, while the domain wall quark action has the advantage of having nearly exact chiral symmetry on the lattice. Figure 5 shows g_A from this and previous lattice calculations as a function of the square of the pion mass, along with a fit using chiral perturbation theory.

The final LHPC result is $g_A = 1.226 \pm 0.084$, in excellent agreement with the experimental value 1.2695 ± 0.0029.

Predictions of Lattice QCD

During the course of the SciDAC Program, the Lattice QCD community moved from the validation of techniques through the calculation of quantities that are well known experimentally, to the successful prediction of quantities that had not yet been measured. Four important predictions that were subsequently confirmed by experiment are:

- One of the major objectives of the field of Lattice QCD is to determine the decay properties of pseudoscalar mesons with one light and one heavy quark. Strong interaction effects in leptonic decays are characterized by decay constants, while in semileptonic decays they are characterized by various form factors. The decay constants and form factors for B and B_s mesons, which contain heavy b quarks, play a critical role in tests of the Standard Model that are currently a major focus of the experimental program in high energy physics. These quantities are very difficult to measure experimentally, so accurate lattice calculations of them would be of great importance. On the other hand, the decay constants and form factors of D and D_s meson, which contain heavy c quarks, are being measured to high accuracy by the CLEO-c Collaboration and other groups. Since the lattice techniques for studying mesons with c and b quarks are identical, these experiments provide an excellent opportunity to validate the lattice approach being used in the study of D and B decays.

  The Fermilab Lattice and MILC Collaborations have calculated the semileptonic form factors for the decay of the D meson into a K meson and leptons [18]. Shortly after this prediction was made, the Focus and Belle Collaborations confirmed it experimentally [19, 20]. The lattice and most recernt experimental results are shown in Fig. 6. The excellent agreement between experimental and lattice results was an important first step in the validation process. This work was featured in Fermi News Today [21]. Preliminary results for the form factors of the B meson are available from the HPQCD and UKQCD Collaborations [22].

- The Fermilab Lattice and MILC Collaborations performed the first calculation the decay constants of the D and D_s mesons that fully takes into account the effects of sea quarks. They found $f_{D^+} = 201 \pm 3 \pm 6 \pm 9 \pm 13$ MeV, and $f_{D_s} = 249 \pm 3 \pm 7 \pm 11 \pm 10$ [23]. where the uncertainties are statistical and a sequence of systematic effects. Within a few days of this result being made public, the CLEO-c Collaboration announced its experimental determination, $f_{D^+} = 223 \pm 16^{+7}_{-9}$ MeV [24]. The lattice and experimental results were the subjects of cover articles in the CERN Courier [25] and the New Scientist [26]. More recently the BaBar Collaboration measured the decay constant for the D_s^+ meson finding $f_{D_s} = 279 \pm 17 \pm 6 \pm 19$ MeV [27].

- A fourth prediction from lattice QCD is the mass of the B_c meson. This exotic particle, consisting of a bottom quark and a charmed anti-quark, was first observed in 1998, but its mass was only poorly measured. The Fermilab Lattice and UKQCD Collaborations used the Fermilab cluster and the MILC configurations to calculate the B_c mass. They found a mass of 6304 ± 20 MeV [28], a dramatic improvement in accuracy over previous lattice calculations.

Soon after this result was made public, the CDF experiment at Fermilab's Tevatron finished a new, precise measurement of the mass: 6287 ± 5 MeV, confirming the prediction from lattice QCD [29]. The fine agreement was covered in the New Scientist (11 December 2004), The Scotsman newspaper (11 June 2005), and a News and Views article in Nature (14 July 2005). The success of the lattice calculation was named one of the The Top Physics Stories for 2005 by Physics News Update [30], which described it as "the best-yet prediction of hadron masses using lattice QCD".

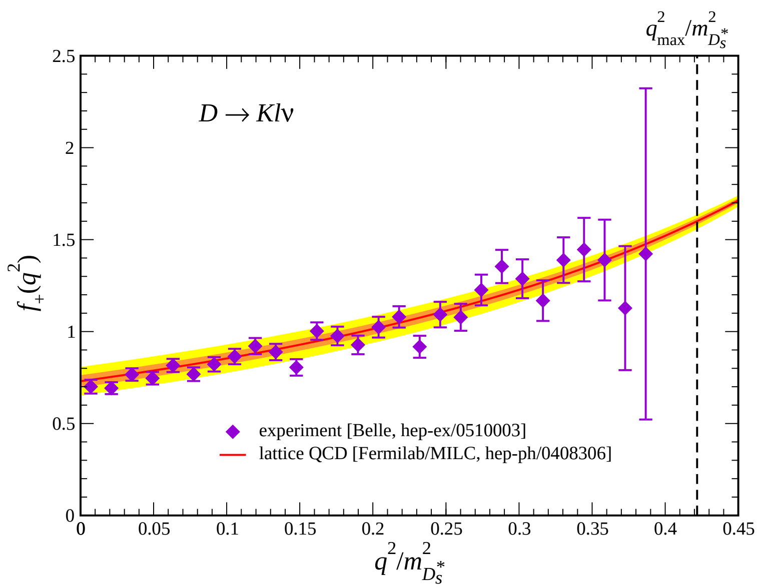

Figure 6: The semileptonic form factor $f_+(q^2)$ for the decay of a D meson into a K meson, a lepton, and a neutrino, as a function of the momentum transfer to the leptons q^2. The orange curve is the lattice result, and the blue points are the experimental results of the Belle Collaboration.

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A Appendices

A.1 Publications Enabled by this Grant

Publications in Refereed Journals

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A.2 Committees and Senior Personnel

In this appendix we list the members of the committees that made up the management team of this project. We also list the senior personnel who participated in it, or have indicated that they would make use of the infrastructure it created. They comprise nearly all of the senior lattice gauge theorists in the United States, as well as computer scientists and engineers who have participated in the project.

Lattice QCD Executive Committee

Richard Brower	Boston University
Norman Christ	Columbia University
Michael Creutz	Brookhaven National Laboratory
Paul Mackenzie	Fermi National Accelerator Laboratory
John Negele	Massachusetts Institute of Technology
Claudio Rebbi	Boston University
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