Project Execution Plan
For the Lattice QCD Computing Project (LQCD)

At
Brookhaven National Laboratory, Brookhaven, New York
Fermi National Accelerator Laboratory, Batavia, Illinois
Thomas Jefferson National Accelerator Facility, Newport News, Virginia

For the
U.S. Department of Energy
Office of Science
Offices of High Energy and Nuclear Physics

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LQCD Project Execution Plan
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Signature Sheet for Original Approval (2006) on File in the LQCD Project Office

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1 INTRODUCTION

The development and operation of a large scale computing facility dedicated to the study of quantum chromodynamics (QCD) plays an important role in expanding our understanding of the fundamental forces of nature and the basic building blocks of matter. Since 2000, members of the United States lattice gauge theory community have worked together to plan the computational infrastructure needed for the study of QCD. With support from the Department of Energy (DOE) High Energy Physics (HEP), Nuclear Physics (NP), Advanced Scientific Research (ASCR) and SciDAC programs, prototype hardware was designed, constructed and tested. In addition, the software needed to effectively use the hardware was developed. By taking advantage of simplifying features of lattice QCD calculations, these R&D efforts demonstrated that it is possible to build computers for this field with significantly better price/performance than commercial machines.

Two tracks for the construction of massively parallel computers for QCD were studied. One involved the design and fabrication of key components, while the other made use of carefully chosen commodity parts. During the 6-year development phase, the QCD on a Chip (QCDOC) machine was designed and developed by lattice gauge theorists at Columbia University in collaboration with colleagues at IBM. The design incorporates CPU, memory and communication on a single chip. Based on the above design, a 12,288-chip QCDOC was constructed at Brookhaven National Laboratory (BNL).

In parallel, commodity-component-based prototype clusters optimized for the study of QCD were developed and tested at Fermilab (FNAL) and Jefferson Lab (JLab) under a grant from the SciDAC program, as well as with the support of these labs' base programs. Research and development performed during the first six years of this period provided the groundwork for the Lattice QCD Computing Project.

The Lattice QCD Computing Project encompasses the design, procurement and operation of dedicated computing hardware for the study of QCD. The 4-year project began in October 2005 and is scheduled to end in September 2009 (FY06-FY09). Total project cost is estimated to be $9.2M. The project meets the criteria for an OMB Exhibit 300 project and is managed as such. The Unique Project (Investment) Identifier is 019-20-01-21-01-1032-00.

Project funds are used to support the operation of existing hardware and the procurement and deployment of new hardware. Specifically, funds are used to procure and deploy new computing hardware in order to meet performance requirements and metrics. Project funds are also used to support the operation of the QCDOC machine; research and development systems procured under the early SciDAC grant; and new commodity clusters as they are brought online.

The hardware is housed at Brookhaven National Laboratory (BNL), Fermi National Accelerator Laboratory (FNAL) and Thomas Jefferson National Accelerator Facility (JLab), and operated as a single distributed computing facility. The computing facility is available to lattice gauge theorists at national laboratories and universities throughout the United States.

2 MISSION NEED

The Lattice QCD Computing Project directly supports the mission of the DOE's High Energy Physics Program “to explore and to discover the laws of nature as they apply to the basic constituents of matter and the forces between them," and of the DOE's Nuclear Physics Program "to foster fundamental research in nuclear physics that provides new insights and advance our knowledge on the nature of matter and energy...". The Project also supports the Scientific Strategic Goal within the DOE Strategic Plan to "Provide world-class scientific research capacity needed to: advance the frontiers of knowledge in physical sciences...; or provide world-class research facilities for the Nation's science enterprise."

To fulfill their missions the HEP and NP Programs support major experimental, theoretical and computational programs aimed at identifying the fundamental building blocks of matter and determining the interactions among them. Remarkable progress has been made through the development of the Standard Model of High Energy and Nuclear Physics. The Standard Model consists of two quantum field theories: the Weinberg-Salam Theory of the electromagnetic and weak interactions, and QCD, the theory of the strong interactions. The Standard Model has been enormously successful; however, our knowledge of it is incomplete because it has been difficult to extract many of the most interesting 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, to make precise calculations of the theory's predictions, and to test the range of validity of the Standard Model. Lattice simulations are necessary to solve fundamental problems in high energy and nuclear physics that are at the heart of the Department of Energy's large experimental efforts in these fields. Major goals of the experimental programs in high energy and nuclear physics on which lattice QCD simulations will have an important impact are to: 1) verify the Standard Model or discover its limits, 2) understand the internal structure of nucleons and other strongly interacting particles, and 3) determine the properties of strongly interacting matter under extreme conditions, such as those that existed immediately after the "big bang" and are produced today in relativistic heavy—ion experiments. Lattice QCD calculations are essential to the research in all of these areas.

The lattice QCD computational infrastructure effort, of which this project is the culmination, was reviewed in February 2003 by a panel of physicists and computer scientists chaired by Frank Wilczek. Among its conclusions were that "The scientific merit of the suggested program is very clearly outstanding." Since then the High Energy Physics Advisory Panel (HEPAP) and the Nuclear Science Advisory Committee (NSAC) have both recommended that the DOE fund dedicated computer hardware for lattice QCD because of the importance of the calculations to their respective fields. Thus, the scientific need for this project has been validated by leading experts in high energy and nuclear physics.

3 FUNCTIONAL REQUIREMENTS

Two classes of computing are done on lattice QCD machines. In the first class, a simulation of the QCD vacuum is carried out, and a time series of configurations, which are representative samples of the vacuum, are generated and archived. Several ensembles with varying lattice spacing and quark masses are generated. This class of computing requires machines capable of sustaining at least on the order of a Tflop/s for days or weeks at a time. The second class, the analysis phase, uses hundreds of archived configurations from each ensemble to calculate quantities of physical interest. A wide variety of different quantities can be calculated from each ensemble. These analysis computations also require large floating-point capabilities; however, the calculations performed on individual configurations are independent of each other. Thus, while configuration sequence generation requires single machines of as large computing capability as practical, analysis computing can rely on multiple machines each capable of sustaining at least on the order of 100 Gflop/s for days at a time, with a total aggregate computing capacity of on the order of Tflop/s.

3.1 Computational Requirements

The fundamental kernels of both configuration generation and analysis are SU(3) algebra. This algebra uses small, complex matrices (3x3) and vectors (3x1). SU(3) matrix-vector multiplication dominates the calculations. For single precision calculations, these multiplications require 66 floating-point operations, 96 input bytes, and 24 output bytes, a 1.82:1 byte-to-flop ratio. Double precision calculations have a 3.64:1 byte-to-flop ratio. The four dimensional space-time lattices used in lattice QCD calculations are quite large, and the algorithms allow very little data reuse. Thus, with lattices spread over even hundreds of processors, the local lattice volumes exceed typical cache sizes. On modern processors, the performance of these fundamental kernels is limited not by the floating-point capacity, but rather by either bandwidth to main memory, or by the delays imposed by the network fabrics interconnecting the processors.

Lattice QCD clusters are composed of hundreds to thousands of interconnected processors. For Tflop scale machines, each processor must be capable of sustaining on the order of 1 Gflop/sec on the fundamental kernels. Memory bandwidths of 2-4 GBytes/sec are necessary to sustain such floating-point rates. Depending on the size of the local lattice, which depends upon the number of processors used for a calculation, sustained network communication rates of tens to hundreds of MBytes/sec per processor are required, using message sizes of order Kbytes in size.

3.2 I/O and Data Storage Requirements

During vacuum configuration generation, data files specifying each representative configuration must be written to storage. These files are of order 1 to 10 Gbytes in size, with a new record produced every few hours. The average I/O rate required for configuration storage is modest, of order 1 MByte/sec. However, high peak rates are desired, to minimize the delays in computation while configurations are written to external storage. The storage volumes required for configurations are of order tens of terabytes. Because configurations are computationally costly to generate, archival-quality storage is mandatory.

During the analysis stage, hundreds of configurations must be loaded into the machines. The propagation of quarks must be calculated on each configuration. This requires the numerical determination of multiple columns of a large sparse matrix. The resulting "propagators" are combined to obtain the target measurements. Propagator files for Clover quarks, for example, are 16 times larger than the corresponding gauge configuration. Often, eight or more propagators are calculated for each gauge configuration. However, because of the large computational resources needed to generate them, they are often written to external storage for later reuse. Because many independent analysis streams can run on a given lattice QCD machine, substantial aggregate I/O rates (hundreds of MBytes/sec) are required during the loading of configurations and the storage of results.

3.3 Data Access Requirements

In the first year of this project, configurations were generated at the BNL QCDOC facility, as well as imported from external facilities. Starting in FY2007, configuration generation was also performed on the "Kaon" cluster at FNAL. Archival storage of these configurations utilizes robotic tape facilities at FNAL and TJNAF. The project maintains software to provide facile movement of files between the three sites. The aggregate size of the files moved between sites is of order 10 Tbytes/year.

4 TECHNICAL SCOPE

The Lattice QCD Computing project consists of the fabrication or purchase of high performance parallel computers, as well as the operation of these systems, the existing SciDAC prototype clusters, and the existing QCDOC system at Brookhaven National Lab. In each year of this project, new systems are built or purchased. In FY2006, a commodity cluster ("6n") was deployed at TJNAF, and another commodity cluster ("Kaon"), was deployed at Fermilab. In FY2007, an additional commodity cluster ("7n") was deployed at TJNAF. For each deployment, the choice of hardware is based upon a determination of what type of machine best advance the science.

A final system will be deployed at FNAL in early FY2009, using funds from the last two years of the project's budget. For this system, one or more alternatives to clusters may prove more cost effective than another commodity cluster. These alternatives include commercial supercomputers, such as the IBM BlueGene/P, Cray XT3, or the SiCortex 5832, as well as tightly integrated blade systems based on commodity processors. For the purposes of defining the cost and schedule of this project we have made the assumption that the final system in FY2009 will be a cluster. This assumption is conservative, because based on current roadmaps a cluster will enable us to meet the project's milestones. Should superior alternatives emerge, the project will adopt the most cost effective design and modify the schedule and budgets accordingly; this would enable the project to surpass the planned milestones, allowing US physicists to accelerate the rate of scientific accomplishments. Full details are described in the *SC LQCD Computing Project Acquisition Plan* and *SC LQCD Computing Project Alternatives Analysis*.

4.1 Computing Systems - Nodes and Networks

Lattice QCD clusters consist of multiple commodity computers interconnected with high performance networks. In each year of this four-year project, new systems are constructed; in the final two years, funds will be combined to construct a single new system. The most cost effective processor and network is used in each year's system design. Evaluations of available processors and networks will be part of this project. In each year commercial supercomputers are also considered as alternatives to clusters.

From 2001-2005, the SciDAC Lattice Gauge Computing project evaluated the performance of all of the then currently available commodity processors, and built a number of prototype clusters based on gigabit Ethernet, Myrinet, and Infiniband networking equipment. At the start of this project, continuing to the present day, the most cost effective commodity computers for these calculations have been systems based on the x64_86 architecture. The most cost effective high performance network fabric since 2005 has been Infiniband.

In FY2006, Fermilab and Jefferson Lab each constructed clusters. Jefferson Lab constructed a 256-node Infiniband cluster based on dual-core Intel processors; through the construction and operation of this cluster, Jefferson Lab acquired expertise in Infiniband networks. The Jefferson Lab cluster was funded through a combination of SciDAC, in kind, and project monies. Fermilab constructed a 2400-processor-core Infiniband cluster based on dual-socket dual-core AMD Opteron systems, funded through a combination of SciDAC and project monies. In FY2007, Jefferson lab constructed a 3168-processor-core Infiniband cluster based on dual-socket quad-core AMD Opteron systems, funded solely by project monies.

Based on current vendor roadmaps and benchmarking, the suitable processors for the final FY2008/FY2009 clusters will be Intel quad-core Pentium, or AMD quad-core Opteron. These processors differ in memory bandwidth, floating-point performance, chipset support, and cost. The cost effectiveness of each will vary according to their performance, the pricing of the available motherboards, SMP scaling efficiency, and the cost of the Infiniband network.

4.2 Operations

The operation of the lattice QCD systems involves physical facilities (buildings, power, cooling), system administration, hardware and software maintenance, configuration management, cyber security, data storage, and data movement.

FNAL, TJNAF, and BNL operate physical facilities in support of the lattice QCD systems. The QCDOC, built in 2005 at Brookhaven, is housed in a refurbished computing room. In FY2006, Fermilab refurbished an existing computer room to supply sufficient power and cooling for the “Kaon” cluster. Jefferson Lab used a new computer facility, completed in early 2006, to house the “7n” cluster. In 2008, Fermilab constructed a new computer room to accommodate the final LQCD compute cluster (JPsi) in early FY2009.

As part of the SciDAC and SciDAC-II Lattice Gauge Computing projects, libraries and application programming interfaces (API's) have been developed that allow high level physics codes to run without modification (after recompilation) on the different hardware platforms available: QCDOC, Myrinet and Infiniband clusters, gigabit Ethernet mesh clusters and commercial supercomputers. At each site, one or more versions of the SciDAC libraries are maintained to support this diverse hardware base. SciDAC project personnel are responsible for building and verifying the correctness of these libraries. Project personnel are responsible for the configuration management of the libraries and the associated utilities.

Archival storage of physics data utilizes tape robots and hierarchal mass storage systems at Fermilab and Jefferson Lab. Tape media and, as necessary, tape drives are procured using operational funds allocated to the project.

On a periodic basis, US collaboration members apply to and receive from the Scientific Program Committee allocations of computing time at one or more of the three sites. Specific physics projects often utilize two of the three sites to take advantage of the specific characteristics of each. For this reason, efficient movement of physics data between the sites is essential.

4.3 Deliverables

Each year, the Lattice QCD project deploys high performance parallel computing systems, as well as operates the systems deployed in the previous years. The project also operates the remaining SciDAC prototype clusters. Each computing system is generally operated for up to 3.5 years after commissioning. The project decommissions individual systems when they are no longer cost effective to operate.

In FY2006 and FY2007, clusters were constructed at FNAL and TJNAF. The final system designed and deployed by the project will be housed at Fermilab; this system will be purchased with a combination of FY2008 and FY2009 funds. Table 1 below shows by year the performance of the clusters deployed by the system, the estimated performance of the FY2008/FY2009 system, and the integrated performance of all project resources.

Table 1 – Performance of Systems Deployed by the Project, and Integrated Performance

Performance Indicator	**FY 2006 (Actual)**	**FY 2007 (Actual)**	**FY2008 (Plan)**	**FY2009 (Plan)**
Performance of deployed system, (Tflops)	2.6	3.0	4.2	2.0
Delivered integrated performance (TFlops-yrs)	6.27	9.7	12.0	15.0

5 MANAGEMENT ORGANIZATION

This section describes the management organization for the LQCD Computing project as defined for the incremental deployment and operation of the resources at three national laboratories. The project management is organized by three major subprojects including hardware deployment and operations at BNL, FNAL and JLab. The management structure also facilitates the involvement of the scientific community that is the ultimate users of the infrastructure. Figure 1 outlines the management structure. Solid lines indicate reporting relationships; horizontal lines indicate advisory relationships.

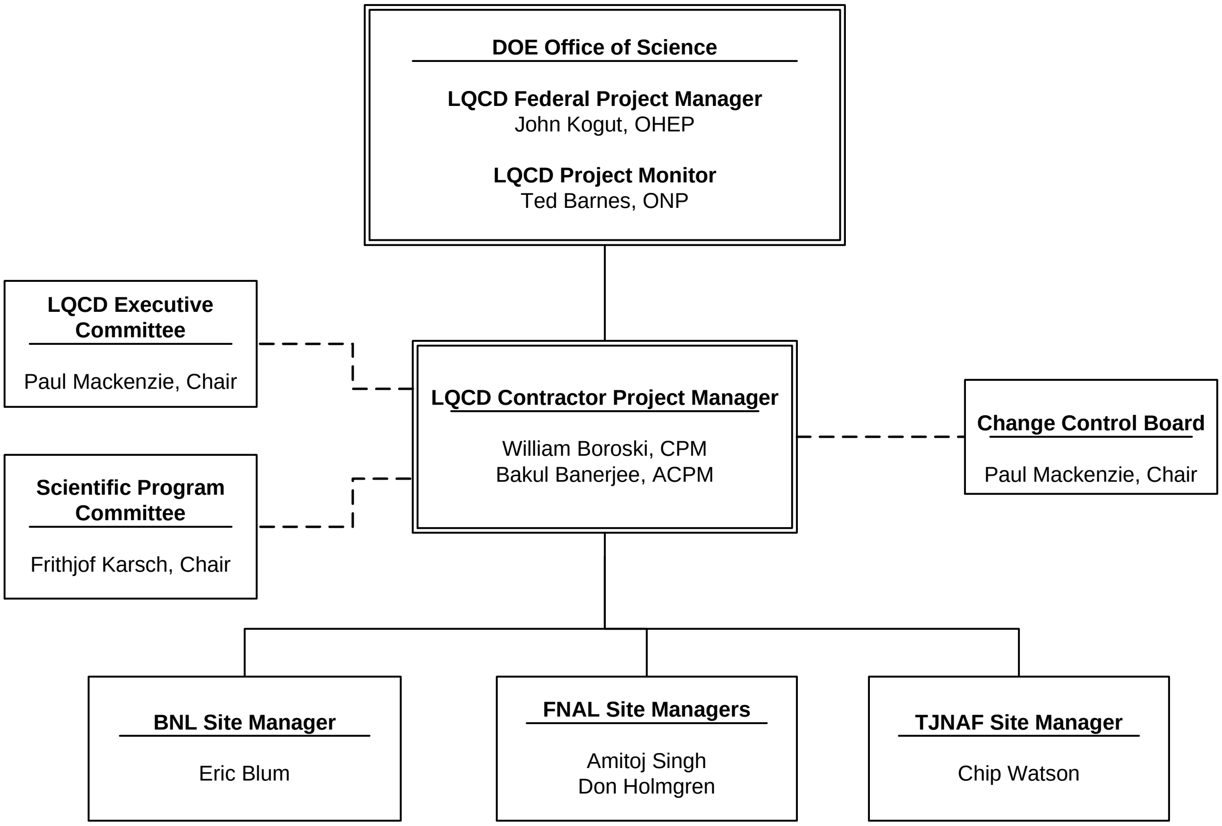

Figure 1. Management Organization Chart for the LQCD Computing Project.

5.1 Project Management Responsibilities

5.1.1 LQCD Project Manager

Within DOE's Office of Science (SC), the Offices of Nuclear Physics (NP) and High Energy Physics (HEP) are the major stakeholders for the project and have overall responsibility for the SC LQCD Computing Project. The LQCD Federal Project Manager is appointed from either of HEP or NP. The Contractor Project Manager is equivalent to the Federal Investment Manager defined in the OMB Exhibit 300. A Project Monitor is also appointed to represent the other stakeholder organization. Responsibilities of the LQCD Federal Project Manager include:

- Provide programmatic direction for LQCD
- Function as DOE headquarters point of contact for LQCD matters
- Oversee LQCD progress and help organize reviews as necessary
- Budget funds for LQCD and act as the key contact to the project office during the preparation of the OMB Exhibit 300 submissions.
- Control changes to the LQCD baselines in accordance with the PEP

5.1.2 Contractor Project Manager

The LQCD Contractor Project Manager (CPM) is responsible for the overall management of the project. This person is the key interface to the Federal Project Manager for financial matters, reporting, and reviews of the project. The CPM has significant budgetary control and is in the approval chain for all major project commitments and procurements.

Specific responsibilities include:

- ensures that the detailed planning documents for the project including a work breakdown structure (WBS) with each task defined at a level that can be externally reviewed, with sites and individuals responsible for those tasks well identified, and with a set of project milestones to rigorously track progress
- prepares OMB Exhibit 300 submission documents for each budgeted year for the duration of the project
- prepares and approves budgets consistent with the detailed planning documents
- provides final approval for the project of all major (> $50K) procurements
- ensures the submission of DOE quarterly progress reports including project financial, performance, and administrative status as required
- provides internal project oversight and reviews, ensuring that funds are being expended according to the project plan, and identifying weaknesses in the execution of the project plan which need to be addressed
- prepares and maintains the LQCD Project Execution Plan
- establishes and manages a project change control mechanism

Interactions

- reports to the LQCD Federal Project Manager
- serves as a point of contact with DOE on matters related to budget and schedule of all funded activities

5.1.3 Associate Contractor Project Manager

The CPM is assisted by the Associate Contractor Project Manager(ACPM). This person prepares and tracks the project WBS, expenditure and milestones and associated performance records of the project at all three labs. This person creates various management documents and maintains other controlled documents as the need arises.

Responsibilities

- prepares detailed planning documents for the project, including the WBS specific for each subproject, project milestones, and expenditure including the tracking of the progress
- assists in the preparation of proposal budgets consistent with the detailed planning documents and assures the proper allocation of the funds received
- assists in the preparation of the OMB exhibit 300 submission to DOE for each budgeted year for the duration of the project and associated documents

- prepares the financial information for the monthly reports to the DOE Project Manager and the DOE quarterly progress reports according to the guidance received from OMB
- prepares other technical and administrative controlled documents and conducts project performance measurement related activities
- develops and maintains project management related communications including the project web site and the repository of project documents, etc.
- assists with the annual reviews.

Interactions

- reports to the CPM
- works with the Site Managers to gather budget and performance data for tracking the project and to preparing quarterly and/or annual reports

5.1.4 Site Managers

The hardware deployment and operations subproject at each host laboratory (BNL, FNAL, and JLab) is headed by a Site Manager (SM) at each site, who has significant authority at his/her site for delivering LQCD computational resources to the community. The SM is responsible for developing and executing the corresponding components of the WBS, and for ensuring that appropriate commitments by the host laboratory are obtained and carried out. The SM is the primary interface between the CPM, ACPM, the host laboratory, and the individuals associated with the work to be performed at that host laboratory.

The SM has authority to reallocate project resources within the laboratory to accomplish the assigned scope and tasks. This person is responsible to provide sufficient details of major procurements to the CPM to facilitate a review and approval for use of funds. The Site Manager has direct management control over that site’s budget each year, with major procurements subject to approval by the CPM. All procurements are subject to host site management procedures and approvals.

Responsibilities

- technical oversight of the LQCD computing resources at the site including the monitoring and reporting of the uptime and usage. The SM also implements the user allocations determined by the Scientific Program Committee
- software deployment consistent with the project plan the integration of the necessary software developed in other projects including the LQCD SciDAC-2 projects and the International Lattice Data Grid (ILDG) project
- specific hardware selection consistent with the project plan, hardware procurement and deployment
- site operations and user support
- assisting in preparation of detailed planning documents for the site sub-project, including the WBS and the milestones at a level which can be externally reviewed
- staff resources needed and deployed to carry out tasks identified in the WBS

- tracking progress of the site project milestones
- preparation of site budgets consistent with the detailed planning documents
- preparation of monthly status reports, including expenditures and effort, for the section of the WBS covering the site and communicating them to CPM and ACPM
- providing necessary information on quarterly reports to DOE
- internal site project oversight and review, ensuring that funds are being expended according to the project plan, and identifying weaknesses in the execution of the project plan which need to be addressed
- preparation of materials for external oversight and reviews
- implementing the user allocations determined by the Scientific Program Committee
- obtaining necessary resources and approvals from laboratory management and coordination of resources contributed by the laboratory

Interactions

- reports to the CPM
- works closely with the ACPM and other Site Managers both to assist in defining milestones and infrastructure deployment schedules, and to ensure a high level of coherency across the project
- oversees all staff responsible for deployment and operation of that site's portion of the national hardware infrastructure

5.1.5 Integrated Project Team

The LQCD Integrated Project Team (IPT) is composed of the LQCD Federal Project Manager, LQCD Project Monitor, CPM, ACPM and Site Managers from the three participating laboratories. The list of names is given in Appendix A. Members of the team meet on an "as-needed" basis. The LQCD Federal Project Manager chairs the IPT.

5.1.6 LQCD Executive Committee

The charter of the Lattice QCD Executive Committee is to provide leadership in developing the computational infrastructure needed by the United States lattice gauge theory community to study quantum chromodynamics (QCD), the theory of the strong interactions of subatomic physics. The Executive Committee has the responsibility for setting scientific goals, determining the computational infrastructure needed to achieve these goals, developing plans for creating the infrastructure, securing funds to carry out these plans, and overseeing the implementation of all of the above..

Current members of the Executive Committee are expected to serve for the duration of the project. If a vacancy occurs, it is filled by a vote of the remaining members of the Executive Committee. The current membership of the Executive Committee is shown in Appendix B.

Responsibilities

- sets the scientific goals and determines the computational infrastructure needed to achieve them
- establishes procedures for the equitable use of the infrastructure by the national lattice gauge theory community
- arranges for oversight of progress in meeting the scientific goals
- arranges regular meetings of the national lattice gauge theory community to describe progress, and to obtain input
- has responsibility for the national lattice gauge theory community's SciDAC grant and provides coordination between work done under that grant and in the current project
- appoints the members of the Scientific Program Committee
- appoints three or more members of the Control Change Board

5.1.7 Spokesperson

The Chair of the Executive Committee serves as the Scientific Spokesperson for the project.

Responsibilities

- determines scientific goals and required computational infrastructure together with the Executive Committee
- chairs Executive Committee
- serves on Change Control Board

Interactions

- principal point of contact for the Department of Energy on scientific matters related to the project
- presents the project's scientific objectives to the Department of Energy, its review committees and its advisory committees
- liaison between the Executive Committee and the CPM, relating the Executive Committee's priorities to the CPM, and transmitting the CPM's progress reports to the Executive Committee

5.1.8 Change Control Board

The Change Control Board (CCB) is composed of three to four members of the executive committee. Members are appointed by the chair of the executive committee for the duration of the project. The spokesperson is also a member of the CCB. The sole purpose of this committee is to assure that the changes to the project are managed with the primary focus on the advancement of the scientific goals of the project. CCB must approve all sub-project related changes resulting in a shift of more than $250K between equipment and labor budgets, or movement of more than $100K between subprojects, or any 3-month or greater delay of a level 1 WBS milestone. The CPM presents such changes to CCB for approval before executing any changes. All changes approved by CCB are reported to DOE.

Responsibilities

- Evaluates feasibility, cost, and impact of proposed changes to the project which results in more than a minimal cost or schedule change.

Interactions

- Gathers input from the project participants and the user community about project scope changes.

5.1.9 Scientific Program Committee

The charter of the Scientific Program Committee (SPC) is to assist the Executive Committee in providing scientific leadership for the Lattice QCD infrastructure development efforts. This committee monitors the scientific progress of the effort, and provides leadership in setting new directions.

The SPC is charged with allocating time on the integrated hardware resources operated under the LQCD computing project: including the SciDAC prototype clusters, the QCDOC, and all new hardware acquired by the project. The SPC has instituted the following allocation process. Once a year it solicits proposals for use of the computational resources that are available to the user community during the allocation period July 1 to June 30. The SPC reviews the proposals, and makes preliminary allocations based on its reviews. It then organizes an open meeting of the user community to discuss the proposals and the preliminary allocations. The SPC makes final allocations at each site following this meeting. The three site managers are responsible for executing these allocations. The objective of this process is to achieve the greatest scientific benefit from the resources through broad input from the community. This process has been used to make the initial allocations of resources on the QCDOC computer and on the SciDAC prototype clusters. The SPC is also charged with organizing an annual meeting of the user community to review progress in the development of the infrastructure and scientific progress achieved with the infrastructure, and to obtain input on future directions.

Members of the SPC are appointed by the Executive Committee. The current members are expected to serve for the duration of the project. If a vacancy occurs, it is filled by the Executive Committee. See Appendix B for names of the current members.

Responsibilities

- organizes annual meeting of the users community
- solicits proposals for using LQCD computational resources
- allocates computing resources

5.2 Interaction of the Laboratory Management and Project

Line management within the three host laboratories (BNL, FNAL, and JLab) provides support to the project in a number of ways, including management and infrastructure support.. Management authorities for DOE and upper management of the laboratories are shown in Figure 2.

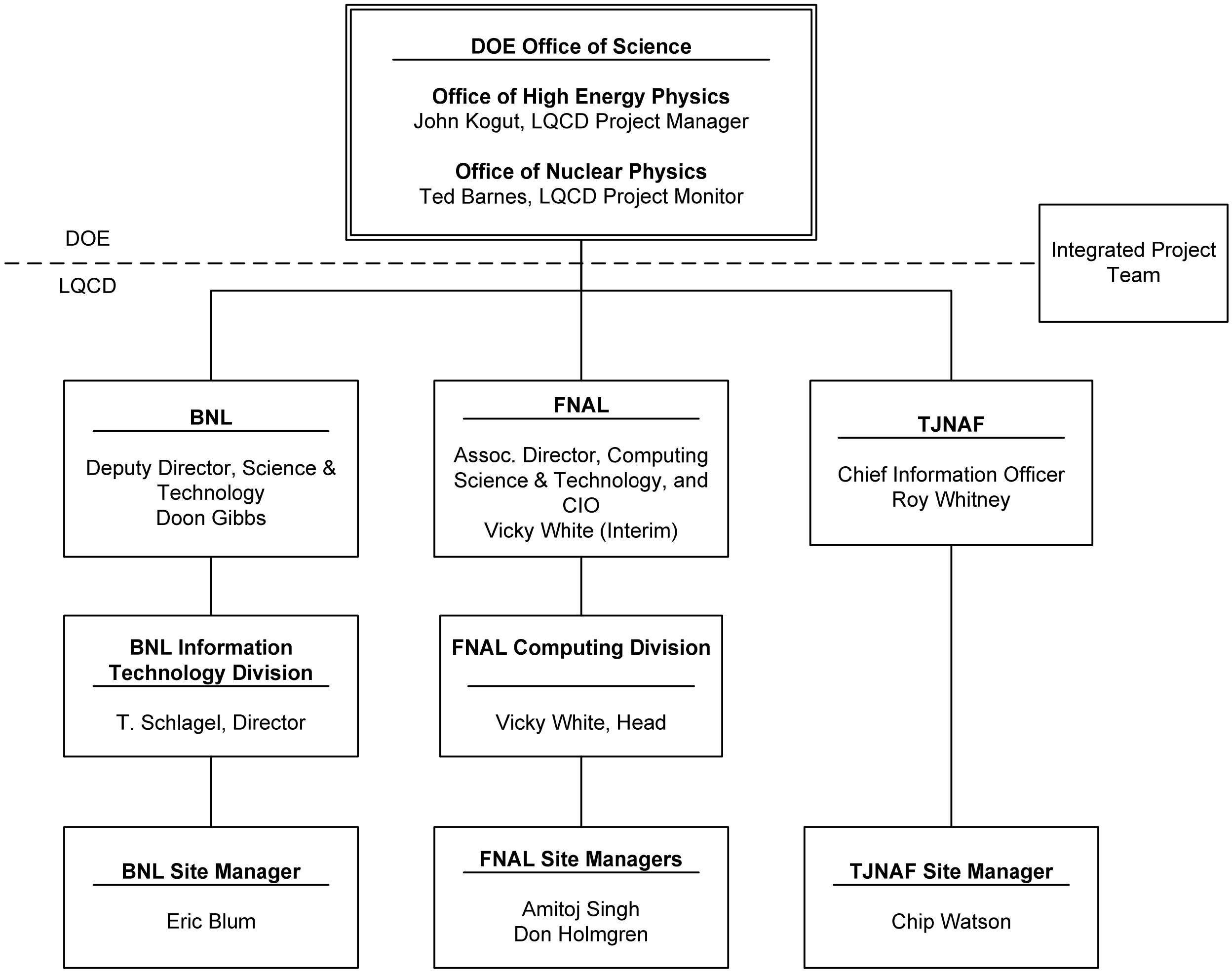

Figure 2: LQCD and Laboratory management

6 SCHEDULE AND COST MANAGEMENT

The LQCD computing project is categorized as an OMB Exhibit 300 Mixed Life Cycle IT investment with a development, modernization, enhancement (DME) component for procurement and a steady state (SS) component. The project is organized using a Work Breakdown Structure (WBS) for purposes of planning, managing and reporting project activities. Work elements are defined to be consistent with discrete increments of project work and the planned method of project control. LQCD has three major WBS Level 2 components based on the facilities at each participating laboratory, BNL, Fermilab, and JLab spanning the period from October 2005 to September 2009. Under each Level 2 component there are multiple Level 3 components. These are:

- Deployment: Includes planning and deployment of new hardware
- Operations: Includes site operation of the existing facility to serve the LQCD researchers. It also includes the maintenance of the software libraries and user support for each laboratory and occasional purchase of consumables, like tapes.

- Acquisition: Includes all hardware acquisitions of the LQCD facility at three laboratories.
- Planning: Includes all project management activities at Fermilab

6.1 Project Milestones

Project milestones are defined in the project WBS. Each laboratory reports the status of completion for each project milestone to the CPM on a monthly basis. Any significant changes to milestone schedules are processed according to the change control procedure described later.

6.2 Scope of the LQCD Computing Facility Hardware

The project acquires new equipment using project funds from FY06 to FY09. The deployment and operation of the new equipment as well as the operation of existing equipment are included within the project scope.

6.3 Cost Scope

The LQCD computing project is funded by both DOE-HEP and DOE-NP. In May 2006, OHEP and ONP held a Technical, Cost and Schedule Review of LQCD at MIT/LNS in May 2006. The OMB Exhibit 300 submission for the project and the Project Execution Plan were assessed by this independent committee. The baselined cost profile is given in Figure 3 in actual year dollars as planned for FY06, the first year of the project. Indirect costs are applied according to agreements between the project and the host laboratories. All estimates were inflated using escalation rates of 0.8 per year for material and 1.04 for labor, assuming a funding profile that covers FY2006 to FY2009. These rates are derived from the FY07 Field Budget Call. These rates are adjusted annually according to the guidance received from DOE.

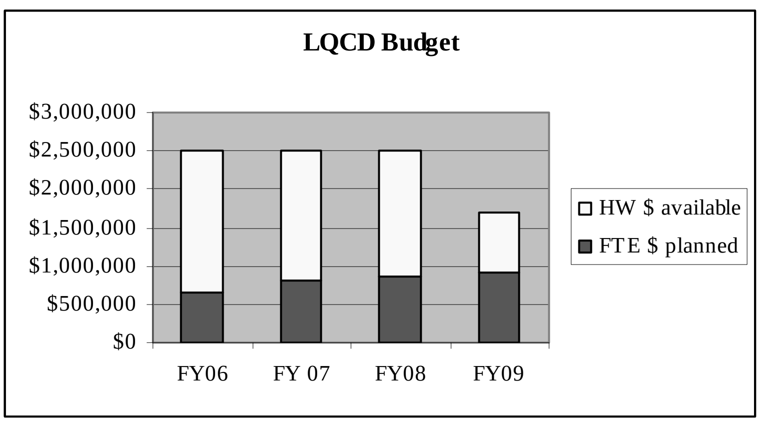

Figure 3: DOE Baseline Funding Profile

6.3.1 Procurement Strategy

Each year, the Lattice QCD project either constructs high performance clusters, or purchase commercial supercomputers, choosing the most cost effective solution available at the time. Each of these annual developments of new computing systems is “built-to-cost”. That is, a fixed budget is determined annually for computer hardware, with the precise number of processors procured determined by the purchase price of systems and network equipment in that year. Variations in purchase price of these components from the estimates used in the budget may result in greater or lesser computing capability from the estimated value. The resulting performance risk is managed by determining the impact on the achievement of the scientific goals of the project. Small negative variances in available computing capability and/or capacity may result in schedule delays in completing scientific computing projects. If a large negative variance is expected that might prevent the completion of computing goals; it triggers the review and modification of the LQCD scientific program, such as through changes or elimination of allocations of computing resources to specific projects. The risk of large variances is minimized through the use of conservative projections in the estimated costs and performance of each future system development. Allocations of computing resources and the planning of the LQCD scientific program are based upon these conservative estimates. Further mitigation of risks follows from steady state operations at each site of older systems as each system developed is operated for three to four years. The computing performance available from any given system becomes well known within months of initial production. At any given time, these established systems represent more than half of the available computing capacity.

Each year, the project operates the computing systems that were developed either during the project, or prior to the start of the project (the SciDAC prototype clusters at FNAL and JLab, and the QCDOC at BNL). The manpower requirements for the operations of these systems, particularly the clusters, have been well established through these years of production. The amount of manpower required to provide end user support, and to maintain the systems, continues to increase as the installed sizes of the systems at FNAL and JLab grow. Using the initial historical data on manpower usage to operate the systems, the project plan attempts to optimize the scientific output by balancing the annual funding level between operational cost and procurement cost of new computing systems. At any given time, there may be a risk that insufficient user support, for example, may limit the scientific productivity of the systems. This risk is managed by adjusting the balance between labor and equipment costs in every procurement cycle, relying on the experience gained in prior operations.

6.3.2 Resource Utilization

Project funds are used to support development/modernization/enhancement (DME) and steady-state (SS) operations and maintenance activities. However, some portion of the SS cost is subsidized by the laboratories, including the system and scientific software support by the base budgets of the three labs. Infrastructure costs of the LQCD facility, such as power and cooling, are contributed by the participating laboratories. The disk and tape storage system infrastructure is mostly provided by the participating laboratories, except the project contributes to the purchase of consumables.

The decommissioning of LQCD resources covers the disposal of standard electronic, computers and network equipment, which must follow accepted standard procedures for disposal of these items. These decommissioning costs are not included in the project.

7 CHANGE CONTROL

Changes to the technical, cost and schedule baselines are controlled using the thresholds described in Table 2.

All changes that exceed Level 3 approval thresholds should first be submitted to the CPM for approval, using a Change Request (CR) form. See Appendix C for the LQCD CR form. For changes exceeding Level 3, the CPM recommends the approval of the request to higher authority or rejects the request. If approved, the CPM transmits the CR to the LQCD CCB with recommendations. If the request exceeds Level 2, the LQCD CCB submits the CR to the DOE LQCD Project Manager for approval or rejects the request. The Scientific Program Committee reviews all CRs for potential scientific impacts on the project.

If a change is approved, a copy of the approved CR, together with any qualifications or further analysis or documentation generated in considering the request is returned to the requestor, and copies are sent to the official at the next higher control level and to the LQCD project office for filing. If approval is denied, a copy of the CR, together with the reasons for denial, is returned to the requestor, and a copy is filed. The official at the next higher control level may review the granted change to ensure proper application of the procedure and consistency of the change with the goals and boundary conditions of the project.

Table 2: Summary of Change Control Thresholds

Level	Cost	Schedule	Technical Scope/Performance
DOE Federal Project Director (Level 1)		6 or more months increase (cumulative) in a Level 1 milestone date	Changes to scope that affect mission need and requirements
LQCD Change Control Board (Level 2)	Change of > $250K in labor/equipment balance or Movement of > $100K between laboratories	3-month or more delay of a Level 1 milestone date	> 10% decrease from baseline of either the targeted computing capability increment (Tflop/s) or integrated delivery (Tflop/s-yrs) in a single project year.
LQCD CPM (Level 3)	Any increase of > $25K in equipment purchase price	> 1-month delay of a Level 2 milestone date	Any deviation from technical deliverables that negatively affects expected performance specifications by more than 3%
LQCD Site Manager (Level 4)	Any increase of $25K or less in equipment purchase price	Less than 1-month delay of a Level 2 milestone date	Any deviation from technical deliverables that negatively affects expected performance specifications by less than 3%

8 ANALYSIS, ASSESSMENTS, AND PLANS

8.1 Project Controls

The project implements a Performance Based Management System (PBMS). Performance goals and measures are fully defined in the annual OMB Exhibit 300 submission for the project.

The investment scope, schedule performance, and cost are evaluated on a monthly basis using the industry-standard project management methodologies currently in place at FNAL. The project office identifies, monitors, and assesses accomplishments or deviations from baseline goals. The IPT reviews and provides suggestions for improving the project management methodologies to ensure that all key milestones and project cost estimates have been adequately adjusted for risk. In addition, monthly operational analysis is utilized to ensure that the investment is performing within baseline cost, schedule and performance goals.

Management processes for the investment is designed according to the Guidance from the DOE M 413.3. In addition, methodologies from the Project Management Institute (PMI) Guide to the Project Management Body of Knowledge (PMBOK) have been adopted as necessary. Overall performance at three host laboratories (BNL, JLab, and FNAL) is managed under the terms of the performance-based management contract with the DOE. Under these terms, the laboratories are expected to integrate contract work scope, budget, and schedule to achieve realistic, executable performance plans. Following existing financial and operational processes at FNAL, BNL and JLab, the project has implemented methods of collecting and analyzing data measured. Additionally, annual self-assessments, aligned with the annual DOE review, are used at the investment level to assess and evaluate results and to improve performance. Finally, annual LQCD User Surveys are conducted to assess facility customer satisfaction and identify areas for improvement.

The CPM and ACPM coordinate project activities across all host sites and are responsible for reporting project status to DOE on a regular basis. Each Site Manager monitors the performance of project activities within their respective organizations.

Before the beginning of each fiscal year, a detailed WBS, including WBS dictionary is developed for the work to be done for the investment during the year with basis of estimates derived from past purchase records and effort reports. This WBS is baselined at the beginning of the year with the concurrence of the three Site Managers. Microsoft Project software is used for this work. After the WBS is defined, it is baselined and status reporting process against the baseline is initiated. Cost and effort report data is collected on a monthly basis from all three laboratories. FNAL uses Oracle-based Project Accounting system to capture actual costs for WBS. Similar data is collected from other laboratories and consolidated. This data is used to create cost and schedule performance reports as well as necessary change requests and exception reports. All costs are reported at a fully burdened level. The budget planning and resource allocation process is based on the financial management system of the respective laboratories, which in turn are based on DOE's general guidance. Details of fund management for the investment that includes both DOE's High Energy Physics and Nuclear Physics organizations has been established. The project deploys existing tools in participating laboratories as deemed necessary.

Memoranda of Understanding (MOU) with the participating laboratories and the LQCD project have been executed. These MOUs include details of the in-kind contributions provided to the project by the host laboratories. The MOUs are updated on an as-needed basis.

The LQCD project office, consisting of CPM and ACPM, creates a set of detailed web-based project management processes, associated plans and procedures to control the project WBS, cost, schedule and documentation. These documents reside in secure or public areas as needed. Primary controlled elements of the project are the schedule and cost as defined in the WBS. Site managers are be responsible for tracking cost and schedule elements, and for reporting these to the ACPM. The ACPM prepares and reviews monthly cost and schedule performance based on schedule, cost, and technical data, and reports the result to the CPM. The CPM submits a monthly report on the overall cost, schedule and technical performance to the DOE Federal Project Manager and other stakeholders. The Offices of High Energy and Nuclear Physics jointly conduct an annual progress review with a committee of external experts.

Each host laboratory uses its official accounting system as a basis for collecting cost data. Each site manager and respective financial officer work with the ACPM to establish a direct one-to-one relationship between each WBS element of Level 2 or higher and a separate account code under their accounting system. Site managers and the ACPM define a common format of reporting data that can be consolidated into the master WBS.

Technical performance is monitored throughout the project to insure conformance to approved functional requirements. Design reviews and performance testing of the completed systems is used to ensure that the equipment meets the functional requirements.

8.2 Project Plans and Analysis

The primary planning document for the project is the OMB Exhibit 300 document for the budgeting year. This document contains detailed tracking information on cost and schedule performance, performance toward project goals, security and privacy, alternative analysis and risk management. Since this is a major Federal IT investment, the project prepares a Performance Reference Model (PRM), mapping all “Measurement Indicators” to the corresponding "Measurement Area" and "Measurement Grouping" identified in the PRM. Other measures associated with the project are measures associated with the Service Component Reference Model (SRM) and Technical reference Model. Details on Federal Enterprise Architecture are given at www.egov.gov.

Supplemental controlled documents for the project include Risk Management Plan, Acquisition Strategy document, and the Certification and Accreditation document for cyber security. These documents are reviewed and updated on an annual basis. More frequent updating may occur as necessary.

The LQCD project office prepares a monthly report for the Office of Science and a monthly meeting is held to inform the Federal Project Manager and Project Monitor about the accomplishments, financial and technical performance, and issues related to the project. The project office also prepares formal DOE Quarterly Reports based on the OMB guidance.

8.3 Project Reviews

To determine the health of the project and to provide guidance on the project progress, an annual DOE Office of Science project review is held, generally in May. During this review, upcoming procurement strategies are presented and reviewed.

8.4 Risk Management

Within the project, risk management is viewed as an ongoing task that is accomplished by continuously identifying, analyzing, mitigating and monitoring risks that arise during the course of project execution. Risk is a measure of the potential of failing to achieve overall project objectives within the defined scope, cost, schedule and technical constraints. The project team plans for and tracks the operational and financial risks associated with the project using the *LQCD Risk Management Plan*. The purpose of risk analysis is not solely to avoid risks, but to understand the particular risks associated with the project and devise strategies for managing them.

The final responsibility for risk management rests with the CPM, in consultation with the LQCD Executive Committee and Site Managers. However, effective risk management is a multi-step process that requires continued involvement of all project members.

Because of the build-to-cost nature of the project, LQCD has minimal risk of overrunning the approved project budget. Cost estimates are based in part on current and past procurements for the prototype computing systems, and on the actual cost of labor for deploying and operating the existing facilities. Actual costs are tracked monthly, allowing for prompt corrective action if necessary.

Notwithstanding, failure to properly manage project costs may impact our ability to deliver on key performance goals. Hardware cost variances result in adjustments to the size of the computing systems developed each year. Likewise, labor cost variances (.e.g., the need to change the level of systems admin or user support) results in adjustments in the allocation of funds between subsequent computing hardware and labor budgets. In either case, significant increases in hardware or labor costs could result in reductions in deployed computing capacity, system uptime, or other key performance metrics.

As documented in the Risk Management Plan, performance risks associated with computing and network system are estimated to be low due to successful R&D efforts and the use of off-the-shelf components whenever possible.

The distributed nature of the LQCD facility partially mitigates the risk of natural disasters. Additionally, the LQCD project employs a disaster recovery strategy for valuable data as follows: gauge configuration data files are stored redundantly at two different locations (FNAL and JLab), and possibly also at NERSC and/or NCSA. Although the equipment at each facility is not being insured against disasters, standard disaster recovery protections are provided by each laboratory.

8.5 Quality Assurance

The LQCD project defines quality as the “fitness of an item or design for its intended use” and Quality Assurance (QA) as “the set of actions taken to avoid known hazards to quality and to detect and correct poor results.” LQCD follows established quality control procedures established at various laboratories. The project has put in place various methodologies to monitor and improve quality. Some of these processes are incoming inspection, performance management, uptime, operations analysis, and the annual user survey.

9 ENVIRONMENT, SAFETY AND HEALTH

Environment, safety and health (ES&H) is integrated into all phases of planning, acquisition and maintenance phases of the LQCD project using appropriate procedures defined by the participating laboratories. The LQCD Project follows the five core functions as described in the DOE guidelines.

1. Define work and identify the potential hazards
2. Analyze potential hazards and design the equipment or activities to appropriately mitigate or eliminate those hazards.
3. Establish controls for hazards that cannot be eliminated through design features
4. Perform work in accordance with the procedures
5. Review the effectiveness of the hazard analyses and controls and provide feedback for improvement.

The LQCD Computing Project is a collaborative effort among three DOE sponsored laboratories with stringent ES&H policies and programs. Those working for the project follow procedures specific to each laboratory.

The line management of each laboratory retains supervisory authority of their personnel and responsibility for the safety of work at their home laboratory. Line management in each laboratory keeps the CPM informed about their laboratory's management and ES&H organization structures. Any safety concerns by LQCD personnel are to be communicated to the line management where the concern occurs and the employee's home laboratory or university.

Site managers at each laboratory work with safety officers at their home laboratories to ensure that any specific hazards associated with project activities are documented according to the plans and procedures of the particular laboratory, and mitigated appropriately. Information pertaining to these hazards are documented as needed using appropriate safety documentation guidelines for the laboratory. Also, laboratory personnel receive specific training required or recommended for project to perform their job in a safe and proper manner.

Applicable electrical, mechanical, etc. codes, standards and practices are used to ensure the safety of personnel, environment, equipment and property. All equipment purchased from manufacturers must comply with Underwriters Laboratories Inc. or equivalent requirements, or reviewed for safety. The procurement of each LQCD system is done under the guidance provided by the procurement organization of the associated laboratory. There has been no direct construction activity associated with the project. However, an assessment of the need for NEPA review will be done if necessary.

10 PARTICIPATION OF OTHER INSTITUTIONS

For the LQCD project, BNL, Fermilab, and JLab are the primary participating laboratories. MOUs are used to define the relationships and expectations between these laboratories and the project.

Researchers from various universities are key customers of the computing systems developed during this LQCD Project. Their feedback is incorporated throughout the duration of the project through the LQCD Executive Committee and the spokesperson.

Appendix A: LQCD Integrated Project Team

LQCD Federal Project Manager	John Kogut (chair)
LQCD Project Monitor	Ted Barnes
Contractor Project Manager	Bill Boroski
Associate Contractor Project Manager	Bakul Banerjee
BNL Site Manager	Eric Blum
JLab Site Manager	Chip Watson
FNAL Site Manager	Don Holmgren/Amitoj Singh
LQCD Executive Committee Chair	Paul Mackenzie

Appendix B: LQCD Committees and Members

The current Executive Committee members are:

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

The current Scientific Program Committee members are:

Tom Blum (U. Connecticut), Chris Dawson (U. Virginia), Robert Edwards (JLab), Frithjof Karsch (Chair, BNL), Andreas Kronfeld (FNAL), Martin Savage (U. Washington), Junko Shigemitsu (Ohio State)

Appendix C: Change Request Form

Log number (provided by project office): [BCA #]		
1) DATE: [date of origination]	2)Laboratory/WBS: [Highest level of WBS affected	3) ORIGINATOR:
4) WBS DESCRIPTION OF PRIMARY AFFECTED TASKS:		
5) TECHNICAL DESCRIPTION AND PRIMARY MOTIVATION OF CHANGE: [Attach in word doc]		
6) ASSESSMENT OF COST IMPACT (identify any change in resources needed as reflected in the WBS) Estimated M&S Cost Increase ($): Estimated Labor Cost Increase ($): Estimated scientific impact (high, medium, and low)		
7) ASSESSMENT OF SCHEDULE IMPACT AND AFFECTED MILESTONES (identify slip or stretch of work or change in plan): [Attach as WBS report]		
8) SECONDARY IMPACT AND OTHER COMMENTS:		
9) APPROVALS Level 1 Signature / Date Level 2 Chair, CCB Signature / Date Level 3 Contract Project Manager Signature / Date		
10) CCB ApprovalS O APPROVED O DISAPPROVED ____________ Signature/date O APPROVED O DISAPPROVED ____________ Signature/date O APPROVED O DISAPPROVED ____________ Signature/date O APPROVED O DISAPPROVED ____________ Signature/date O APPROVED O DISAPPROVED ____________ Signature/date		

Appendix D: LQCD Controlled Documents

The set of documents submitted to DOE are designated as controlled project documents. These documents are tracked using the Document Database Control system installed in the Computing Division at Fermilab. This document control area is password protected and only accessible by the IPT. The project ACPM may be contacted to obtain the user id and password. The following documents are considered as primary controlled documents

1. Project Execution Plan (this document)
2. Risk Management Plan
3. Acquisition Plan
4. Alternatives Analysis
5. Certification and Accreditation Documentation

The following documents are considered to be of significant importance to the project. Copies are maintained by the LQCD Project Office.

1. Project Review reports
2. OMB Exhibit 300 submission documents
3. Memoranda of Understanding
4. LQCD monthly progress reports
5. DOE quarterly reports