

**Program Execution Plan  
for  
Lattice QCD Research Program Extension III  
(LQCD-ext III)**

**Unique Program (Investment) Identifier: 019-20-01-21-02-1032-00**

*Operated at*  
Fermi National Accelerator Laboratory  
Brookhaven National Laboratory

*for the*  
U.S. Department of Energy  
Office of High Energy Physics

Version 0

DRAFT  
July 7, 2019

**Program Execution Plan for  
Lattice QCD Research Program Extension III  
Version 0**

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**LQCD-ext III Program Execution Plan  
Change Log**

| <b>Version No.</b> | <b>Description / Pages Affected</b>              | <b>Effective Date</b> |
|--------------------|--|-----------------------|
| <b>0</b>           | Updated to reflect LQCD ext III operations model | In progress           |
|                    |  |                       |

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## 1 INTRODUCTION

This document describes the program and related methodologies to be followed while executing the Lattice Quantum Chromodynamics Computing Research Program Extension III (hereon referred to as LQCD) for the period FY2020 through FY2024. The official name of this capital asset investment is **Lattice QCD Research Program Extension III**, and the Unique Program (Investment) Identifier is 019-20-01-21-02-1032-00.

The LQCD research program is an extension of the LQCD-ext II Computing Project, which is funded through FY2019. LQCD will support the continued acquisition and operation of institutional computing hardware at existing facilities located at Brookhaven National Laboratory (BNL) and Fermi National Accelerator Laboratory (FNAL). BNL and FNAL will provide facilities and infrastructure that deliver the mid-scale computing required by the LQCD Program. They will also provide computing professionals to plan, design, deploy, and operate the computing systems.

LQCD was initially classified as an OMB Exhibit 300 IT investment project. In August 2010, the OMB Exhibit 300 investment classification criteria were modified and LQCD was re-classified as an OMB Exhibit 53 IT investment.

This plan has been prepared in accordance with DOE Order O413.3B, *Program and Program Management for the Acquisition of Capital Assets* (dated 29-Nov-2010).

## 2 HISTORICAL BACKGROUND

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. In February 2003, the lattice QCD computational infrastructure effort was reviewed by a panel of physicists and computer scientists chaired by Frank Wilczek. One of its conclusions was: "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 DOE funds should be allocated for dedicated computer hardware for lattice QCD simulations because of the importance of the calculations to their respective fields. Thus, the scientific need for this Program has been validated by leading experts in high energy and nuclear physics.

The LQCD-research Program continues to meet the planning, budgeting, and reporting criteria for an OMB Exhibit 53 IT investment; therefore, this classification remains intact.

In fall 2017, the LQCD Program began transitioning from a dedicated compute cluster model to a new cooperating model under which program funds were used to purchase computing cycles

from institutional clusters (ICs) operating at BNL and FNAL. LQCD began purchasing compute cycles from BNL in January 2017 and Fermilab in FY18.

Beginning in FY18 and concluding in FY19, LQCD partnered with FNAL on the design and implementation of a new institutional cluster. Building on an acquisition strategy and annual planning process that was used by LQCD for many years, a joint committee was formed to understand computing needs, create viable options, and supply a recommendation to LQCD and FNAL management regarding a preferred solution for the FY19 Fermilab institutional cluster procurement.

The Acquisition Planning Committee was asked to provide input into the FY18 computing hardware planning process. Specific activities included:

1. Gather and review computing needs of the LQCD, CMS, neutrino Program user groups
2. Understand the capabilities of the existing hardware portfolio available to LQCD
3. Assess the vendor landscape for viable architecture options
4. Prepare an Alternatives Analysis of viable options
5. Present a recommendation, with technical design and cost estimates to the LQCD and FNAL computing leadership on the most cost-effective hardware solution

A strong alignment of the LQCD hardware portfolio with anticipated computing needs for the USQCD scientific Program were provided by completing the above tasks. This also assisted with the alignment of the new FNAL Institutional Cluster with anticipated future computing needs for the scientific Program.

Based on recommendations and data the team agreed that the preferred solution for the new FNAL institutional cluster was to deploy and commission a conventional cluster of 89 nodes and a GPU accelerated cluster of 2 hosts (4 GPU's per host total 8 GPUs capable of delivering respectively at least 39 TF and 11 effective TF, 50 TFlops total, with at least a memory capacity of 12TB . The committed hardware funds were used in exchange for compute cycles on the new Fermilab Institutional Cluster machine.

### **3 JUSTIFICATION OF MISSION NEED**

LQCD directly supports the mission of the DOE's SC HEP Program "to explore and to discover the laws of nature as they apply to the basic constituents of matter and the forces between them". LQCD 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 program supports 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 these areas.

## 4 PROGRAM DESCRIPTION

The purpose of the LQCD computing program is to provide the USQCD user group with the mid-scale computing resources required to meet the computational needs of the lattice quantum chromodynamics (QCD) research program for fiscal years 2020-2024. The LQCD computing program is an extension of the LQCD-ext II computing project, which currently runs through FY2019. LQCD will support the continued acquisition and operation of institutional computing hardware at existing computing facilities located at Brookhaven National Laboratory (BNL), and Fermi National Accelerator Laboratory (FNAL).

Following the current model, the two host laboratories (BNL and FNAL) will provide computing facilities and infrastructure support to host the LQCD computing systems. The host laboratories will also provide computing professionals who plan, design, deploy, and operate the computing hardware systems at each site. In addition, Fermilab will provide the LQCD Program Manager and Associate Program Manager, who will be charged with the management and oversight of all program activities at the two host laboratories; the Program Office will be located at Fermilab. A detailed description of the roles and responsibilities of these positions can be found later in this document. The budget associated with this proposal provides salary and travel support for Program management and computing professional staff. It also provides for the procurement and deployment of new computing hardware in order to archive Program goals

### 4.1 *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. For the planned scientific program, this class of computing requires machines capable of sustaining at least 10 Tflop/s on jobs lasting at least 2 hours. The total memory required for such jobs will be at least 4 TB. 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. For the planned scientific program, these analysis jobs will require systems capable of sustaining at least 0.5 Tflop/s on jobs lasting at least one hour. The total memory required by such jobs will be up to 2 TB. During the final two years of the Program, all requirements (sustained performance and required memory) for both classes of lattice QCD computing will at least double.

Depending on funding and the needs of the scientific community, a new system will be deployed per year during the period FY2020-FY2024. “System” denotes a cluster or other hardware of uniform design; typically, either a conventional or an accelerated cluster may be deployed in a given year. Table 1 shows the planned total computing capacity of the new deployments and planned delivered (integrated) performance. Currently the Program uses effective Tflop/s-yrs as the metric for delivered computing capacity on the clusters. In all discussions of performance, unless otherwise noted, the specified figure reflects an average of the sustained performance of domain wall fermion (DWF) and highly improved staggered quark (HISQ) algorithms.

Table 1: Annual Capacity Deployment Goals for Aggregate Sustained Performance on LQCD Applications

|  | <b>FY<br/>2020</b> | <b>FY<br/>2021</b> | <b>FY<br/>2022</b> | <b>FY<br/>2023</b> | <b>FY<br/>2024</b> |
|--|--------------------|--------------------|--------------------|--------------------|--------------------|
| Planned delivered performance by resource type (conventional/accelerated) (TFlop/s-yr) | 41/13              | 42/13              | 58/26              | 56/58              | 59/61              |
| Planned delivered performance total (TFlop/s-yr)                                       | 54                 | 55                 | 84                 | 114                | 120                |

**Performance of New System Deployments, and Integrated Performance** (DWF+HISQ averages used). Integrated performance figures assume an 8760-hour year. The delivered performance figures (conventional/accelerated) shown in each year reflect the total across all sites.

In each year of the program, the combination of institutional cluster resources that best accomplishes the scientific goals for LQCD calculations will be purchased. Determining the appropriate mix of conventional and GPU-accelerated resources occurs as part of the annual acquisition planning process and is based upon several factors, including cost effectiveness, availability of software, user demand, and scientific impact.

As in past years, for each annual hardware planning cycle, the LQCD team will consider alternative hardware designs suitable for LQCD computing that may become available.

## 4.2 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. Average memory bandwidths of at least  $F \cdot 1.82$  GBytes/sec per processor core are necessary to sustain a  $F$  GFlop/sec per core single precision floating point rate for SU(3) matrix vector multiplication. We note that some optimized QCD algorithms take good advantage of half-float precision (0.91:1 byte-to-flop ratio) which

requires less memory bandwidth per Flop. 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 thousands of processor cores, the local lattice volume often exceeds the processor's cache sizes. On modern processors, the performance of these fundamental kernels is limited not by the floating-point capability, but rather by either bandwidth to main memory, or by the delays imposed by the network fabrics interconnecting the processors. LQCD computing clusters are composed of thousands of interconnected processor cores. Depending on the size of the local lattice, which depends upon the number of processors used for a calculation, sustained network communication rates of at least 200 MBytes/sec per processor core are required, using message sizes of at least 10 Kbytes in size. LQCD software frameworks maintain performance scalability by using strategies to increase data reuse, exploit data locality, and to overlap computation with communications in order to mitigate network latencies.

### ***4.3 I/O and Data Storage Requirements***

During vacuum configuration generation, data files specifying each representative configuration must be written to storage. These files are at least 10 GBytes in size, with a new file produced every two hours. Thus, the average I/O rate required for configuration storage is modest at only 1.4 Mbytes/sec. However, higher peak rates of at least 100 Mbytes/sec are desired, to minimize the delays in computation while configurations are written to or read from external storage. The total storage volume required for configurations generated in the first two years of the Program is at least 400 TB. 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. To minimize the time for writing to and subsequently reading from scratch storage space, the sustained I/O rate for each independent analysis job may be as high as 300 Mbytes/sec for a fraction of the duration of the job. The mix of jobs on a given cluster may be manipulated using the batch system to preclude saturation of the I/O system.

### ***4.4 Data Access Requirements***

The bulk of configuration generation is performed at the DOE Leadership Computing Facilities and other capability facilities. Archival storage of ensembles of these configurations utilizes robotic tape facilities at Brookhaven, Fermilab, and Jefferson Lab, in addition to tape storage available at facilities producing configurations. LQCD maintains services to provide facile movement of data sets among sites involved with the generation and analysis of gauge ensembles. The aggregate size of data moved between sites is at least 200 terabytes per year and although the 200 terabytes number is difficult to verify, it is considered a lower bound.

#### ***4.5 Hardware Acquisition Model***

The LQCD Program Office will maintain a 5-year hardware portfolio plan that will define current and planned mid-scale computing assets available to the research program from the host laboratories. Based on experience, the production lifecycle for suitable hardware clusters is typically 5 years.

On an annual basis, the Program Office and USQCD leadership will meet with computing leadership from the host laboratories to review past performance, LQCD computational needs, vendor and Leadership Class Facility (LCF) roadmaps, institutional hardware roadmaps, and future acquisitions plans. The purpose of these meetings will be for all parties to update each other on current and future plans and needs, to ensure alignment of objectives. Outcomes from the meetings will include updating the 5-year hardware portfolio plan, determining the optimal mix of computing resources that will be procured from the host laboratories in the next fiscal year, and formulating plans and timelines for expansions of existing cluster resources.

For the acquisition of new laboratory computing resources applicable to the research program, a joint evaluation committee will be formed to evaluate options. The joint committee will consist of subject matter experts (SMEs) representing the needs of LQCD and other laboratory user groups who will use the system. The committee will be charged with gathering user requirements, identifying potential solutions and formulating software benchmarks to use in measuring performance. The committee will evaluate potential solutions against anticipated usage and performance objectives. Available hardware will be benchmarked and compared against scientific requirements and planned milestones. An alternatives analysis will be performed to determine the most cost-effective solution for a given year. The committee will make a recommendation to laboratory computing leadership and the LQCD Contractor Program Manager (CPM) regarding the preferred solution. The recommendation will be included in a written report that summarizes and present the results of the committee's work.

The CPM will review the recommendation and forward a copy of the written report to the USQCD Executive Committee (EC) for their consideration. If appropriate, the CPM will approve the recommendation with the concurrence of the EC.

The host laboratory will be responsible for procuring, installing, commissioning and deploying new systems. A deployment schedule will be communicated to the LQCD Program Office, where it will be tracked to completion.

The procurement of new computing hardware will be done in accordance with the procurement policies and procedures of the laboratory hosting the new system. All procurements will utilize a multi-step process that includes the issuance of Requests for Information (RFIs) and Requests for Proposals (RFPs). Procurement documentation will clearly define performance requirements and specifications. Purchase contracts will be awarded to the winning vendor based on a set of pre-defined selection criteria designed to ensure "best-value" procurements. Upon receipt and installation, each new system will undergo a series of rigorous acceptance tests to verify performance against specified requirements. The system must successfully pass all acceptance tests before final payment is made to the vendor. Should a system fail to pass specific acceptance tests, negotiations will be conducted between the host laboratory procurement office, laboratory

technical staff and vendor to mitigate and successfully resolve discrepancies between required and actual performance.

Full details of the acquisition planning and procurement process, as well as a description of the minimum set of acceptance tests required to verify system performance, will be contained in the following document: *Acquisition Strategy for the Lattice QCD Computing Program*.

#### **4.6 Operations**

LQCD operation associated with the use of institutional clusters includes user support, system administration, system performance monitoring (e.g., capacity utilization and system availability), configuration management, cyber security, data storage, and data movement.

Archival storage of physics data utilizes tape robots and hierarchal mass storage systems at BNL, and FNAL. Tape media is procured using program funds.

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

The planned lifecycle for institutional computing hardware used by LQCD is five years after commissioning. Specific systems may be operated beyond five years if it is determined that continued operation is cost-effective by the host institution.

#### **4.7 Major Interfaces**

As noted earlier, BNL and FNAL are the primary participating laboratories. Memoranda of Understanding (MOU) will be established between LQCD and each host laboratory to define the relationships and expectations between both parties.

#### **4.8 Key Stakeholders**

Key stakeholders include the DOE Office of Science, the DOE Office of High Energy Physics, and the laboratories hosting LQCD computing facilities. Members of the USQCD collaboration are key customers of the LQCD computing facilities. These include laboratory and university researchers, as well as post-docs and students. Their feedback will be provided throughout the Program through the USQCD Executive Committee and spokesperson.

### **5 MANAGEMENT STRUCTURE AND INTEGRATED PROGRAM TEAM**

This section describes the management organization for LQCD and defines roles and responsibilities for key positions. The management structure is designed to facilitate effective communication between the management team and key stakeholders. The LQCD organization chart for management and oversight is shown in Figure 1. Solid lines indicate reporting relationships; dashed lines represent advisory relationships.

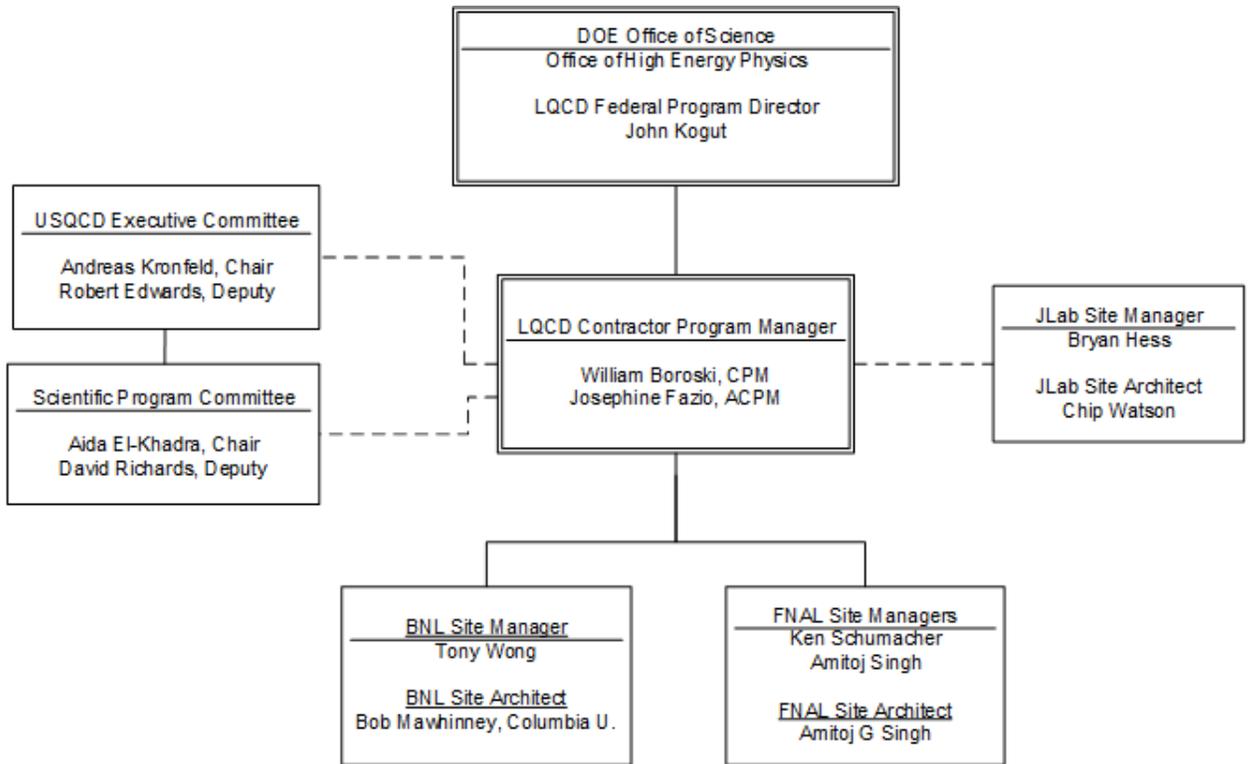


Figure 1: LQCD Management Organization Chart

## 5.1 Roles and Responsibilities

### 5.1.1 LQCD Federal Program Director

Overall management and oversight are provided by the DOE Office of Science, through OHEP. The LQCD Federal Program Director is appointed by OHEP. The LQCD Federal Program Director is John Kogut; he is a certified DOE Level 1 Qualified IT Project Manager

Specific responsibilities of the Federal Program Director include the following:

- Provide Program management direction for the LQCD Program.
- Serve as the primary point of contact to DOE SC headquarters for LQCD matters
- Oversee LQCD progress and help organize reviews as necessary
- Budget funds for LQCD and act as the key contact to the Program office during the preparation of annual OMB Exhibit 53 submissions and reports.
- Control changes to the approved Program baseline in accordance with the change control process defined later in this document.

### 5.1.2 Contractor Program Manager

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

for all major Program commitments and procurements. The Contractor Program Manager is Bill Boroski from Fermilab. He is a certified DOE Level 1 Qualified IT Project Manager.

Specific responsibilities for the Contractor Program Manager include the following:

- Provide management and oversight for all planning, deployment, and steady-state activities associated with program execution.
- Ensure that critical program documents exist and are kept up to date, such as the Program Execution Plan, Risk Management Plan, Acquisition Plan, Alternatives Analysis, and Certification & Accreditation Documentation.
- Develop and maintain a work breakdown structure (WBS) with tasks defined at a level appropriate to successfully manage the program, and that can be externally reviewed. The WBS should include program milestones at a level appropriate to track progress.
- Establish and maintain MOUs with the DOE laboratories hosting LQCD computing facilities.
- Provide support to the LQCD Federal Program Director in the preparation of annual OMB Exhibit 53 Budget Year (BY) submissions in accordance with DOE and OMB guidance and schedules.
- Gather and summarize financial information for the monthly progress reports to the LQCD Federal Program Director.
- Present monthly progress reports to the LQCD Federal Program Director. These reports cover cost and schedule performance, performance against established key performance metrics, review of annual acquisition strategies and progress against deployment plans, and other significant issues related to execution as appropriate.
- Prepare and submit to DOE annual operating budgets and financial plans consistent with the program plan and performance objectives and manage costs against the approved budget.
- Provide final approval of all major (> \$50K) procurements
- Provide internal oversight and reviews, ensuring that funds are being expended according to the program plan and identifying weaknesses in the execution of the plan that need to be addressed.

Interactions of the Contractor Program Manager:

- Reports to the LQCD Federal Program Director.
- Serves as the primary point of contact with DOE SC, through the LQCD Federal Program Director, on matters related to budget and schedule for all funded activities.
- Interacts with host laboratory senior management regarding program-related matters.
- Provides direction and oversight to LQCD Site Managers on program-related matters.
- Interacts with the Chair of the USQCD Executive Committee and the Chair of the Scientific Program Committee to ensure collaboration needs are being met.

### ***5.1.3 Associate Contractor Program Manager***

The CPM is assisted by the Associate Contractor Program Manager (ACPM). The CPM delegates to the ACPM many activities, including preparing and tracking the Program WBS and schedule; managing the Risk Management Plan; and gathering and analyzing performance data from the host laboratories. Performance data includes actual expenditures, progress towards

milestones, and other relevant performance data. The ACPM assists with the creation of various management documents and maintains other controlled documents as appropriate. The Associate Contractor Program Manager is Josephine Fazio from Fermilab.

Specific responsibilities of the ACPM include the following:

- Prepares detailed planning documents for the Program, including the overall Program WBS and WBS sections specific to certain activities. Included in the WBS are key tasks and performance milestones that allow for the tracking of progress and expenditures against the baseline plan.
- Prepares and manages the Risk Management Plan and Risk Register. Coordinates periodic risk assessments and updates with the LQCD program team.
- Prepares and manages other technical and controlled documents as requested.
- Monitors and reports on activities related to performance assessment.
- Assists in the preparation of annual financial plans consistent with the detailed planning documents and ensures that funds received by the host laboratories are in accordance with annual financial plans.
- Assists in the preparation of OMB Exhibit 53 submission documents.
- Develops and maintains program-management-related communications including the Program web site and the repository of program documents, etc.
- Leads the annual user survey process, which includes preparing the survey, analyzing and reporting on survey results, and preparing annual user survey reports.
- Assists with the annual reviews.

Interactions of the Associate Contractor Program Manager:

- Reports to the CPM
- Works with the Site Managers to coordinate the development of program documents, updates the Risk Management Plan and Risk Register and gathers budget and other data for tracking performance against plan.
- Works with the LQCD Federal Program Director in the CPM's absence.

#### ***5.1.4 Site Managers***

Steady-state operations and new hardware deployment activities at each host laboratory are led by a designated Site Manager (SM) who is located at that site. Each SM has significant authority at his/her site over the resources necessary to deliver the appropriate level of computing resources to the USQCD community. The SM is responsible for developing and executing the corresponding components of the WBS and making sure 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 the authority to reallocate program resources within their host laboratory to accomplish their assigned scope and tasks, in consultation with the CPM. The SM provides enough details of major procurements to the CPM to facilitate review and approval for the use of funds. The SM has direct management control over their site's LQCD budget, with major procurements subject to approval by the CPM. All procurements are subject to host site management procedures and approvals.

Specific site manager responsibilities include the following:

- Provide day-to-day management and oversight of the LQCD computing facilities at his/her site. This includes providing adequate user support to the USQCD community
- Ensure that funds are being expended according to the program plan and identifying weaknesses in the execution of the plan that need to be addressed.
- Obtain necessary resources and approvals from laboratory management and coordinate resources contributed by the laboratory
- Provide technical oversight of the LQCD computing resources at the host site including the monitoring and reporting of system performance metrics such as uptime and usage.
- Implement and monitor user allocations as determined by the Scientific Program Committee.
- Participate in the hardware selection process for deployments at his/her site, representing their host laboratory facilities and operations capabilities.
- Lead the hardware deployment activities at his/her site.
- Assist in the annual budget planning and allocation process, and in the preparation of detailed planning documents, including the WBS and performance milestones at a level appropriate for external review.
- Track progress of site-specific performance milestones.
- Prepare and submit monthly status reports, including expenditures and effort, to the CPM and ACPM
- Prepare materials for external oversight and reviews and participate in external review activities, as necessary.

Interactions of the Site Manager:

- 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.
- Oversees all staff responsible for deployment and operation activities at their respective site.

### ***5.1.5 Site Architects***

The Site Architect (SA) is responsible for technical design and architecture at their host site. The Site Architect assists the Site Manager on strategic issues, monitoring, and reviews, but does not have day-to-day operations responsibilities.

Specific site architect responsibilities include the following:

- Participates in hardware selection activities at their host laboratory, working with host laboratory management and the Site Manager who represents the host laboratory facilities and operations capabilities.
- Leads the architectural design effort at their host laboratory, working with the Site Manager who represents the host laboratory facilities and operations capabilities.

- Architectural design covers computing, storage, networking, monitoring, facilities (space, power, cooling), and integration of these components into a holistic system.
- Establishes performance goals and benchmarks for LQCD systems located at or to be located at their site.
- Assist the SM in the monitoring and assessment of actual performance versus planned performance.
- Assists the CPM in documenting and communicating:
  - Hardware selection information for acquisition planning (target audience is USQCD Executive Committee)
  - Performance goals and benchmarking information for allocation process (target audience is Scientific Program Committee)

Interactions of the Site Architect:

- Reports to the CPM
- Works closely with the ACPM, Site Managers, and other Site Architects both to assist in defining milestones, and to ensure a high level of coherency across the program.
- Works closely with technical staff at the host laboratory in communicating LQCD computing needs and participating in the design and selection of new institutional clusters.

#### ***5.1.6 Integrated Program Team***

The LQCD Integrated Program Team (IPT) is composed of the LQCD Federal Program Director, CPM, ACPM, Site Managers and Site Architects from the host laboratories. The LQCD Federal Program Director chairs the IPT. The current membership of the IPT is given in Appendix A.

The full IPT meets on an as-needed basis, however subsets of the IPT meet on a regular basis. For example, monthly meetings are held between the Federal Program Director, CPM and ACPM to review progress against goals and milestones. The CPM, ACPM and Site Managers meet bi-weekly to discuss operations and review performance on a more detailed, technical level. These meetings often involve planning for subsequent deployments and sharing lessons learned. Site Architects participate in these meetings as well when they involve acquisition planning, architectural design, or other Site Architect responsibilities, or at least every other bi-weekly meeting as a touchpoint.

#### ***5.1.7 USQCD Executive Committee***

The charter of the USQCD 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 is responsible 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 the above. The Executive Committee advises the CPM regarding scientific priorities and the computing resources

needed to accomplish them. The Executive Committee appoints the Scientific Program Committee, which allocates the Program's computational resources.

Members of the Executive Committee rotate at the rate of around one per year. Around half of the members of the Executive Committee are expected to remain during the lifetime of the Program. If a vacancy occurs, it is filled by a vote of the remaining members of the Executive Committee. Appendix B contains a list of the current members of the Executive Committee.

#### 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
- Oversees the national lattice gauge theory community's SciDAC grants and provides coordination between the work done under those grants and in the current Program
- Appoints the members of the Scientific Program Committee

#### **5.1.8 Spokesperson**

The Chair of the Executive Committee serves as the Scientific Spokesperson for the LQCD Research Program.

#### Responsibilities

- Determines scientific goals and required computational infrastructure together with the USQCD Executive Committee
- Chairs the USQCD Executive Committee

#### Interactions of the Spokesperson:

- Principal point of contact to DOE on scientific matters related to the Program
- Presents the Program's scientific objectives to the DOE, 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

#### **5.1.9 Scientific Program Committee**

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

The Scientific Program Committee is charged with allocating time on the integrated hardware resources operated within the scope of the LQCD computing program. This committee has

instituted the following allocation process. Once a year, proposals are solicited for the use of computational resources that are available to the user community during the allocation period July 1 to June 30. The Committee reviews the proposals and makes preliminary allocations based on its reviews. An open meeting of the user community is then held to discuss the proposals and the preliminary allocations. The Committee makes final allocations for each site following this meeting. The LQCD Site Managers are responsible for executing these allocations. The objective of this process is to achieve the greatest scientific benefit from the computing resources through broad input from the community. The committee 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 Scientific Program Committee are appointed by the Executive Committee. The committee chair rotates every two years. Current members have staggered terms of four years. When a vacancy occurs, the open slot is filled by the Executive Committee. The current membership of the SPC is shown in Appendix B.

## 5.2 Program Communications

In addition to the interactions defined under Roles and Responsibilities, the following formal communications touchpoints are to occur annually, as appropriate:

| Touch Point and Timing     | Attendees   | Actions and Goals  |
|----------------------------|---|--|
| Early Acquisition Planning | CPM,<br>Executive Committee                           | CPM leads discussion of acquisition planning, timeline.<br><br>Goal: Concurrence on scope, non-technical considerations as input.  |
| Late Acquisition Planning  | CPM, Site Architects,<br>Executive Committee          | CPM presents acquisition plan.<br><br>Goal: Concurrence on proposed acquisition plan.  |
| Early Allocations Process  | CPM, Site Architects,<br>Scientific Program Committee | CPM presents performance benchmarks, deployed capacity.<br><br>Goal: Address questions from SPC related to their Allocations process.  |
| Late Allocations Process   | CPM, Site Managers,<br>Scientific Program Committee   | SPC presents allocations including expectations for Class B, C allocations in coming year.<br><br>Goal: Address questions from Site Managers related to their monitoring of allocations. |

### 5.3 Interaction with Host Laboratory Management

Line management within the two host laboratories (BNL and FNAL) provides support to the program in several ways, including management and infrastructure support. Management authorities for DOE and senior management of the laboratories are shown in Figure 2. The primary flow of communication regarding LQCD program matters between the DOE Federal Program Director and laboratory management is through the LQCD Program Office.

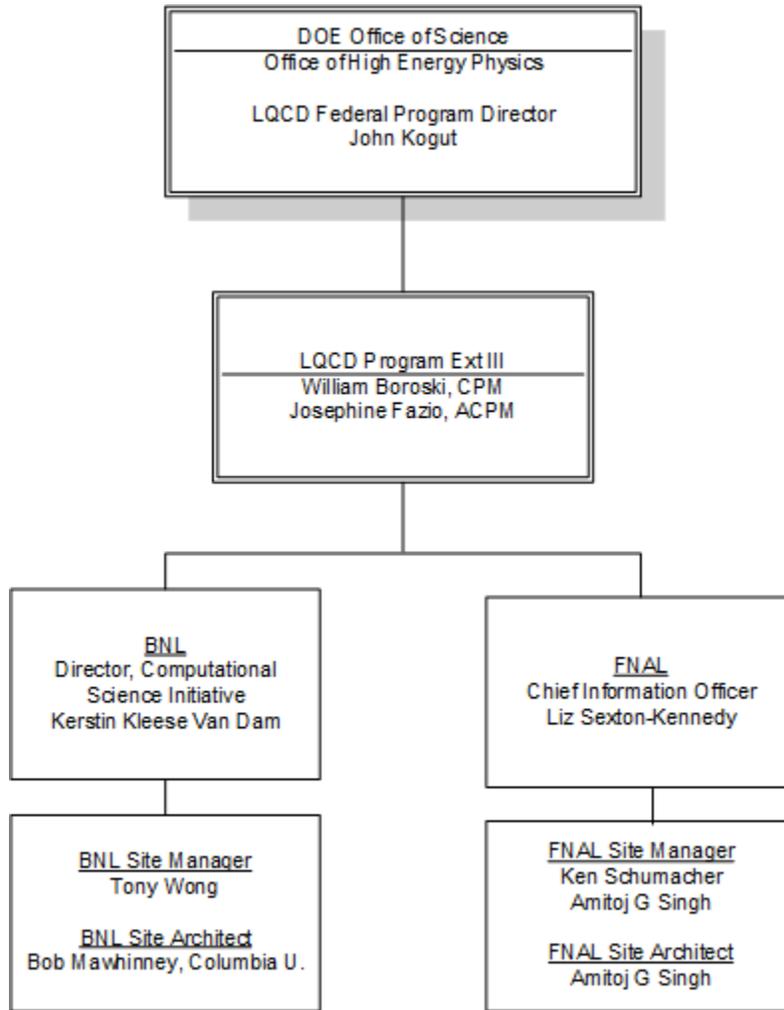


Figure 2: LQCD and Laboratory Management

## 6 COST AND SCHEDULE MANAGEMENT

### 6.1 Program Scope

The scope of the LQCD program include the operation of existing clusters at BNL and FNAL, and the acquisition and operation of new systems in FY2020-2024. Existing systems will be operated through end of life as determined by cost effectiveness (typically 4-5 years). All new systems

acquired during the program will be operated from purchase through end of life, or through the end of the program, whichever comes first.

## **6.2 Work Breakdown Structure**

The LQCD computing program is categorized as an OMB Exhibit 53 mixed life-cycle investment. Program work is organized into a Work Breakdown Structure (WBS) for purposes of planning, managing and reporting activities. Work elements are defined to be consistent with discrete increments of work and the planned method of control. The LQCD program plan has three major WBS Level 2 components based on the work performed at each participating laboratory (BNL & FNAL). Under the Level 2 components are the following Level 3 components:

**Steady-State Operations:** Includes all activities associated with the steady state operation of the LQCD computing facilities at the two host laboratories. The budget associated with Operations supports Site Manager and Site Architect activities as defined above, along with a modest level of travel support.

**New Hardware Deployment:** Includes all activities performed by Site Architects and Site Managers associated with developing acquisition strategies and plans for institutional computing system hardware procurements; and activities associated with the deployment of new computing system and storage hardware. Planning activities typically include gathering vendor roadmap information, performing benchmarking tests, preparing procurement documents, etc. Deployment activities occur from the time new hardware arrives at the site until it is released for production use. Typical activities include unit acceptance tests, system acceptance tests, release in friendly user mode and analysis of results, and preparations for production release. The budget associated with New Hardware Deployments includes labor costs for planning and deployment activities and equipment costs for new hardware.

**Program Management:** Includes all activities associated with program management and oversight, as described above. The budget associated with Program Management supports salary costs for the Contractor Program Manager and Associate Contractor Program Manager, as well as a modest amount for travel and miscellaneous Program Office expenses.

Before the beginning of each fiscal year, a WBS is developed for the work to be performed in the coming year, with bases of estimates derived from past purchase records and effort reports. The WBS is developed with the concurrence of the Site Managers. Once defined, the WBS is baselined and a process for reporting status against the baseline is initiated. The WBS is developed and maintained using Microsoft Project.

Program milestones are defined in the WBS. Site Managers report the status of completion for each milestone to the ACPM on a monthly basis. Any significant changes to milestone schedules are processed according to the change control procedure described later.

### 6.3 Program Milestones

Table 2 shows the Level 1 Program milestones that are tracked by the DOE Federal Program Director and Program Monitor. These milestones are also defined and tracked in the WBS. The target levels for new computing capacity deployed and aggregate computing delivered are defined in Appendix D - Computing Facility Performance Metrics.

Table 2: Level 1 Milestones

| No. | Level 1 Milestone   | Fiscal Year |
|-----|---|-------------|
| 1   | Computer architecture planning for the FY20 procurement complete & reviewed               | Q1 FY20     |
| 2   | Procurement of <i>Combined Resources</i> in FY20  | Q3 FY20     |
| 3   | Target level of aggregate <i>Combined Resource</i> computing deployed & delivered in FY20 | Q4 FY20     |
| 4   | Computer architecture planning for the FY21 procurement complete & reviewed               | Q1 FY21     |
| 5   | Procurement of <i>Combined Resources</i> in FY21  | Q3 FY21     |
| 6   | Target level of aggregate <i>Combined Resource</i> computing deployed & delivered in FY21 | Q4 FY21     |
| 7   | Computer architecture planning for the FY22 procurement complete & reviewed               | Q1 FY22     |
| 8   | Procurement of <i>Combined Resources</i> in FY22  | Q3 FY22     |
| 9   | Target level of aggregate <i>Combined Resource</i> computing deployed & delivered in FY22 | Q4 FY22     |
| 10  | Computer architecture planning for the FY23 procurement complete & reviewed               | Q1 FY23     |
| 11  | Procurement of <i>Combined Resources</i> in FY23  | Q3 FY23     |
| 12  | Target level of aggregate <i>Combined Resource</i> computing deployed & delivered in FY23 | Q4 FY23     |
| 13  | Computer architecture planning for the FY24 procurement complete & reviewed               | Q1 FY24     |
| 14  | Procurement of <i>Combined Resources</i> in FY24  | Q3 FY24     |
| 15  | Target level of aggregate <i>Combined Resource</i> computing deployed & delivered in FY24 | Q4 FY24     |

In addition to these Level 1 milestones, the WBS contains lower level milestones that provide the means for tracking progress at a more granular level. Table 3 contains an example of the type of Level 2 milestones contained within the WBS that are associated with each annual computing system purchase and deployment.

Table 3: Example of Level 2 Milestones in the WBS associated with each Hardware Procurement

| <b>Level 2 Milestones</b>                         |
|---|
| Preliminary System Design Document prepared       |
| Request for Information (RFI) released to vendors |
| Request for Proposal (RFP) released to vendors    |
| Request for Proposal (RFP) responses due          |
| Purchase subcontract awarded                      |
| Approval of first rack                            |
| Remaining equipment delivered.                    |
| Successful completion of Acceptance Test Plan     |
| Release to “Friendly User” production testing     |
| Release to full production                        |

Progress against all milestones is tracked and reported by the LQCD Program Office. Site Managers at each host laboratory report the status of completion for each milestone to the Program Office on a monthly basis. Any significant changes to milestone schedules will be processed according to the change control procedure. Progress against Level 1 and Level 2 milestones is discussed with the DOE Federal Program Director during monthly progress conference calls.

#### 6.4 Total Program Cost

The total program cost for LQCD is \$10.82 million. The program is supported by the DOE SC Office of HEP. The HEP planning budget for LQCD is shown in Table 4.

Table 4: \$10 million Planning Budget for LQCD (in millions)

| <b>FY20</b> | <b>FY21</b> | <b>FY22</b> | <b>FY23</b> | <b>FY24</b> | <b>Total</b> |
|-------------|-------------|-------------|-------------|-------------|--------------|
| 2.030       | 2.095       | 2.165       | 2.230       | 2.300       | 10.820       |

Program funds will be used to procure and deploy new systems and provide labor support for steady-state operations (e.g., site management, system administration, hardware support, and deployment of LQCD software) and program management. Software development is not in the scope for the LQCD Program.

Each host site will continue to contribute in-kind support to the Program in the form of infrastructure facilities and equipment, such as suitable computer room space, utility costs for power and cooling, and mass storage facilities. Each host site also provides administrative and technical support and services to the program in areas such as environment, safety, and health (ESH&Q), cyber security, disaster planning and recovery, networking, procurement, financial

management services, and administrative support. The program contributes to the pool of funds at each site used to cover these costs, through the assessment of overhead charges by each host site in accordance with standard laboratory policies.

Table 5 shows the LQCD obligation budget profile in terms of commonly recognized expenditure types, by fiscal year. The personnel budget provides salary support for Site Managers, Site Architects and program management. All labor cost estimates are based on fully loaded average labor rates at the host laboratories and have been inflated using an annual escalation rate of 3%. The travel budget covers costs for the Program Office, site architects and site managers to participate in annual DOE reviews and the USQCD All-hands Meeting. The compute services budget covers the cost of computing cycles delivered from institutional clusters. The data storage services budget covers the cost of disk and tape storage. Indirect charges will be applied according to agreements established between the Program and the host laboratories and documented in approved MOUs.

Table 5: Obligation Budget Profile by Expenditure Type (\$K)

| Expenditure Type      | FY20         | FY21         | FY22         | FY23         | FY24         | Total         |
|-----------------------|--------------|--------------|--------------|--------------|--------------|---------------|
| Personnel             | 175          | 155          | 160          | 165          | 167          | 825           |
| Travel                | 15           | 15           | 15           | 15           | 15           | 75            |
| Compute Services      | 1,625        | 1,710        | 1,775        | 1,835        | 1,900        | 8,845         |
| Data Storage Services | 215          | 215          | 215          | 215          | 215          | 1,075         |
| <b>Total</b>          | <b>2,030</b> | <b>2,095</b> | <b>2,165</b> | <b>2,230</b> | <b>2,300</b> | <b>10,820</b> |
| HEP Planning Guidance | 2,030        | 2,095        | 2,165        | 2,230        | 2,300        | 10,820        |

Figure 4 shows the proportional cost breakdown by expenditure type. Approximately 90% of the total budget will be allocated to new compute and storage hardware. The level of personnel support is based on past operating experience. Program funds allocated to support travel have been kept to a minimum, with budgeted levels based on and consistent with past operating experience.

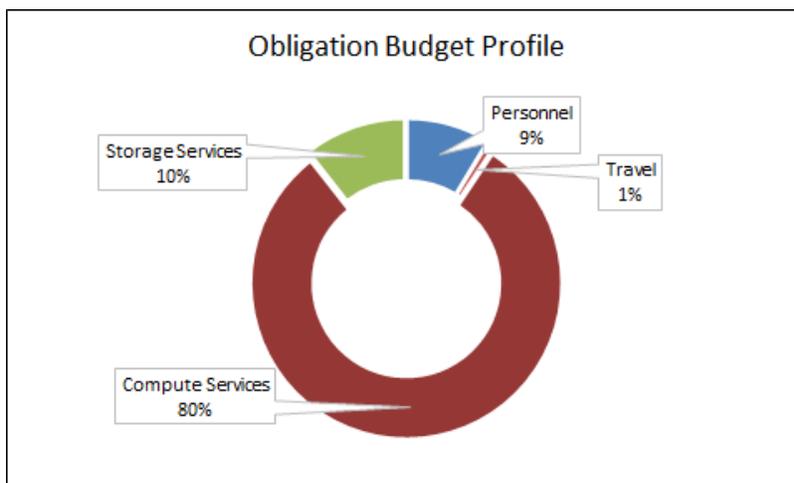


Figure 4: LQCD Total Program Budget Fraction by Expenditure Type

Figure 5 shows in graphical form the data presented in Table 5. The budgets for personnel, travel and storage services are relatively flat. Growth due to inflation is most visible in the compute services budget, which increases from \$1.6M to \$1.9M over the five-year period.

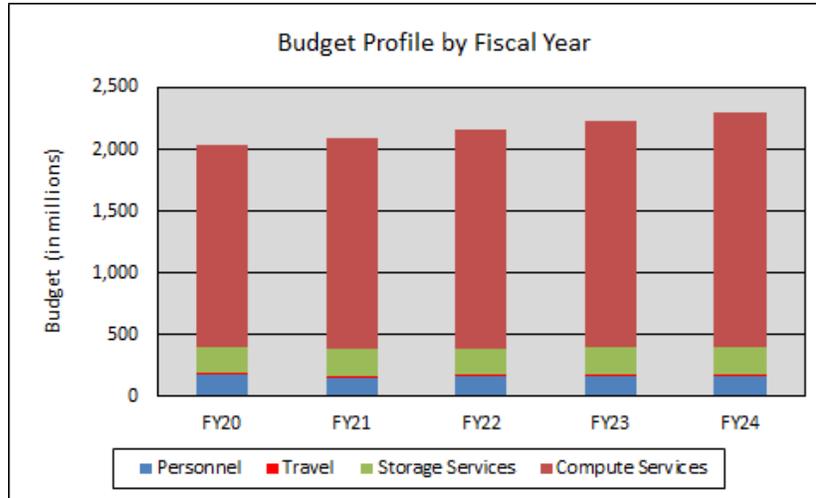


Figure 5: LQCD-ext III Budget Profile by Fiscal Year

#### 6.4.1 Management Reserve

No funds have been set aside for management reserve. The program will be managed to fit within the budget guidance. Any unplanned cost increases in any category will be offset by decreasing the budget for other categories. The categories with the most built-in contingency are the compute and storage services budgets. Knowing that decreasing budget allocation in these categories directly impacts the amount of computing and storage delivered to the science program, all costs will be managed very carefully.

#### 6.4.2 Deployment Performance Contingency

Table 7 shows the planned budget for compute and storage services. In each year of the LQCD program, the LQCD team will choose the most cost-effective mix of computing and storage services that meets the needs of the science program. The selection of “node-hrs delivered” from the available cluster portfolio and the volume of data storage capacity contracted will be constrained by the available budget. Given this cost constraint, contingency is in the form of delivered performance.

Table 6: Compute and Storage Services Budget (in \$K)

| Fiscal Year | Compute Services | Storage Services | Total |
|-------------|------------------|------------------|-------|
| FY20        | 1,625            | 215              | 1,840 |
| FY21        | 1,710            | 215              | 1,925 |
| FY22        | 1,775            | 215              | 1,990 |
| FY23        | 1,835            | 215              | 2,050 |
| FY24        | 1,900            | 215              | 2,115 |
| Total       | 8,845            | 1,075            | 9,920 |

All institutional cluster hardware procurements will utilize firm fixed-price contracts and will be “built-to-cost” in accordance with approved budgets. Given fixed budgets, the precise number of processors procured will be determined by the purchase price of systems and network equipment in that year. Variation in purchase price of these components, from the estimates used in the budget, will result in greater or lesser computing capability from the estimated value. Variation in performance of the components from the estimates will also result in greater or lesser computing capability. The resulting performance risk is managed by the fact that the scope of the Program is fluid; small negative variances in available computing capability and/or capacity may result in schedule delays in completing scientific computing Programs. Large negative variances will prevent the achievement of computing goals; these may trigger review and modification of the USQCD scientific program, such as through changes or elimination of allocations of computing resources to specific science projects.

The risk of large performance variances is minimized using conservative projections in the estimated costs and performance of each future system development. Allocations of computing resources, and the planning of the USQCD scientific program, will be based upon these conservative estimates.

Figure 6 shows historical price/performance data for FY10 through FY19 and extrapolated performance through FY26. The blue squares and blue trend line are the price/performance figures for conventional clusters deployed through FY19 (10q, 12s, Pi0, BNL-KNL, BNL-SKY, FNAL LQ1). The red squares and trend line are the price/performance figures for GPU clusters deployed through FY19 (Dsg, 12k, Pi0g, BNL-IC).

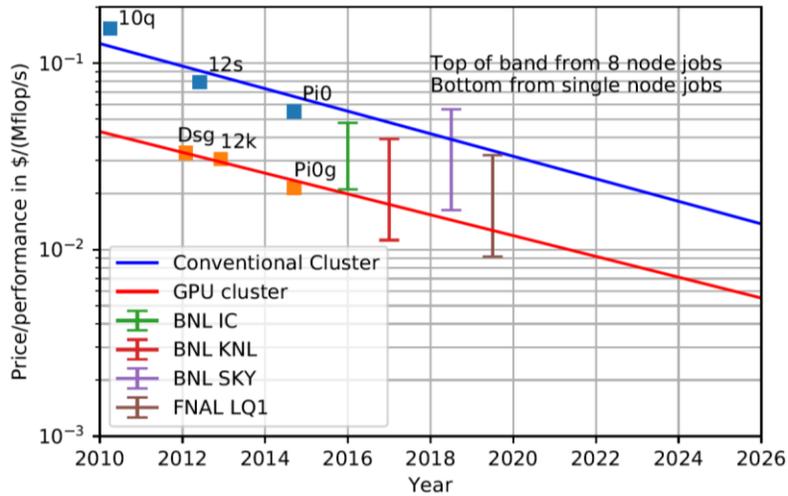


Figure 6: Development of Performance Contingency

For the purpose of extrapolating future price/performance figures, the Program assumes that the exponential trends observed in FY10 through FY19 will continue. The “deployed TFlops” goals shown in Table 1 are based on this assumption.

In each year, the host laboratories procuring new clusters will continue to build to cost and LQCD will commit to procuring computing cycles in accordance with the approved baseline budget. Based on experience, price/performance has occasionally exceeded our conservative forecasts. Barring significant market fluctuations and/or technological delays, we anticipate this trend to continue and actual computing capacity deployed, and computing cycles delivered, will be in excess of the stated goals. This excess is the contingency.

A full description of the LQCD program procurement strategy can be found in the following Program document: *Acquisition Strategy for the Lattice QCD Computing Program*.

### 6.5 Cost and Schedule Management Controls

Overall performance at the two host laboratories is managed under the terms of the performance-based management contract with the DOE. Under these terms, laboratories are expected to integrate contract work scope, budget, and schedule to achieve realistic, executable performance plans. The table in Appendix C shows the cost and work performance metrics for the LQCD program. The table in Appendix D lists all facility performance metrics for the entire LQCD program. The metrics in these tables are associated with a \$10.8 million Program budget. The values in these tables will be revised once the final funding profile is approved.

Following existing financial and operational procedures and processes at FNAL and BNL, the program has implemented methods of collecting and analyzing program performance data. The LQCD Program Office, consisting of CPM and ACPM, is responsible for the overall management of the Program and for implementing controls to ensure that cost, schedule, and technical performance requirements are met.

Memoranda of Understanding (MOU) are executed between the Program and the participating laboratories that detail work scope, level of funding, and the in-kind support provided to the Program by the host laboratories.

The LQCD Program Office has implemented a performance-based management system in which cost and effort data are collected from both laboratories and analyzed on a monthly basis. Site Managers are responsible for tracking cost and schedule elements, and for reporting these to the ACPM monthly. The ACPM prepares and reviews monthly cost and schedule performance data against schedule, cost, and technical goals, and reports the result to the CPM. Every month the CPM reports on the overall cost, schedule and technical performance to the Federal Program Director.

Technical performance is monitored throughout the Program to ensure conformance to approved functional requirements. Design reviews and performance testing of the completed systems are used to ensure that equipment and systems meet functional requirements.

On an annual basis, the DOE Office of High Energy Physics organizes an external review of Program performance. The review typically covers aspects of scientific, technical, cost, and schedule performance against goals. Results are recorded in a written report; all recommendations are carefully considered and implemented as appropriate. The Contractor Program Manager is responsible for preparing a document summarizing the Program's response to each recommendation.

## **7 PROGRAM MANAGEMENT**

### ***7.1 Security Management***

The institutional clusters at the host laboratories are computing enclaves of the host laboratory. Each computing enclave is protected according to the procedures implemented by the corresponding laboratory. The LQCD Program Office maintains copies of the Certification and Accreditation documents for each laboratory.

Performance is monitored by the DOE site office at each laboratory, in accordance with the requirements specified in the contracts between the DOE and the respective contracting agencies (Brookhaven Science Associates (BSA) for BNL and Fermi Research Alliance (FRA) for FNAL). These contracts include requirements for compliance with pertinent government (NIST 800-53) and DOE Computer Security policies (e.g. DOE O 205.1 Department of Energy Cyber Security Management Program). At each laboratory, contractor security procedures are monitored, verified, and validated by numerous external entities including: 1) DOE-OCIO, 2) DOE Office of Performance Management and Oversight Assessment, 3) the DOE-IG, and 4) external reviews.

### ***7.2 Privacy Management***

None of the computing systems being used by LQCD contain, process, or transmit personally identifiable information. These systems are not privacy systems of record.

### **7.3 Risk Management**

Risk management is viewed as an ongoing task that is accomplished by continuously identifying, analyzing, mitigating and monitoring risks that arise during program execution. Risk is a measure of the potential of failing to achieve overall program objectives within the defined scope, cost, schedule and technical constraints. The purpose of risk analysis is not solely to avoid risks, but to understand the risks associated with the program and devise strategies for managing them.

The final responsibility for risk management rests with the CPM, in consultation with the USQCD Executive Committee and LQCD Site Managers. However, effective risk management is a multi-step process that requires the continuous involvement of all program team members. The LQCD team plans for and tracks operational, technical and financial risks the LQCD Risk Management Plan. The Risk Management Plan is reviewed and updated whenever changing conditions warrant a review and revision of the risk register. The Risk Management Plan is also reviewed on a periodic basis to review the status of identified risks and to consider the potential existence of new risks. During these reviews, the risk register is updated by adding and/or closing risks, and initiating and revising risk mitigations, as needed.

A full discussion of potential risks and mitigation strategies is contained in LQCD Risk Management Plan. The following paragraphs provide a brief insight into some of the more salient risks associated with Program execution, including cost overruns, failure to meet performance goals, and data loss due to catastrophic events. Because of the build-to-cost nature of the Program, the Program has minimal risk of overrunning the approved program 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 Program costs may impact the 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 computing facility partially mitigates the risk of natural disasters. Additionally, the Program employs a disaster recovery strategy for valuable data by storing data files redundantly at two different locations. Although the equipment at each facility is not insured against disasters, standard disaster recovery protections are provided by each laboratory.

## **7.4 Quality Assurance**

Quality is defined 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.” Program personnel follow quality control procedures established at the three host laboratories. In addition, the Program has put into place various methodologies to monitor and improve quality, as described in the following document: *Quality Assurance Plan for the LQCD Computing Program*. All new hardware is inspected for physical quality defects upon initial delivery. As new systems are brought online, a series of tests are conducted to verify quality at the component and system level. Nodes are tested individually and then as a racked unit. Racks are then interconnected and tested. When various components of a new cluster have been tested, the cluster is release to “user-friendly mode” for a short period of more intense testing and use to verify operational readiness, before being turned over to full-production use. Other quality assurance processes include incoming inspection of replacement components, performance management, uptime monitoring, operations analysis, and user satisfaction surveys.

## **7.5 Program Oversight**

The LQCD Program Office prepares a monthly progress report and a monthly meeting is held to inform the Federal Program Director of cost, schedule and technical performance, along with other issues related to program execution.

To determine the health of the program and to provide guidance on progress, an annual DOE Office of High Energy Physics progress review is held, generally in May. During this review, past performance and future plans are presented and reviewed. Review results are presented in written form and transmitted to the Contractor Program Manager via the DOE Office of High Energy Physics. The CPM is responsible for responding to all review recommendations.

## **8 ENVIRONMENT, SAFETY AND HEALTH**

The LQCD program is a collaborative effort among the two DOE-sponsored laboratories with stringent environment, safety, and health (ES&H) policies and programs. LQCD integrates ES&H into all phases of the program (planning, acquisition, operations and maintenance) using appropriate procedures defined by the participating laboratories. All individuals supported by Program funds follow procedures specific to the laboratory at which they work.

The LQCD program follows the five core functions associated with integrated safety management:

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.

Line management at each laboratory retains supervisory authority of their personnel and responsibility for the safety of work performed. Line management keeps the CPM informed about

their laboratory's management and ES&H organization structures. Any safety concerns by personnel assigned to the LQCD program are to be communicated to the line management where the concern occurs and if appropriate, the employee's home laboratory or university.

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

Applicable electrical and mechanical 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 new system or component is done under the guidance provided by the procurement organization of the host laboratory.

There is no direct construction activity under the direction and control of this Program. Any facility upgrades or improvements involving construction activities will be managed by the host laboratory. The LQCD program will comply with all necessary rules, regulations, policies and procedures related to working in or around construction areas. Any required NEPA reviews related to facility upgrades associated with the LQCD computing facilities will be coordinated and/or conducted by the host laboratory.

### Appendix A: Integrated Program Team

|   |                              |
|---|------------------------------|
| LQCD Federal Program Director (HEP)       | John Kogut (chair)           |
| Contractor Program Manager (CPM)          | Bill Boroski                 |
| Associate CPM (ACPM)                      | Josephine Fazio (Jo)         |
| BNL Site Manager                          | Tony Wong                    |
| BNL Site Architect                        | Bob Mawhinney                |
| FNAL Co-Site Managers                     | Amitoj Singh, Ken Schumacher |
| FNAL Site Architect                       | Amitoj Singh                 |
| USQCD Executive Committee Chair           | Andreas Kronfeld             |
| USQCD Executive Committee Deputy          | Robert Edwards               |
| USQCD Scientific Program Committee Chair  | Aida El-Khadra               |
| USQCD Scientific Program Committee Deputy | David Richards               |

## **Appendix B: Committees and Members**

### ***USQCD Executive Committee***

Andreas Kronfeld (chair), Richard Brower, Norman Christ, Carleton E. DeTar, William Detmold, Robert Edwards (deputy), Aida El-Khadra (ex officio, SPC chair), Anna Hasenfratz, Christoph Lehner, Swagato Mukherje, Kostas Orginos

### ***Scientific Program Committee***

Alexei Bazavov, Aida El-Khadra (chair), Jack Laiho, Meifeng Lin, Keh-Fei Liu, Ethan Neil, David Richards (co-chair)

### Appendix C: Cost and Schedule Performance Metrics

| ID | Description of Activity   | Total Cost         |                   | Current Baseline (xx/xx/2019) |                   |                         |                        |
|----|---|--------------------|-------------------|-------------------------------|-------------------|-------------------------|------------------------|
|    |   | Planned Cost (\$M) | Actual Cost (\$M) | Planned Start Date            | Actual Start Date | Planned Completion Date | Actual Completion Date |
| 1  | FY20 SS - Aggregate sustained computing delivered to USQCD community. Goal level: KPI #1  | \$2.030            |                   | 10/01/2019                    |                   | 09/30/2020              |                        |
| 2  | FY21 SS - Aggregate sustained computing delivered to USQCD community. Goal level: KPI #6  | \$2.095            |                   | 10/01/2020                    |                   | 09/30/2021              |                        |
| 3  | FY22 SS - Aggregate sustained computing delivered to USQCD community. Goal level: KPI #11 | \$2.165            |                   | 10/01/2021                    |                   | 09/30/2022              |                        |
| 4  | FY23 SS - Aggregate sustained computing delivered to USQCD community. Goal level: KPI #16 | \$2.230            |                   | 10/01/2022                    |                   | 09/30/2023              |                        |
| 5  | FY24 SS - Aggregate sustained computing delivered to USQCD community. Goal level: KPI #21 | \$2.300            |                   | 10/01/2023                    |                   | 09/30/2024              |                        |
|    | <b>Total</b>  | <b>\$10.820</b>    |                   | <b>10/1/2019</b>              |                   | <b>09/30/2024</b>       |                        |

## Appendix D: Computing Facility Key Performance Indicators (KPIs)

The metrics shown in the following table are associated with the \$10.8 million budget.

| ID | Fiscal Year | Measurement Category         | Measurement Indicator   | Target  | Actual Results       | Rating |
|----|-------------|------------------------------|---|---|----------------------|--------|
| 1  | 2020        | Scientific Program Support   | TF-Yrs delivered towards the completion of the Scientific Program – <i>Combined Resources</i>             | 54 TF-Yrs   | Available in Q4 FY21 |        |
| 2  | 2020        | Responsiveness               | % of tickets resolved within 2 business days  | ≥95%  | Available in Q1 FY21 |        |
| 3  | 2020        | Security and Privacy         | Frequency of vulnerability scans performed at each site on nodes visible from the Internet                | Vulnerability scans performed at least weekly at each host site (minimum of 52 scans per year per site) | Available in Q1 FY21 |        |
| 4  | 2020        | Reliability and Availability | % of average machine uptime across all LQCD computing sites   | ≥95%  | Available in Q1 FY21 |        |
| 5  | 2020        | Quality of Service Delivery  | Customer satisfaction rating (Customers rate satisfaction with the service provided on a scale of 1 to 5) | ≥92%  | Available in Q1 FY21 |        |
| 6  | 2021        | Scientific Program Support   | TF-Yrs delivered towards the completion of the Scientific Program – <i>Combined Resources</i>             | 55 TF-Yrs   | Available in Q1 FY22 |        |
| 7  | 2021        | Responsiveness               | % of tickets resolved within 2 business days  | ≥95%  | Available in Q1 FY22 |        |
| 8  | 2021        | Security and Privacy         | Frequency of vulnerability scans performed at each site on nodes visible from the Internet                | Vulnerability scans performed at least weekly at each host site (minimum of 52 scans per year per site) | Available in Q1 FY22 |        |
| 9  | 2021        | Reliability and Availability | % of average machine uptime across all LQCD computing sites   | ≥95%  | Available in Q1 FY22 |        |
| 10 | 2021        | Quality of Service Delivery  | Customer satisfaction rating (Customers rate satisfaction with the service provided on a scale of 1 to 5) | ≥92%  | Available in Q1 FY22 |        |
| 11 | 2022        | Scientific Program Support   | TF-Yrs delivered towards the completion of the Scientific Program – <i>Combined Resources</i>             | 83 TF-Yrs   | Available in Q1 FY23 |        |
| 12 | 2022        | Responsiveness               | % of tickets resolved within 2 business days  | ≥95%  | Available in Q1 FY23 |        |
| 13 | 2022        | Security and Privacy         | Frequency of vulnerability scans performed at each site on nodes visible from the Internet                | Vulnerability scans performed at least weekly at each host site (minimum of 52 scans per year per site) | Available in Q1 FY23 |        |
| 14 | 2022        | Reliability and Availability | % of average machine uptime across all LQCD computing sites   | ≥95%  | Available in Q1 FY23 |        |
| 15 | 2022        | Quality of Service Delivery  | Customer satisfaction rating (Customers rate satisfaction with the service provided on a scale of 1 to 5) | ≥92%  | Available in Q1 FY23 |        |
| 16 | 2023        | Scientific Program Support   | TF-Yrs delivered towards the completion of the Scientific Program – <i>Combined Resources</i>             | 114 TF-Yrs  | Available in Q1 FY24 |        |
| 17 | 2023        | Responsiveness               | % of tickets resolved within 2 business days  | ≥95%  | Available in Q1 FY24 |        |
| 18 | 2023        | Security and Privacy         | Frequency of vulnerability scans performed at each site on nodes visible from the Internet                | Vulnerability scans performed at least weekly at each host site (minimum of 52 scans per year per site) | Available in Q1 FY24 |        |
| 19 | 2023        | Reliability and Availability | % of average machine uptime across all LQCD computing sites   | ≥95%  | Available in Q1 FY24 |        |
| 20 | 2023        | Quality of Service Delivery  | Customer satisfaction rating (Customers rate satisfaction with the service provided on a scale of 1 to 5) | ≥92%  | Available in Q1 FY24 |        |

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| ID | Fiscal Year | Measurement Category         | Measurement Indicator   | Target  | Actual Results       | Rating |
|----|-------------|------------------------------|---|---|----------------------|--------|
| 21 | 2024        | Scientific Program Support   | TF-Yrs delivered towards the completion of the Scientific Program – <i>Combined Resources</i> | 121 TF-Yrs  | Available in Q1 FY25 |        |
| 22 | 2024        | Responsiveness               | % of tickets resolved within 2 business days  | ≥95%  | Available in Q1 FY25 |        |
| 23 | 2024        | Security and Privacy         | Frequency of vulnerability scans performed at each site on nodes visible from the Internet    | Vulnerability scans performed at least weekly at each host site (minimum of 52 scans per year per site) | Available in Q1 FY25 |        |
| 24 | 2024        | Reliability and Availability | % of average machine uptime across all LQCD computing sites                                   | ≥95%  | Available in Q1 FY25 |        |

## **Appendix E: Controlled Documents**

The set of documents submitted to DOE are designated as controlled Program documents. These documents are tracked using DocDB, the Document Database Control system managed by the Fermilab Core Computing Division. The LQCD document control area is password protected and only accessible by the IPT. Access requests should be made to the ACPM.

The following are considered controlled documents, with formal version control and signature approval.

1. Program Execution Plan
2. Risk Management Plan
3. Quality Assurance Program
4. Acquisition Strategy
5. Annual Acquisition Plans
6. Certification and Accreditation Document
7. Cyber Security Plan (formerly called the Security Vulnerability Assessment Report)

In addition to controlled documents, the following documents are also stored in DocDB under limited access.

1. Memoranda of Understanding
2. DOE Annual Review Reports