Memorandum of Understanding
between
Brookhaven National Laboratory (BNL)
and the
SC Lattice QCD Computing Project Extension II (LQCD-ext II)

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

Operated at
Brookhaven National Laboratory
Fermi National Accelerator Laboratory
Thomas Jefferson National Accelerator Facility

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

Version 1.1

Approved: (TBD)

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Change Log

Revision No.	Description/Pages Affected	Effective Date
0.0	Entire Document (LQCD-ext Project)	April 20, 2010
0.5	Revised entire document (LQCD-ext Project)	April 11, 2013
0.9	Adapted & updated entire document for LQCD-ext II Project	February 3, 2016
1.0	Adjust document for CR16-01 where necessary. Declare v1. Add description of project funds management and allocation. Adjust document text for feedback. Add Appendix 1.	March 31, 2016 April 20, 2016 May 24, 2016
1.1	Adjust wording of BNL-specific terms in Section 3 and Subsection 7.2 to better capture the intent, remove ambiguity. Update and sync to PEP v2.0 org chart. Reformat Appendix 1.	August 11, 2016 August 11, 2016 October 17, 2016

CONCURRENCES:

_____   _____
William Boroski   Date
LQCD-ext II Contract Project Manager
Fermilab

_____   _____
Kerstin Kleese van Dam   Date
Director, Computational Science Initiative
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1 Project Overview

The Lattice Quantum Chromodynamics (LQCD) computing project (LQCD Project) provides for the acquisition and operation of computational systems that will serve as a principal computational resource for the national USQCD scientific community. The LQCD Project is operated as an OMB Exhibit 53 IT Investment project under the direction of the DOE Offices of High Energy Physics (OHEP) and Nuclear Physics (ONP).

The numerical study of QCD requires very large computational resources and has been recognized as one of the great challenges of computational science. Recent advances in computer technology, coupled with major improvements in scientific algorithms, have brought the field to a new level. A limited number of crucial quantities have been calculated to a level of accuracy comparable to their experimental determination. Moreover, the experience that has been gained allows confident predictions of the computing resources required for determinations of a broad range of fundamental quantities to an accuracy required for support of the experimental program and to provide guidance to the program in some areas. As a result, there are opportunities to make major scientific advances.

The main objective of the LQCD Project is to support the achievement of the scientific goals described in the Project Execution Plan. Using the computational resources made available through the LQCD Project, members of the USQCD scientific collaboration can better provide theoretical insight and guidance to the community of approximately 4,500 particle and nuclear physicists. In fact, this investment is crucial to advance scientific discovery in the QCD discipline.

The LQCD Project has been funded through a series of proposals and funding extensions. The initial LQCD project was funded from FY2006-2009. The LQCD extension project (LQCD-ext) was funded from FY2010-2014. The LQCD extension II project (LQCD-ext II) is currently funded from FY2015-2019. References to LQCD-ext II in this document refer specifically to this latest funding period.

2 Purpose

This Memorandum of Understanding (MOU) describes the collaboration between Brookhaven National Laboratory (herein referred to as BNL or the Institution) and the OMB Exhibit 53 Investment project titled "SC Lattice Quantum Chromodynamics Computing (LQCD) project" (herein referred to as the LQCD Project). The LQCD Project's Unique Project (Investment) Identifier is 019-20-01-21-02-1032-00. Other collaborating laboratories include Fermi National Accelerator Laboratory (FNAL) and Thomas Jefferson National Accelerator Facility (TJNAF).

This document outlines the general agreement between the project and BNL regarding the use of laboratory personnel, infrastructure and facilities to meet the performance goals and requirements defined in the approved baseline plan. It will remain effective throughout the lifetime of the LQCD Project, which is currently funded through September 30, 2019.

3 Scope of Work

The scope of work for the LQCD Project is defined in detail in the LQCD Project Execution Plan (PEP)[i] and the LQCD Acquisition Strategy[ii]. In summary, the scope of work for the LQCD Project includes:

- Operation through end-of-life of computing hardware purchased and deployed at BNL, FNAL, and TJNAF during FY2010-2014 using LQCD-ext and LQCD-ARRA project funds;
- Acquisition, deployment, and operation of new computing hardware at BNL, FNAL, and TJNAF in FY2015-2019.

The scope of work for the LQCD Project excludes:

- Scientific software development
- System and scientific software support activities

The scope of work specific to BNL includes:

- Steady-state operations: This includes continuous operation, until an appropriate end-of-life, of:
  - Maintenance and operation of the LQCD BG/Q computer system (half-rack) through a mutually-agreed upon decommissioning date or the end of FY2017, whichever comes first.
  - Maintenance and operation of the BNL-owned prototype BG/Q computer system (DD2 rack) through a mutually-agreed upon decommissioning date or the end of FY2017, whichever comes first.
  - Newly deployed hardware at BNL during the current MOU period as described above.

  Operations may also include software development specifically driven by project operation needs, such as improvements to storage, network, monitoring, or computing system software that are stressed by LQCD operations.

- New hardware planning and deployments: This includes the acquisition and deployment of new computing hardware during the period FY2015 to FY2019 in accordance with the LQCD-ext II Acquisition Strategy and annual LQCD-ext II Acquisition Plans. Project funds are to be used for the purchase of the new hardware and for the labor needed to plan for and deploy this new hardware. Full details of the deployment plan are found in the Acquisition Strategy document.

The LQCD Integrated Project Team (IPT) will determine planned decommissioning dates of computing hardware purchased with project funds after evaluating the cost effectiveness of continued operation. Based on over 10 years of operational experience, the nominal operational lifetime for LQCD computing project hardware is approximately 5 years. LQCD Site Managers will work closely with computing facility managers at each host institution to ensure that LQCD facility needs and project decommissioning timelines are understood and mutually agreeable. Decommissioning and disposal of retired LQCD equipment is the responsibility of the host site. The host site may repurpose, sell, or dispose of retired LQCD equipment as it deems most appropriate.

Work on the LQCD Project will be performed in accordance with the LQCD Project Execution Plan (PEP) and the Work Breakdown Structure (WBS), subject to the availability of funding from OHEP and ONP. Detailed activities to be performed at BNL and the required level of effort for technical personnel are specified in the LQCD Project WBS document. The project WBS will be reviewed on an annual basis and updated as necessary to reflect changing conditions or needs.

4   Funding and Costs

Funding for the LQCD Project will be provided by OHEP and ONP over the project lifetime in accordance with the approved baseline plan and funding profile. BNL expenditures will be covered by funds provided by DOE and allocated to the laboratory on an annual basis, following the guidance contained in the annual financial plan that is prepared by the CPM and submitted to the LQCD Federal Project Director and the LQCD Project Monitor prior to the start of each fiscal year. The LQCD Federal Project Director is responsible for managing the allocation of funds from OHEP. The LQCD Project Monitor is responsible for managing the allocation of funds from ONP. BNL agrees not to exceed the site budget defined in the annual approved financial plan.

The project funding profile for host sites is provided in Appendix 1. The actual amount of funds allocated to each host site will likely vary from this profile as described in Section 4.1. The current project funding profile involves changes described by project change request CR16-01 which affects some modest site budget items as early as June 2016 and the overall project funding profile beginning in FY17.

4.1   Project Funds Management and Allocation

In August of each year, the LQCD Project Office works with the LQCD Site Managers to forecast expenditures through the end of the current fiscal year and estimate the potential level of unspent funds remaining at each site, including Management Reserve. The LQCD Project Office factors these estimates of unspent funds into the upcoming year's financial plan to optimize the allocation of new DOE funds across the three host sites to achieve the levels of site funding necessary to accomplish project goals. The optimized financial plan is prepared by the CPM, who shares the plan with the LQCD Site Managers and transmits the plan to the LQCD Federal Project Director and the LQCD Project Monitor. The LQCD Federal Project Director is responsible for managing the allocation of funds from OHEP to each host laboratory. The LQCD Project Monitor is responsible for managing the allocation of funds from ONP to each host laboratory. As the new fiscal year begins, the Project Office works with the LQCD Site Managers to ensure that new project funds have been received and that the funds distribution from DOE to the host sites is in agreement with the allocation guidance provided in the LQCD annual financial plan.

Project funds are not transferred from project site to project site as a rule, and would invoke project change control if such transfers were required for some reason. The LQCD Project Office holds the project funds necessary for its function, project management. Site managers hold the project funds necessary to support their site operations and deployment responsibilities.

4.2   Project Funds Allocated to the Site

Project funds will be allocated to BNL to cover costs in the following categories:
- Labor support for the deployment of new LQCD Project computing systems. This includes new hardware deployment planning and support.

- Labor support for the steady-state operation of LQCD Project computing systems, including system administration, hardware support, storage (including tape costs), and site management. The budget also provides a modest amount of funds for travel and materials/services.
  - Project funds will also be allocated to cover 10% of the labor support for the BNL-owned prototype BG/Q DD2 rack in exchange for the LQCD Project to be allocated 10% compute time (time-averaged over 1 month) on the DD2 rack.
- Construction and purchase of new computing systems, including clusters or equivalent computing hardware, network switches, tapes, disks, etc. The size, makeup and location of the equipment will be defined on an annual basis to optimize the cost and performance of the machines. New system deployments also include a modest amount of hardware required for the near-line storage.

5 Resources

5.1 Project Management Personnel

- LQCD Contract Project Manager (CPM): William Boroski
- LQCD Associate Contract Project Manager (ACPM): Robert D. Kennedy

William Boroski and Robert D. Kennedy are FNAL employees.

5.2 Site Management Personnel

- BNL Site Manager: Tony Wong
- BNL Site Architect: Shigeki Misawa and Bob Mawhinney

Tony Wong and Shigeki Misawa are BNL employees. Bob Mawhinney is a Visiting Senior Scientist at the RIKEN-BNL Research Center at BNL and an employee of Columbia University. Some functions of these roles may be delegated to others.

5.3 Technical Personnel

Project work at BNL will be performed by BNL staff members and/or BNL-designated personnel. Job categories required may include computer professionals, engineers, and engineering technologists. The estimated level-of-effort for each year is contained in LQCD Project 5-Year Operating Budget Forecast. On an annual basis and as part of developing each year's financial plan, the Project Office reviews resource needs with each Site Manager and makes mutually-agreed upon adjustments as necessary. These adjusted amounts are used in the preparation of each annual financial plan.

5.4 Equipment

New equipment for the computing system at the BNL site will be procured using DOE funds made available to BNL through the process described in Section 4. Existing computing equipment deployed at BNL to carry out LQCD computing work at the beginning of FY2015 falls within the scope of the LQCD Project computing system covered under this document.

6 Project Management Responsibilities

The LQCD project management infrastructure and the Project Office reside at FNAL. The LQCD CPM is responsible for the overall management of the project. This person reports to the LQCD

Federal Project Director and is the key interface to the Federal Project Director for financial matters, reporting, and project reviews.

6.1   Organization Chart of the LQCD-ext II Project

Please refer to the LQCD-ext II Project Execution Plan, Section 5, Figure 1.

6.2   Laboratory Management at LQCD Project Sites

Please refer to the LQCD-ext II Project Execution Plan, Section 5.1.6, Figure 2.

6.3   Coordination and Reporting

The BNL Director of the Computational Science Initiative is a signatory to this MOU and represents the Institution to the LQCD Project. This person will carry out the coordination with the senior management of the Institution, and possibly other institutions within the LQCD Project collaboration.

During the deployment of a new cluster, the technical progress of the design, implementation, and testing of computer equipment will be reported to the Project Office by the BNL Site Manager on a monthly basis, by WBS element. The Site Manager is also responsible for reporting to the LQCD CPM operations metrics and performance measures defined for the project. The LQCD CPM will, in turn, report the consolidated progress report to the DOE Federal Project Director.

Any changes to the scope of work and the associated cost and schedule must be documented in consultation with the LQCD CPM and pre-approved using the change control mechanism established in the LQCD PEP.

6.4   Procurement Authorization

The LQCD CPM approves procurement plans and delegates procurement obligation authority to the Site Manager and as necessary, the appropriate financial officer at the site. The procurement cost ceilings at each host site are documented in the LQCD computing hardware budget. These cost ceilings must not be exceeded without the authorization of the CPM and, when necessary, by invoking change control processes as defined in the PEP.

6.5   Reporting to LQCD Project Management

BNL will report all LQCD Project-related expenditures and labor charges in each item of work by LQCD WBS category (cost element level). This detailed reporting will be done on a monthly basis through the Site Manager to the LQCD CPM. Any request for variance from the base cost must be immediately reported to the Site Manager. Any significant variance in schedule from the base schedule must be immediately reported through the Site Manager to the LQCD CPM.

BNL agrees to furnish complete documentation of the quality assurance (as defined in the LQCD Project Quality Assurance Plan[iii] and applicable BNL Integrated Quality Assurance Program documents), risk management information (as defined in the LQCD Project Risk Management Plan[iv]) and performance testing that is carried out for LQCD. Further, the institution agrees to furnish accurate documentation of all software that it provides to the LQCD Project in electronic format.

BNL agrees to set up and maintain ledger cost accounts in a manner compatible with the one used by LQCD Project management. The Institution agrees to provide and maintain this ledger so as to provide timely information to the LQCD Project Office. By this MOU, standard practices used at BNL for cost accounting will be applied to the LQCD Project activities by BNL.

6.6 Collaboration with Other Groups and Institutions

FNAL and TJNAF are the two other institutions participating in the LQCD Project. The LQCD CPM and ACPM will coordinate with these two institutions and present consolidated reports to the DOE Federal Project Director.

7 BNL Contributions

Subject to available funding from DOE, BNL will provide additional support to the project during this period of performance.

7.1 Effort

BNL will provide support for additional scientific and technical personnel as an in-kind contribution. This contribution refers only to system and scientific software support provided outside of the scope of the LQCD Project.

7.2 Services

BNL agrees to provide support services to the LQCD Project to the degree required to carry out relevant responsibilities, some of which are covered by the overhead paid by the LQCD Project. Support services provided by BNL may include:
- Services for generic computing infrastructure, including networking
- Services for the lab-wide infrastructure for mass storage. This includes backups of operating systems and non-volatile data by the BNL Information Technology backup server.
- Services for computer security infrastructure
- Services of the responsible financial officer
- Services for building facilities
- Services for administrative staff.

In addition, BNL agrees to provide the following services as part of an agreement for the LQCD Project to acquire cluster systems at BNL in FY17 and FY18:
- Sufficient compute cycles on the BNL Institutional Cluster (IC) to make up the deficit in the project's Delivered Computing due to acquiring and supporting LQCD clusters at BNL.
  a. BNL will grant the LQCD project an allocation of about 40 BNL IC node equivalents from June 2016 to September 2019 inclusive.
     i. The allocation size may be revised if benchmark tests prove these nodes are 15% more or less performant than initial estimates based on a previous generation GPU-based LQCD cluster.
  b. LQCD usage will be based on a monthly average.
     i. More or fewer nodes may be used by LQCD at any one time.

     c. The same rules for managing allocations applied to USQCD proposals will be used for the LQCD-BNL IC allocation, for instance, in the partial loss of unused allocations from quarter to quarter.
- 100-200 TB of disk storage on the 1 PB Institutional Cluster storage system.
     a. This storage system will have a peak bandwidth of 24 GB/s that is shared between all users of the BNL Institutional Cluster.
- 0.5 PB of older disk storage for scratch and/or intermediate-term storage on the existing storage systems for BG/Q systems at BNL.
     a. This storage will have lower bandwidth than the Institutional Cluster storage system.
     b. As a result of the above storage contributions, $80k of project budget in FY17 and FY18 is freed up that would have been assigned to BNL disk storage purchases.
- Use and access of BNL mass storage systems, including tape robot and intermediate disk caching system.
     a. LQCD users will see a standard file system interface to this mass storage system.
     b. LQCD users may be required to bundle their files to a minimum file size before storing them to tape.

7.3 Facilities and Equipment

Adequate facility infrastructure will be made available to the LQCD Project to the degree necessary to carry out the implementation and operation of LQCD Project computing systems at the BNL site. BNL agrees to pay for all facility and utility costs, such as the power needed to support the computing and HVAC systems.

7.4 Operating Costs

BNL, subject to available funding from DOE, will support the normal operating expenses related to the LQCD Project but not listed in the project scope of work in Section 3, such as administrative support and miscellaneous office supplies.

8 General Considerations

8.1 System Engineering Practices

BNL management agrees to support the implementation of standard system engineering best practices. All major system components will undergo appropriate quality control and validation testing.

BNL agrees to provide a high level of reliability and availability for the system, sufficient to meet the Key Performance Indicators defined in the Project Execution Plan. Any outage or abrupt maintenance shutdown shall be recorded and analyzed to minimize future disruptions. Adequate notices must be given to the LQCD Project site management for routine maintenance and upgrades.

8.2 Project Management Practices

BNL management agrees to support project management best practices and guidelines prescribed by DOE, within the scope of the PEP, and within the terms of BNL's contract with DOE. Note that during the initial approval of the LQCD-ext II computing project, it was determined by the

DOE Federal Project Director that the LQCD-ext II computing project is exempt from the implementation of the Earned Value Management System (EVMS).

All procurement documents must be transmitted to the LQCD Project Office. All procurements must be accompanied by adequate backup documents, including the appropriate LQCD Project charge codes established for the site. All project labor costs must be reported by the appropriate charge codes to the LQCD Project Office on a monthly basis. All equipment items purchased using DOE funds will be properly marked as the property of DOE and identifiable as a part of the LQCD Project computing system.

8.3 Schedules and Milestones

BNL will make every effort to carry out its institutional responsibilities consistent with the schedule and milestones for the LQCD Project. It is understood that these schedules may need to be adjusted as the LQCD Project progresses. BNL agrees to notify the LQCD Project Office as soon as possible of any significant changes that would affect the scope, cost, performance, or schedule of the LQCD Project. These changes must be documented in writing and approved using the change control process described in the LQCD PEP. Status of the project milestones for BNL will be reported on a monthly basis to the LQCD Project Office.

Appendix 1. LQCD-ext II Project Funding Profile

The LQCD-ext II project funding profile for host sites is shown below. The actual amount of funds allocated to each host site will likely vary from this profile as described in Section 4.1.

LQCD-Ext II Cost Forecast - $14 Million
(as of 08/25/2016)

Project Budget, by Site - Baseline 2 (in $k)

BNL LQCD SITE BUDGET	FY15	FY16	FY17	FY18	FY19	Total
Steady-state Operations	280	283	466	365	409	1,804
New Hardware Deployment	0	0	708	807	0	1,515
Project Management	0	0	0	0	0	0
Management Reserve	0	0	74	50	0	124
Total BNL LQCD Site Budget	280	283	1,248	1,222	409	3,442

FNAL LQCD SITE BUDGET	FY15	FY16	FY17	FY18	FY19	Total
Steady-state Operations	809	915	763	728	750	3,966
New Hardware Deployment	0	0	15	377	1,199	1,591
Project Management	118	135	139	144	148	685
Management Reserve	46	0	0	22	94	161
Total FNAL LQCD Site Budget	974	1,051	917	1,271	2,191	6,404

TJNAF LQCD SITE BUDGET	FY15	FY16	FY17	FY18	FY19	Total
Steady-state Operations	746	562	471	486	380	2,646
New Hardware Deployment	0	1,021	332	21	19	1,394
Project Management	0	0	0	0	0	0
Management Reserve	0	83	32	0	0	115
Total TJNAF LQCD Site Budget	746	1,667	835	507	400	4,154

LQCD-EXT II PROJECT BUDGET	FY15	FY16	FY17	FY18	FY19	Total
Steady-state Operations	1,836	1,760	1,701	1,579	1,540	8,415
New Hardware Deployment	0	1,021	1,055	1,205	1,219	4,500
Project Management	118	135	139	144	148	685
Management Reserve	46	83	105	72	94	400
Total LQCD-ext II Project Budget	2,000	3,000	3,000	3,000	3,000	14,000

DOE Project Funding by Fiscal Year	2,000	3,000	3,000	3,000	3,000	14,000

Notes:
1. All unspent funds in one year, including Management Reserve, are assigned primarily to New Hardware Deployment in following year.

Appendix 2. List of Acronyms

ACPM	Associate Contract Project Manager
ARRA	The American Recovery and Reinvestment Act of 2009
BG/Q	IBM Blue Gene/Q model computer
BNL	Brookhaven National Laboratory
CIO	Chief Information Officer
CPM	Contract Project Manager
DOE	Department of Energy
EVMS	Earned Value Management System
FNAL	Fermi National Accelerator Laboratory, a.k.a. Fermilab
IPT	Integrated Project Team
LQCD	Lattice Quantum Chromodynamics
LQCD-ext II	Lattice Quantum Chromodynamics Extension II Computing Project
MOU	Memorandum of Understanding
OHEP	DOE Office of Science-Office of High Energy Physics
OMB	Office of Management and Budget
ONP	DOE Office of Science-Office of Nuclear Physics
PEP	Project Execution Plan
QCD	Quantum Chromodynamics
SC	DOE Office of Science
TJNAF	Thomas Jefferson National Accelerator Laboratory
WBS	Work Breakdown Structure

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[i] LQCD-ext II Project Execution Plan
[ii] LQCD-ext II Acquisition Strategy
[iii] LQCD-ext II Quality Assurance Plan
[iv] LQCD-ext II Risk Management Plan