

**Acquisition Strategy
for the
SC Lattice QCD Computing Project Extension
(LQCD-Ext)**

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

for the
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**Acquisition Strategy
Change Log**

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Revision 0.9	LQCD II plan draft drawn from LQCD FY08/FY09 Plan	Dec 30, 2008
Revision 1.0	Pre-ARRA version.	March 19, 2009
Revision 1.1	Combined FY2010/FY2011 buy. LQCD II → LQCD-Ext	April 13, 2009
Revision 1.2	Added performance basis, Section 508 and M-07-11 compliance, and cyber security sections.	April 15, 2009
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Introduction

The Lattice QCD Computing Extension Project (LQCD-Ext) develops and operates new and existing systems in each year from FY2010 through FY2014. These computing systems are deployed at Fermilab (FNAL), Jefferson Lab (JLab), and Brookhaven (BNL). Table 1 shows the actual and planned total computing capacity of the new deployments, as well as the actual and planned delivered (integrated) performance; the FY2013 and FY2014 numbers reflect the addition of the ARRA-project computing capacity (JLab 9q, 10q, 9g, and 10g clusters).

	FY 2010	FY 2011	FY 2012	FY 2013	FY 2014
Actual (FY10) and <i>Planned</i> (FY11-FY14) Computing capacity of new Deployments, Tflop/s	12.5 <i>11</i>	9 <i>9</i>	<i>10-15*</i>	<i>15-22*</i>	<i>22-33*</i>
Actual (FY10) and <i>Planned</i> (FY11-FY14) delivered Performance (JLab + FNAL + QCDOC), Tflop/s-yr	19.2 <i>18</i>	31.5 <i>22</i>	<i>34</i>	<i>50-55*</i>	<i>60-78*</i>
Actual and <i>Planned</i> (FY11) GPU Deployment, number of Fermi-equivalent NVIDIA GPUs	-	152 <i>128</i>	<i>360-540**</i>	<i>570-860**</i>	<i>930-1400**</i>
Estimated and <i>Planned</i> delivered GPU computing capacity, Fermi-GPU-Mhrs	-	-	<i>0.92</i>	<i>4.6-6.9**</i>	<i>7.5-11.2**</i>

Table 1 – Performance of New System Deployments, and Integrated Performance (DWF+asqtad averages used). Integrated performance figures use an 8000-hour year. * FY2012 through FY2014 deployments and delivered conventional cluster performance reflects 40:60 range on budget split between conventional and accelerated clusters; FY2013 and FY2014 numbers include JLab ARRA resources (9q and 10q conventional clusters). ** FY2012 through FY2014 GPU-accelerated cluster acquisitions and operations reflect the 40:60 range on the budget split between conventional and accelerated clusters; FY2013 and FY2014 numbers include JLab ARRA resources (9g and 10g accelerated clusters).

In FY2011, the LQCD-Ext project for the first time deployed a mixture of conventional and GPU-accelerated clusters; in FY2012-FY2014, the split between these types of clusters will be determined based upon a number of factors, including cost effectiveness, availability of software, demand, and scientific impact. Currently the project uses Fermi-GPU-hrs (“Fermi” is the current NVIDIA GPU architecture) as the metric for delivered computing capacity on GPU-accelerated clusters; this unit may change in the future to better reflect scientific production. In all discussions of conventional cluster and supercomputer performance, unless otherwise noted, the specified figure reflects an average of the sustained performance of domain wall fermion (DWF) and improved staggered (asqtad) algorithms.

All LQCD-Ext Project cluster hardware procurements will utilize firm, fixed-price contracts. Cluster purchases will use contracts with vendors specializing in COTS hardware. The steady-state operations of the project computing facilities are performed by the three host laboratories, each of which is a government-owned contractor-operated facility.

In each year of the project, the hardware that best accomplishes the scientific goals for LQCD calculations will be purchased. In FY2010, an Infiniband cluster was deployed at Fermilab. In FY2011, the project determined that two deployments, consisting of an expansion of the FY10 cluster at Fermilab, plus a

GPU-accelerated Infiniband cluster, would best optimize the scientific capabilities of the portfolio of hardware operated by the LQCD-Ext project. In FY2012, the IBM BlueGene/Q supercomputer was considered to be an important hardware candidate in addition to conventional and GPU-accelerated clusters; by August 2011, following a similar decision process to that outlined in this document, a BlueGene/Q acquisition was ruled out because pricing, performance, and a firm delivery schedule were not available. In FY2013, the IBM BlueGene/Q architecture is again considered to be an important hardware candidate. Also in FY2013, accelerators other than NVIDIA GPUs, such as the Intel “MIC” architecture, will be important contenders. Project personnel will also consider alternative hardware designs suitable for LQCD computing that may become available.

In the rest of this document we first discuss the design considerations and strategies that we will use for all of the procurements of the LQCD-Ext Project. We then discuss the process by which the project will determine the best hardware combination for the FY13 acquisition. This document will be updated each year to concentrate on the upcoming year’s hardware acquisition.

Previous LQCD Computing Project

From FY2006 through FY2009, the DOE High Energy Physics (HEP) and Nuclear Physics (NP) program offices funded the DOE Office of Science LQCD Computing Project (SC LQCD). The total project cost of \$9.2M funded the deployment and operation of four clusters at Jefferson Lab and Fermilab, the QCDOC supercomputer at Brookhaven, and several SciDAC LQCD clusters at JLab and FNAL acquired in 2003 through 2005.

The clusters developed during SC LQCD were as follows:

- “6n”, at JLab in 2006, based on single-socket dual-core Pentium processors and single-data-rate Infiniband
- “Kaon”, at FNAL in 2006, based on dual-socket dual-core Opteron processors and double-data-rate Infiniband
- “7n”, at JLab in 2007, based on dual-socket dual-core Opteron processors, upgraded to quad-core processors, and double-data-rate Infiniband
- “J/Psi”, at FNAL in 2008 and 2009, based on dual-socket quad-core Opteron processors and double-data-rate Infiniband

The “J/Psi” cluster was procured using funds from both FY2008 and FY2009. The FY2008 piece of “J/Psi” was awarded late in the fiscal year under a purchasing contract that allowed, via an option, additional compute nodes and network hardware of the same configuration to be purchased in the first half of FY2009. The FY2008 portion of the cluster was released to physics production at the beginning of January, 2009, and the FY2009 portion from the exercise of the purchase option was released to physics production in mid-April of 2009.

By executing a combined purchase, a single request for information (RFI) and a single request for proposal (RFP) were used, reducing project labor costs, laboratory labor costs, and the overhead (G&A) charged to the project.

Overview of LQCD-Ext Project Deployments

When the LQCD-Ext project began in FY2010, the most effective hardware for the calculations performed on the existing SC LQCD project compute resources in FY2009 were commodity clusters built using Intel or AMD x86_64 processors and an Infiniband interconnect. We predicted this to be the case in both FY2010 and FY2011, and so proposed a combined cluster purchase in FY2010 and FY2011 at Fermilab similar to the SC LQCD FY2008/FY2009 purchase of “J/Psi”. In 2010, FNAL purchased the “Ds” cluster, based on quad-socket eight-core Opteron processors and quad-data-rate Infiniband. In FY2011, the “Ds” cluster was expanded from 245 nodes to a total of 421 nodes, utilizing an option in the FY2010 purchase contract. This expansion consumed approximately 60% of the FY2011 project hardware budget. Based on the successes of the JLab GPU-accelerated clusters procured in 2009 and 2010 via ARRA (American Recovery and Reinvestment Act of 2009) funding, the LQCD-Ext project designed and acquired a GPU-accelerated cluster, consuming the remaining approximately 40% of the FY2011 project hardware budget. Because of extensive Congressional continuing budget resolutions, both the Ds cluster expansion and Dsg GPU-accelerated clusters were deployed later than the schedule given in the baseline and modified project plans (Ds expansion occurred in two halves, rather than a single expansion, with release to production of June 6 and Aug 1, respectively, rather than March 31 baseline date; Dsg release to production occurred March 1, 2012, rather than the Oct 31, 2011 modified plan approved at the May 2011 Project Progress Review).

In FY2012, because an IBM BlueGene/Q was removed from consideration in August 2011, all deployment funds were allocated to JLab. Similar to FY2011, the project proposed a split acquisition, with between 40% and 60% of funds to be used for a conventional cluster, and between 60% and 40% for a GPU-accelerated cluster. The split will be determined by the end of May, 2012. The first 40% of the FY2012 budget was awarded on April 2, 2012, for a 212-node conventional cluster based on Intel “Sandy Bridge” processors and quad-data-rate Infiniband. The contract for this purchase allows additional racks to be purchased, should the project elect to allocate additional funds up to 60% of the total budget. JLab will begin the procurement of the GPU-accelerated FY2012 cluster in late May to early June.

In the second half of calendar 2012, the next generation of the IBM BlueGene series, BlueGene/Q, will be available for purchase. This machine, like its BG/L and BG/P predecessors, should perform very well on LQCD applications and may be competitive with commodity cluster and accelerated cluster hardware. The LQCD-Ext project will therefore evaluate BG/Q for deployment at BNL in FY2013. Significant BlueGene expertise resides at BNL. If other hardware, such as a conventional cluster or an accelerated cluster, or a mixture of the two, is determined to be more cost effective and would better meet scientific demands in FY2013, the project will instead deploy that alternative.

In FY2014, the project will procure one or two additional systems, using the most cost-effective hardware as determined by the anticipated usage. Similar to the acquisition of the Ds cluster in FY2010 and FY2011, should combined purchases of conventional and/or accelerated clusters across FY2013/FY2014 be determined to be more cost effective and would better meet scientific demands, the project will execute such procurements using FY2013 contracts that allow additional hardware to be purchased in FY2014.

All procurements will be performed by the host laboratory chosen for the particular hardware deployment. Such purchases will utilize firm, fixed-price contracts. The typical sequence for new deployments will be:

1. In consultation with the USQCD community (through the Executive Committee and Scientific Program Committee), determine anticipated usage profiles for new deployments (*e.g.*, distribution of job types and sizes, file I/O requirements)
2. Complete preliminary design
3. Issue a Request for Information (RFI) to likely vendors
4. Evaluate the RFI responses and complete a final design
5. Obtain host laboratory purchase approvals via the local requisition process
6. Issue a Request for Proposal (RFP) to likely vendors
7. Evaluate RFP responses and award purchase contract
8. Approve sample node and sample scalable unit (rack)
9. Test and approve vendor-integrated final system (acceptance test)
10. Operate final system in “friendly user” mode and tune the configuration
11. Release the final system to users

Design Considerations and Strategies for LQCD-Ext Deployments

Compute Nodes

Lattice QCD codes are floating point intensive, with a high bytes-to-flops ratio (1.45 single precision, 2.90 double precision for SU(3) matrix-vector multiplies). When local lattice sizes exceed the size of cache, which is nearly always the case, high memory bandwidths are required.

Commodity processors that were available at the time of the FY2010 deployment with the greatest memory bandwidths were Intel x86_64 processors with 1066 and 1333 MHz front side buses (Xeon “Nehalem-EP”, “Nehalem-EX”, and “Westmere”) and AMD Opteron processors (“Istanbul” and “Magny-Cours”). Xeon and Opteron processors can be used in dual and quad processor systems. In past years, the total cost of quad processor systems of both types, including the cost of the high performance network, exceeded the cost of two dual processor systems with network because of the high cost of the quad-capable processor variants. However, in 2010, the AMD “Magny-Cours” processors did not have a special quad-socket variant, but rather could be used in either dual or quad-processor systems. Quad processor systems based on these processors were as cost effective, or even more cost effective, as dual processor systems. Commodity processors that were available and suitable at the time of the FY2012 conventional cluster deployment were Intel x86_64 processors (“Sandy Bridge”) and AMD Opteron processors (“Magny Cours” and “Interlagos”).

Since late 2006, Intel and AMD have switched all new processors of relevance to lattice QCD to multi-core (initially dual core, now quad core, eight core, and twelve core). The JLab “7n” and Fermilab “J/Psi” clusters purchased and deployed in 2007 and 2008, respectively, use quad core processors; both use motherboards that accommodate two Opteron “Barcelona” processors. The Fermilab “Ds” cluster purchased and deployed in 2010 uses eight-core AMD processors. Lattice QCD production on these clusters has shown that multi-core processors scale very well on MPI jobs when the cores are treated as independent processors. Multi-core processors typically have lower clock speeds than the older analogous single core processors; however, the degree of scaling on MPI jobs is sufficient to make these

processors a more cost effective choice. Roadmaps from both Intel and AMD indicate that all forthcoming designs will be multi-core.

In 2007, all commodity dual processor Xeon motherboard designs used a single memory controller to interface the processors to system memory. As a result, the effective memory bandwidth available to either processor was half that available to a single processor system. At that time, AMD Opteron processors had integrated memory controllers and local (to the processor) memory buses, with a high-speed link (HyperTransport) allowing one processor to access the local memory of another processor. This NUMA (Non Uniform Memory Access) architecture made multiprocessor Opteron systems a better choice for lattice QCD codes because of increased memory bandwidth. In the 2007 and 2008 LQCD project acquisitions of the “7n” and “J/Psi” clusters, and the 2010 LQCD-Ext project acquisition of the “Ds” cluster, multiprocessor Opteron systems were chosen, as these were the most cost effective designs. Since 2009, Intel systems, beginning with the “Nehalem” processor family, have also used NUMA architectures. The 2009 and 2010 JLab ARRA “9q” and “10q” clusters use processors from this Intel family (“9q”) and its successor “Westmere” (“10q”). The 2011 FNAL Dsg cluster also used “Westmere” processors.

Starting in 2008, various LQCD scientists implemented codes to run on NVIDIA graphics processing units (GPUs) using the “CUDA” extensions to the C and C++ languages. Typically these codes accelerated part of the overall computational work performed during LQCD configuration generation and analysis. Although very labor intensive to implement, these codes greatly accelerated those portions of LQCD computations, and GPU-accelerated clusters clearly can have greater cost efficiency than conventional Infiniband clusters for some of the calculations of interest. In early 2009, the LQCD project acquired a small GPU-accelerated cluster based on “J/Psi” host nodes and NVIDIA Tesla S1070 GPUs, with a total of 16 GPUs deployed across 8 “J/Psi” hosts. In 2009 and 2010, via an ARRA-funded project, the “9g” and “10g” GPU-accelerated clusters were purchased and deployed at JLab. The “9g” cluster utilizes NVIDIA GPUs based on the GeForce 200 series (such as the GTX-280, GTX-285, Tesla C1060, and Tesla S1070), and the “10g” cluster utilizes NVIDIA GPUs based on the “Fermi” GeForce 400 and 500 series (such as the GTX-480, GTX-580, and Tesla M2050). The “Dsg” cluster purchased at Fermilab with FY2011 funds utilizes NVIDIA Tesla M2050 GPUs. Starting in 2012, the successor to “Fermi,” “Kepler,” is expected to be available from NVIDIA. “Kepler” will likely have as much as double the throughput of “Fermi”, and will have twice the GPU-to-host bandwidth because of its use of the third generation of the PCI Express I/O bus.

NVIDIA GPUs are available in two forms: the “Tesla” series, which are intended for computations, and the “GTX” or “GeForce” series, which are intended for graphics. The Tesla GPUs have a number of numerical advantages, including error correcting memory (ECC) for the detection of memory errors and the correction of all single-bit errors, hardware double precision, and optimized GPU-to-GPU and GPU-to-Infiniband communications. The graphics GPUs tend to have less memory (1.5 GBytes, for example, compared to 3 or even 6 GBytes on recent Tesla models), but their memory bandwidth is higher due to faster clocking of the GPU processor, and their cost is much lower than the Tesla models. On Tesla models, use of ECC further erodes memory bandwidth and also reduces memory capacity. LQCD calculations have higher throughput on the graphics models because of their higher memory bandwidth. For calculations that can check on the validity of results, such as those that only do Dirac operator inversions, the graphics cards can be more cost effective. However, since many LQCD computations now do more than just matrix inversions, for FY2012 through FY2014 it is very likely that the project will

restrict acquisitions to Tesla models. One final advantage to Tesla models involves warranties; NVIDIA will replace Tesla GPUs that produce numerical errors, but the vendors of graphics cards in general will not. In the GPU acquisition at JLab in 2009 and 2010, failures of the graphics cards were observed on numerical calculations.

For those calculations to which GPUs can be applied, significant accelerations have been observed. Comparing the “JPsi” cluster with the “9g” and “10g” clusters, users in the fall of 2010 reported relative throughputs of between 5:1 and 15:1 when comparing a single GPU to a single “JPsi” node. This represents a significant increase in cost effectiveness. From 2011 forward, the LQCD-Ext expects to use portions of the hardware budget in each year for GPU-accelerated systems. The portion to be used in any year will depend upon the scientific demand for this hardware, which in turn is related to the fraction of the LQCD calculations that can take advantage of GPU acceleration because of the availability of code.

High Performance Network

Based on LQCD SciDAC prototypes in FY 2004 and FY 2005, the “6n” and “Kaon” clusters purchased in FY2006, the “7n” cluster purchased in FY2007, and the “J/Psi” cluster purchased in FY2008 and FY2009, Infiniband was the preferred choice for the first LQCD-Ext cluster “Ds”, and is the likely choice for any later clusters. These clusters will use quad data rate (QDR) or faster Infiniband parts.

Current QDR switch configurations from multiple Infiniband vendors include 24, 36, 108, 144, 216, 288, 324, and 648-port switches. For the large clusters to be built in this project, leaf and spine designs are preferred. Because QDR 4X HCA bandwidths exceed the requirements for lattice QCD codes, oversubscribed designs can be used. A 2:1 design, for example, would have 24 computers attached to a 36-port switch, with the remaining 12 ports used to connect to the network spine.

Service Networks

Although Infiniband supports TCP/IP communications, we believe that standard Ethernet will still be preferred for service needs. These needs include booting the nodes over the network (for system installation, or in the case of diskless designs, for booting and access to a root file system), IPMI access (IPMI-over-LAN) for remote hardware control and management, serial-over-LAN, and NFS access to “home” file systems for access to user binaries. All current motherboard candidates support two or more embedded gigabit Ethernet ports.

In our experience, serial connections to each computer node are desirable. These connections can be used to monitor console logs, to allow login access when the Ethernet connection fails, and to allow access to BIOS screens during boot. Serial-over-LAN (standard with IPMI 2.0) will be used to provide these serial connections.

Network Plan

For LQCD-Ext project clusters, we will replicate the network layout currently used on all of the FNAL and JLab lattice QCD clusters. In these designs all remote access to cluster nodes occurs via a “head node”, which connects to both the public network and to the private network that forms the sole connection to the computer nodes. Secure ID logon (Kerberos at FNAL, ssh at JLab) is required on the head node. “R-utility” (rsh, rlogin, rcp) or host authenticated ssh are used to access the compute nodes.

File I/O

Particularly for analysis computing, large aggregate file I/O data rates (multiple streams to/from diverse nodes) are required. Data transfers over the high performance Infiniband network, if reliable, will be preferred to transfers over Ethernet. Conventional TCP/IP over Infiniband relies on IPoIB (“IP over IB”, one of the protocols supported by the Open Fabrics Enterprise Distribution, or OFED, Infiniband software stack).

NFS has not proven to be reliable on our prior lattice QCD clusters for extensive file reading and writing, though it has been reliable for access to binaries and for smaller writing activities, such as job log files. Instead, command-based transfers using TCP, such as *rcp*, *scp*, *rsync*, *bbftp*, *etc.*, have been adopted for the transfer of large data files. On the JLab and FNAL clusters, multiple raid file systems available at multiple mount points have been used. Utility copy routines have been implemented to throttle access, and to abstract the mount points (*e.g.*, copy commands refer to */data/project/file*, rather than */data/diskn/file*).

FNAL and JLab use *Lustre* as an alternative to NFS. *Lustre* provides a POSIX-compliant file system visible from all worker nodes and from the cluster head node. *Lustre* has the property that the storage volume and aggregate performance (instantaneous rate of data movement summed across all active transfers) can be scaled upwards by adding additional storage server nodes (known as *OSS* nodes, which serve *OST* disk volumes). Each new storage server node adds additional independent spindles of disks to the file system.

The LQCD-Ext project will carefully watch developments in the parallel file system area for changes that can impact the deployed systems. LQCD-Ext will leverage work in this area performed by the large high energy physics experiments such as Atlas and CMS at the Large Hadron Collider. Relevant issues in this area include concerns over the long term viability of *Lustre* given the pending acquisition of Sun by Oracle, and the emergence and/or maturation of parallel file systems such as GPFS, pNFS (the parallel version of NFSv4), and Hadoop.

Procurement Strategy

LQCD-Ext will procure approximately five separate lattice QCD computing systems, one in each of the five years of the project; here we are considering a mixed conventional and GPU-accelerated cluster purchase to be a single procurement, as these would take place at a single host laboratory. The guiding principal of all of these procurements is that the most cost effective hardware will be deployed, where effectiveness is judged by the quantity of science (and of course, quality of science in terms of the reliability of the numerical results) that will be produced during the lifetime of the individual lattice QCD system. In addition to commodity hardware and GPU-accelerated clusters, similar to those deployed during the preceding LQCD Computing Project and in the JLab LQCD ARRA project, we will evaluate alternatives such as the IBM BlueGene family of computers, traditional supercomputers such as the Cray XT series, purpose built machines such as the QCDOC, and other hardware suitable for lattice QCD calculations that may emerge.

At each of the annual project progress reviews, scheduled in or about the month of May of each fiscal year, LQCD-Ext will present the plans for the deployment that will occur in the next fiscal year. For example, in spring of calendar year 2010, the project presented the plans for the procurement that

occurred in FY2011. The only exception to this schedule occurred during the first year of LQCD-Ext; the plans for the FY2010 acquisition were presented at the CD2/CD3 (Critical Decision 2 / Critical Decision 3) review in August of 2010. The annual presentation of procurement plans will include the selection of hardware designs that will be considered, or the procedure that will be used to determine this selection, cost and performance estimates and their justifications, and a detailed schedule.

All procurements will utilize a multistep process:

1. Identify and characterize candidate computer and network hardware
2. Create a preliminary system design
3. Solicit vendor feedback on the preliminary system design through an RFI (Request for Information) solicitation
4. Create a system design based on vendor feedback and any new information that has emerged
5. Solicit vendor cost proposals for the system design through an RFP (Request for Proposal) solicitation
6. Evaluate RFP responses and award purchase order(s) to the winning vendor(s), issuing a final system design as necessary
7. Accept or reject the delivered system(s) based on acceptance testing

Both the preliminary system design and final system design may include two or more selections of hardware; for example, in a given year, both commodity clusters and GPU-accelerated clusters may be included. Throughout the five years of the project, LQCD-Ext personnel will actively monitor the market, identifying and characterizing through benchmarking candidate hardware for upcoming procurements. Project personnel will also interact closely with computer and network manufacturers to understand product features and schedule roadmaps.

The evaluation and selection of hardware for the preliminary system design, and the evaluation of vendor responses to the RFP, will rely on the projected performance of the anticipated lattice QCD applications that will be run on the hardware during its lifetime. The particular mixture of lattice QCD applications to be used will be determined by LQCD-Ext Project staff in consultation with the USQCD Executive Committee and the USQCD Scientific Program Committee.

All awards will utilize firm, fixed-price contracts. Vendors will be encouraged to include modifications to the system designs in their RFI and RFP responses that would maximize the value of the delivered systems. Purchase awards will be based on best value evaluations that will include factors such as price/performance, quality of the vendor, quality of the proposed hardware, power consumption of the proposed hardware, impact on the facility infrastructure of the host laboratory, and usability of the delivered system.

LQCD-Ext will procure storage for *Lustre* and NFS file systems separately from the computing systems. The amount of storage purchased will be determined in part from the requests that are required for all proposals to the Scientific Program Committee for allocations of time. The incremental storage added at each site annually will increase aggregate storage to provide at least as great as the sum of requested storage in the annual allocations proposals. Further, the storage will be deployed using a sufficient number of servers to meet the anticipated I/O bandwidth needs of the coming allocation year.

Strategy for the FY2013 LQCD-Ext Deployment

As discussed in the sections above, in FY2013 the hardware candidates are an IBM BlueGene/Q system at BNL, a conventional Infiniband cluster at Fermilab, a GPU-accelerated Infiniband cluster at Fermilab, or some mixture of the three.

As of the time of the preparation of this document, the precise schedule for the availability of BlueGene/Q (BG/Q) hardware is not known, but based on deployment of such hardware at Argonne National Lab (the “Mira” facility) in spring 2012, general availability should occur in the second half of calendar 2012. Also, because BG/Q software systems and LQCD code optimizations are still under development, performance data are not available. Performance data for the principal LQCD algorithms (asqtad, clover, DWF) will be measured by the USQCD collaboration using prototype hardware at BNL, and the released BlueGene/Q hardware at Argonne National Laboratory by August 2012. Given the expertise of BNL in the operation of BlueGene hardware and the laboratory’s interest in hosting BG/Q systems, should this hardware be selected for the FY2013 purchase, the LQCD-Ext budget will be altered to provide for the hardware purchase and for operations support at BNL during the operational lifetime of the BG/Q (FY2013 through FY2014). Should BG/Q hardware not be chosen in FY2013, the current LQCD-Ext budget, which calls for hardware funds to be allocated to Fermilab for 2013 conventional and/or accelerated cluster acquisitions and their subsequent operations, will be executed.

The LQCD-Ext strategy for determining the hardware for FY2013 will take into account the availability of hardware, pricing, hardware performance, and full life-cycle costs. Because the project must request the distribution of FY2013 funds among the three laboratories by mid-August 2012, a sequence of information gathering steps will occur as listed in Table II below, culminating in the selection of the laboratory to host the FY2013 hardware. The possible hardware acquisition scenarios include:

- A full rack (1024 nodes) of BG/Q hardware at BNL
- A half rack of BG/Q hardware at BNL, and a combination of conventional and GPU-accelerated clusters at Fermilab
- A combination of conventional and GPU-accelerated clusters at Fermilab

If it is determined in August 2012 that hardware will be procured at Fermilab, the budget breakdown between conventional and GPU-accelerated cluster types will be determined by January 2013. Hardware at Fermilab will be released to production by the end of September 2013.

Table II – FY2013 Acquisition Planning Process

Step	Description	Target Due Date
1	The LQCD-Ext Computing Project team (i.e., “the Project”) will provide the LQCD Executive Committee (EC) with data summarizing the distributions of job types and sizes during the prior year on the hardware operated by the Project (Infiniband clusters, GPU-accelerated clusters, and the QCDOC). The Project will request that the EC provide the anticipated scientific program requirements for various architectures (i.e., leadership-class machines, BG/Q rack or Infiniband cluster, and GPU-accelerated cluster). Information on USQCD hardware usage will be presented to the collaboration at the 2012 All-Hands Meeting May 4-5.	Apr 15

2	The Project will prepare the F13 Acquisition Strategy document for presentation and review at the FY2012 DOE Annual Progress Review. The Acquisition Strategy will outline the various options under consideration and the proposed process for selecting the mix of computing hardware that will be procured and deployed in FY13 using project funds.	May 16-17
3	The Project will request that the BNL site manager prepare a plan for procuring and operating a BG/Q rack, detailing estimating hardware, storage, deployment, and operations costs.	Jun 1
4	The EC, with input from the Scientific Program Committee (SPC), will provide the Project with the anticipated scientific program requirements for various architectures (i.e., leadership-class machines, BG/Q rack or Infiniband cluster, and GPU-accelerated cluster). A helpful way of conveying this information would be for the EC to provide an estimate of the relative fractions of “analysis core-hours” and “cost-equivalent GPU-hours” needed to support the scientific program over the next 1 to 2 years. Ideally, the EC will provide the Project with anticipated needs on a per year basis for FY13 and FY14.	Jun 15
5	The BNL site manager will provide the Project with a preliminary plan for procuring and operating a BG/Q, including estimated costs and schedule.	Jul 1
6	The BNL site manager will provide the Project with a final plan for procuring and operating a BG/Q, including costs (hardware, storage, costed manpower for deployment and operations) and schedule.	Jul 22
7	The Project will review the technical landscape, conduct an alternatives analysis of the various options, and propose a cost-effective solution for the FY12 hardware deployment. When considering viable options, the Project will need to factor in the total cost of ownership (TCO) for each solution. In addition to hardware and deployment costs, TCO also includes on-going operations and support costs. Hardware costs will include any necessary storage acquisitions. For solutions involving Infiniband clusters and GPU-accelerated clusters, an operations cost model already exists. For a BG/Q option, the Project will need to understand the cost model for operating a BG/Q at BNL. Information on cost and availability of production BG/Q hardware will also be needed. Results of the analysis and an overview of the proposed solution will be summarized in the Alternatives Analysis document. The Project will verify the host laboratory’s ability and willingness to provide the necessary space, power, and cooling for each alternative.	Jul 29
8	The EC will review the Alternatives Analysis document and proposed FY13 hardware solution, and will provide advice on how to proceed to the Project Manager.	Aug 10
9	The Project will analyze the advice of the Executive Committee as well as any new data that might have been obtained, and will produce the final plan for the FY13 hardware deployment. The Project Manager will advise the EC, the host laboratories, the Federal Project Director, and Project Monitor of the planned FY13 hardware acquisition.	Aug 15
10	The Project Manager will revise the project budget as necessary to accommodate the FY13 hardware solution. Depending on the alternative selected, changes may be required in the planned allocation of funds across the three host laboratories.	Aug 20
11	The Project Manager will provide the Federal Project Director with the FY13 Financial Plan, containing the requested distribution of project funds to the three host laboratories.	Aug 20 (est.)
12	The Project will develop a detailed acquisition plan, with timeline, based on the approved FY13 architecture solution.	Sep 30, 2012
13	The Project will execute the FY13 acquisition plan in a manner that meets approved performance goals and milestones.	Sep 30, 2013