

\\Scnas2p\SC-33\CPIC\BY 2007\April 2005 Data Call\Exhibit 300 Downloads from eCPIC\Exhibit 300 eCPIC downloads\July 22 2005 eCPIC downloads\SC LQCD eCPIC download July 22 2005.Doc
 SC Lattice Quantum ChromoDynamics Computing (LQCD)
 Additional changes added Aug 8-15, submitted to Jehanne Simon-Gillo
 Change control shows changes to the Aug 15 document.

INITIATIVE DEFINITION BY07	
Initiative Definition BY07	
Template Name	IT Investment BY2007
Investment Name	SC Lattice Quantum ChromoDynamics Computing (LQCD)
Is this investment a consolidated business case?	No
Point of Contact	Midlam, Thomas
Revision Comment	
Class	IT
DOE Identifier	110200
Agency	Department of Energy
Full UPI Code	019-20-01-21-01-1032-00-109-026
Bureau	Energy Programs
Exhibit 53 Part	IT Investments by Mission Area
OMB Exhibit 53 Major Mission Area	Science
Investment Type	Major Investment
Four Digit UPI Code	1032
Two Digit UPI Code	00
OMB Short Description	SC supports large experimental programs in high energy and nuclear physics. This IT investment is to provide the computational infrastructure needed to carry out scientific research in theoretical physics in support of these experimental programs.
DESCRIPTIVE INFORMATION BY07	
Background BY07	
Budget Account Number	Office of Science
Account number of any other budget accounts funding this investment:	019-20-0222
Account Name	Science
Program Name	
Program Name	
This Investment is	Initial Concept
Program Activity	High Energy Physics; Nuclear Physics
Investment Initiation Date	10/1/2005
Investment Planned Completion Date	9/30/2009
Investment/useful segment is funded	Fully
PY Full UPI Code	019-20-01-21-01-1032-00-109-026
Screening Questions BY07	

Was this investment approved by OMB for previous Year Budget Cycle?	Yes
Did the Executive/Investment Review Committee approve funding for this investment this year?	Yes
Did the CFO review the cost goal?	Yes
Did the Procurement Executive review the acquisition strategy?	Yes
Did the Project (Investment) Manager identified in Section 1.D review this?	Yes
Is this investment included in your agency's annual performance plan or multiple agency annual performance plans?	Yes
Does this investment support homeland security?	No
If this investment supports homeland security, Indicate by corresponding number which homeland security mission area(s) this investment supports?	
Is this investment information technology? (See Section 53 for definition)	Yes

IT Investment Screening Questions BY07

Is this project (investment) a financial management system? (see section 53.2 for a definition)	No
If so, does this project (investment) address a FFMIA compliance area?	No
If yes, which compliance area?	
Does this investment implement electronic transactions or record keeping that is covered by the Government Paperwork Elimination Act (GPEA)?	No
If so, is it included in your GPEA plan (and does not yet provide an electronic option)?	
Does the investment already provide an electronic option?	No
If this is a new or significantly altered investment involving information in identifiable form collected from or about members of the public, has a Privacy Impact Assessment (PIA) with the investment's unique identifier been provided to OMB (at PIA@omb.eop.gov) for this funding cycle?	No
Was this investment reviewed as part of this FY Federal Information Security Management Act review process?	No
If yes, were any weaknesses found?	
Have the weaknesses been incorporated into the agency's corrective action plans?	
Has this investment been identified as a national critical operation or asset by a Project Matrix review or other agency determination?	No
If no, is this an agency mission critical or essential service, system, operation, or asset (such as those documented in the agency's COOP Plan), other than those identified as above as national critical infrastructures?	No
Was this investment included in a Performance Assessment Rating Tool (PART) Review?	No
If Yes, what is the name of the PARTed program (i.e., the program that was reviewed with the PART)? (For more details regarding the PARTed Programs, please see the PART website at OMB www.whitehouse.gov/omb/part/)	

PARTed Program

Does this investment address a weakness found during the PART Review?	No
Is this investment for new construction or retrofit to a federal building or facility?	No
If yes, are sustainable design practices included in the requirement?	
If yes, is an UESC or ESPC being used to fund the	

requirement?	
Will you use Share-in-Savings Contract to support this investment?	No

FINANCIAL BY07

Summary of Spending BY07

Percentage of Total Project Spending for Financial Management:	
Percentage of Total Project Spending for IT Security:	3.2
SUMMARY OF SPENDING FOR PROJECT STAGES	

	PY-1 and Earlier	PY 2005	CY 2006	BY 2007	BY+1 2008	BY+2 2009	BY+3 2010	BY+4 and beyond	Total
Planning									
Budgetary Resources	0	0	25	114	119	123	0	0	381
Outlays	0	0	25	114	119	123	0	0	381
Acquisition									
Budgetary Resources	0	0	1850	1694	1630	798	0	0	5972
Outlays	0	0	1850	1694	1630	798	0	0	5972
Total Sum of Stages									
Budgetary Resources	0	0	1875	1808	1749	921	0	0	6353
Outlays	0	0	1875	1808	1749	921	0	0	6353
Maintenance									
Budgetary Resources	0	0	625	692	751	779	0	0	2847
Outlays	0	0	625	692	751	779	0	0	2847
Total all Stages									
Budgetary Resources	0	0	2500	2500	2500	1700	0	0	9200
Outlays	0	0	2500	2500	2500	1700	0	0	9200
Government, FTE Costs									
Budgetary Resources	0	0	50	50	50	100	0	0	250

Funding Sources BY07

Funding Sources

	Row Type	PY - 6 1999	PY - 5 2000	PY - 4 2001	PY - 3 2002	PY - 2 2003	PY - 1 2004	PY 2005	CY 2006	BY 2007	BY + 1 2008	BY + 2 2009	BY + 3 2010	BY + 4 2011	BY + 5 2012	BY + 6 2013	BY + 7 2014	BY + 8 2015	Total
019-20-0222 Science	DME	0	0	0	0	0	0	0	1875	1808	1749	921	0	0	0	0	0	0	6353
	SS	0	0	0	0	0	0	0	625	692	751	779	0	0	0	0	0	0	2847
	Total	0	0	0	0	0	0	0	2500	2500	2500	1700	0	0	0	0	0	0	9200
Total Yearly Budgets	DME	0	0	0	0	0	0	0	1875	1808	1749	921	0	0	0	0	0	0	6353
	SS	0	0	0	0	0	0	0	625	692	751	779	0	0	0	0	0	0	2847
	Total	0	0	0	0	0	0	0	2500	2500	2500	1700	0	0	0	0	0	0	9200

I.A INVESTMENT DESCRIPTION BY07

Description and Status BY07

Provide a brief description of this investment and its status through your capital planning and investment control (CPIC) or capital programming "control" review for the current cycle.

The Lattice Quantum ChromoDynamics (LQCD) Computing Investment is for the acquisition of computational systems that will serve as the principal computational resource for the national LQCD user community. Using these computational resources, the LQCD theorists can better provide theoretical insight and guidance to the community of approximately 4,500 particle and nuclear physicists.

The funding included in this document covers the procurement, operation, and maintenance of these computational LQCD systems, as well as the operation and maintenance of the LQCD systems that were initially part of an R&D program that led to the development of the new systems.

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. In fact, this investment is crucial to advance scientific discovery in the QCD discipline. Given the known computational requirements, configurable commercial off-the-shelf components will be acquired through fixed-price contracts as approved by the acquisition executive.

The scientific drivers and computational requirements for these investments are further explained in the following paragraphs. A major goal of the Department Of Energy (DOE) Office of Science is to identify the fundamental building blocks of matter and to understand how the forces among them give rise to the observed physical world. To this end, the Office of Science supports large experimental programs in high energy and nuclear physics investing approximately \$750M per year in high-energy physics (HEP) and \$400M per year in nuclear physics (NP). In addition, the National Science Foundation (NSF) provides approximately \$70M per year in high-energy physics and \$35M per year to nuclear physics. The purpose of the Information Technology (IT) investment described in this document is to provide the computational infrastructure needed to carry out research in theoretical physics in support of these experimental programs. Because of the direct relevance to weak decays of strongly interacting particles at BaBar (SLAC), the Tevatron B-Meson Program (Fermi National Accelerator Lab, FNAL), and the CLEO-c Program (Cornell) physics, roughly 60% of the investment in the high energy program will be directly impacted by these calculations. Because of the direct relevance of QCD to the hadron physics programs at CEBAF (Thomas Jefferson National Accelerator Facility, TJNAF) and RHIC (Brookhaven National Lab, BNL) and the direct relevance of QCD to the quark-gluon plasma research at RHIC (BNL), roughly 50% of the investment in nuclear physics is impacted by these calculations. There are two key goals: the first goal is to achieve results from theoretical calculations that are comparable to the experimental results thereby demonstrating an understanding of the science producing the experimental results. The second goal is to use the understanding of the science to provide guidance to the experiments, design next generation instrumentation and facilities and achieve scientific discoveries. To achieve these goals, high performance and cost-effective computational systems are required.

Important progress has been made towards understanding the fundamental laws of nature through the development of what is known as the Standard Model of High Energy Physics. As indicated above, the Standard Model forms the principal understanding for approximately half of nuclear physics. The Standard Model provides fundamental theories of the strong, electromagnetic, and weak interactions, three of the four fundamental forces of nature. It has been successful in explaining a wealth of experiments conducted with particle accelerators and cosmic rays. However, knowledge of the Standard Model is incomplete because it has proven difficult to extract many of the predictions of quantum chromodynamics (QCD), the component that describes the strong forces of subatomic physics. The only means of doing so is through very large-scale numerical simulations within a framework known as lattice gauge theory. These simulations are necessary to solve fundamental problems in high energy and nuclear physics that are at the heart of the DOE's large experimental efforts in these fields. Major objectives of the experimental programs are to: 1) verify the Standard Model, or discover its limits, 2) determine the properties of strongly interacting matter under extreme high energy and density conditions, such as those that existed immediately after the "big bang" and are produced today in heavy-ion collision experiments, and 3) understand the structure of protons and neutrons and other strongly interacting particles. QCD simulations are essential to research in all of these areas. Computers sustaining tens of teraflop/s will be needed over the next several years if the calculations are to reach the level of accuracy required to enable the Office of Science to effectively capitalize on the investments it is making in current experiments.

The performance of LQCD on a given computational resources is measured by the floating point operations per second (flop/s) using the actual production scientific codes. The total capacity of a given system is then rated as million (mega) or trillion (tera) flop/s of sustained performance. The price performance for LQCD of a given computational resource is measured as dollars per megaflop/s (\$ per megaflop/s, sustained). Throughout this document computer performance or price/performance, refers to performance sustained by production codes, not to theoretical peak rates.

Currently two formulations for LQCD are used: improved staggered action and domain wall action. Certain results are better calculated using one or the other of the formulations and some results are calculated using both formulations as a quality check on results. Approximately half of the LQCD computational resources are used for each of the two formulations.

Typically, the megaflop/s rate for the improved staggered action is 70% of that for the domain wall action on the same hardware for all computer architectures used today. Milestones are specified by giving the average performance of the sparse matrix inversion routine that consumes the bulk of the floating point operations in any

LQCD calculation, averaged over the two actions with the anticipated mix (50:50) for production running. The objective for FY 2007 is to acquire an additional 3.1 (average) teraflop/s for production calculations with an average price/performance of \$0.5 per sustained megaflop/s. Thereafter, the objective is to take advantage of the improvements in technology implied by Moore's law, as well as the specific nature of QCD calculations to advance a series of increasingly powerful capabilities for science. The hardware could be maintained at Brookhaven National Laboratory (BNL), Fermi National Accelerator Laboratory (FNAL), and the Thomas Jefferson National Accelerator Facility (TJNAF), and would operate as a unified user facility. The location(s) of the hardware will be determined by peer review and availability of funding. The effort will be highly leveraged, benefiting from the expertise of the existing computer staffs and infrastructure of these laboratories. The facilities will be available to the entire U.S. lattice QCD community.

The study of QCD is an international endeavor, and its value has been widely recognized by physicists in other countries. Many foreign programs are already moving rapidly to build the computational infrastructure needed to capitalize on QCD. The U.S. cannot retain its leadership position it has traditionally held in this field without new investments.

Assumptions BY07

What assumptions are made about this investment and why?

The assumptions for this investment follow:

- + The DOE will continue to pursue research in the physical sciences as part of its strategy of providing world-class scientific research capacity, with its consequent economic benefits.
- + As part of the DOE strategy for the physical sciences, the DOE Office of Science will continue its research in nuclear physics and high energy physics as these areas are key to understanding the origin and dynamics of the universe.
- + For over 30 years QCD has been proven to be the underlying theory for nuclear and particle physics. It is assumed that this will continue to be the case. Using LQCD to solve the QCD equations and comparing the results to experiments will be pushing to the limits of QCD in the search for new physics.
- + It is necessary to exploit the most cost-effective methods to perform LQCD calculations. Advantage has been taken of the simplifying features of lattice QCD calculations, such as regular grids and uniform, predictable communications between processors. Consequently it is possible to develop computers for lattice QCD that are far more cost effective than general purpose supercomputers, which must perform well for a wide variety of problems including those requiring irregular or adaptive grids, non-uniform communication patterns, and massive input/output capabilities. In addition, lattice gauge theory calculations require significantly less memory and lower disk I/O bandwidth than most large scale applications, which also serves to reduce the cost of computers dedicated to this field relative to those that must serve a broad range of disciplines.
- + In terms of the performance of computational systems, Moore's Law will continue to provide a doubling of the price performance roughly every 21 months. This figure has been surpassed during research and development efforts funded by the DOE HEP and NP programs and the Scientific Discovery through Advanced Computing (SciDAC) Program.
- + Due to uncertainties in the evolution of custom and commercial off the shelf technologies, two hardware strategies are pursued for the foreseeable future. The balance of the investment in the two different technologies will be established by peer review.
- + It is assumed that the DOE will continue to support software development and hardware prototyping for LQCD through its SciDAC program.
- + The following baseline resources are assumed to exist by the end of FY 2006, based on acquisitions during FY06 by this investment plus the resources delivered by the prototypes developed through HEP, NP and SciDAC research and development efforts, including those prototypes developed during the first year of this project:
 - o ~1.1 teraflop/s aggregate clusters at TJNAF
 - o ~3.3 teraflop/s aggregate clusters at FNAL
 - o ~4.2 teraflop/s QCDOC at BNL

Supporting Information BY07

Provide any other supporting information derived from research, interviews, and other documentation.

Two federal advisory committees have endorsed the LQCD effort:

The High Energy Physics Advisory Panel (HEPAP) at a 2004 February meeting agreed that the U.S. should maintain a world class program in lattice gauge theory in order to realize its investment in theoretical and experimental high energy physics. They agreed that the research and development of dedicated hardware is needed to match the accuracy of important experimental measurements, and recommended a long term development program.

Two Nuclear Science Advisory Committee (NSAC) reports endorse LQCD computational efforts. The Report of the NSAC Subcommittee on Nuclear Theory in its November 2003 report stated, "We urge the funding agencies to actively seek new resources, such as SciDAC or new initiative money to fund these facilities", and recommended support of this effort, even under flat budgets.

The mission need of this work is reflected in the NSAC April 2002 Long Range Plan, Opportunities for Nuclear Science:

"Advances in computational physics and computer technology represent great opportunities. To exploit these opportunities, dedicated facilities must be developed with world-leading computational capabilities for nuclear physics research.

Lattice QCD is crucial for answering fundamental questions in strong-interaction physics, and it is widely recognized that definitive lattice QCD calculations require multi-teraflops resources now available at reasonable cost. In addition, successful nuclear physics programs at TJNAF and RHIC urgently need to make connection to QCD. An aggressive and dedicated effort is needed for the U.S. to regain a competitive edge, an edge that lattice QCD can give to understand hadronic physics. The nuclear science component of an internationally competitive lattice effort requires dedicated facilities providing sustained performance of 0.5 teraflops by 2002, growing to 15 teraflops by 2005."

This mission need of LQCD computing was also endorsed in 2003 by a panel of physicists and computer scientists. Among its findings were:

"The scientific merit of the suggested program is very clearly outstanding."

"It is proposed to pursue two separate hardware tracks, one using specially designed systems-on-a-chip that leverage industrial intellectual property cores, the other using general-purpose computing systems. ... We therefore feel it is prudent, as well as interesting, to pursue both tracks, at least until a clear winner or a synthesis emerges."

"The software development component of the proposal is also novel in this context and extremely important. ... The pursuit of two separate hardware tracks will aid in the development of robust, portable software. If successful, the software component could be very valuable both in itself and as a model for other scientific enterprises."

"The proposed programs are of considerable interest from the point of view of computational science, since they could provide convincing models and demonstrations of the use of cost effective special architectures for scientific problems."

"Both the proposers and the DOE should recognize that this is an endeavor that is not likely to be exhausted in 4 years or even in 10."

In May 2005 a review of this project was held as requested by the Offices of High Energy Physics and Nuclear Physics of the Office of Science of the Department of Energy. The review was lead by Dan Hitchcock of the Office of Advanced Scientific Computing Research. The reviewers noted in their final report:

"The review committee is supportive of the goals of this project and believes that there are significant science opportunities that will both optimize the effectiveness of existing and planned experiments and enable new applications of QCD to problems at the forefront of high energy and nuclear physics."

"Within the duration of the project, several calculations that are essential to do justice to important experiments in high energy and nuclear physics will be performed. These include, notably, calculations of matrix elements that figure into standard model predictions for flavor and CP violating processes, in order to bring the precision of the predictions up to the level achieved by recent experiments. Several ideas for extension of the standard model predict discrepancies at this level. This confrontation between theory and experiment is a major frontier of nuclear and high energy physics, to which enormous human and capital resources have been devoted over the last decade."

"The committee enthusiastically endorses both the short- and long-term scientific potential of this endeavor."

The proposed effort is a result of the U.S. lattice QCD community working together since 1999 to plan the needed computational infrastructure. Nearly all senior lattice gauge theorists in the country are involved in this effort, and the infrastructure will be available to researchers through a proposal review process. The DOE HEP, NP, ASCR and SciDAC Programs have supported these research and development activities. Collaborations have been formed with IBM, the British lattice gauge theory group UKQCD, and the Japanese funded RIKEN Research Center. Assistance has been provided by computer scientists and engineers at universities and national laboratories, and by leaders of the National Science Foundation (NSF) Partnership for Advanced Computing Infrastructure (PACI) Program.

I.B JUSTIFICATION BY07

Strategic Goals BY07

How does this investment support your agency's mission and strategic goals and objectives?

This project directly supports the Science Strategic Goal in the Department of Energy's Strategic Plan: "To protect our national and economic security by providing world-class scientific research capacity and advancing scientific knowledge." The investment will support this goal by providing world-class supercomputing capacity for theoretical high energy physics and nuclear physicists who will use them to advance our knowledge of the fundamental forces of nature.

In order to implement the Science Strategic Goal, the DOE has adopted the long term general goal:

"General Goal 5, World-Class Scientific Research Capacity: Provide world-class scientific research capacity needed to ensure the success of Department missions in national and energy security, to advance the frontiers of knowledge in physical sciences and areas of biological, medical, environmental, and computational sciences, and to provide world-class facilities for the Nation's science enterprise."

Again, the investment supports this goal by providing world-class computing capabilities to high energy physics and nuclear physicists in support of their efforts to advance the frontiers of knowledge in their fields. More specifically, the DOE has adopted eight strategies for meeting General Goal 5. Three of them are directly relevant to this investment:

1. Advance the fields of high-energy physics and nuclear physics including the understanding of dark energy and dark matter, the lack of symmetry in the universe, the basic constituents of matter, the structure of nuclear matter in its most extreme conditions, and the possible existence of other dimensions, collectively revealing key secrets of the universe.
6. Significantly advance scientific simulation and computation applying new approaches, algorithms, and software and hardware combinations to address the critical science challenges of the future.
8. Provide or support the Nation's science community access to world-class scientific computation and networking facilities that support advancements in practically every field of science.

These three strategies are closely followed in this investment:

1. The computing resources in this project will enable studies of QCD that will advance the fields of high-energy physics and nuclear physics by increasing our understanding of the lack of symmetry in the universe through the study of the decays of particles containing heavy quarks, the basic constituents of matter through the calculation of the masses of strongly interacting particles and the study of the internal structure of these particles, and the structure of nuclear matter in its most extreme conditions by obtaining a quantitative understanding of QCD at high temperatures and densities.
6. The investment utilizes a novel approach to computer hardware, specifically designing it to meet the requirements of the problems for which it will be used. It combines this hardware with software developed specifically for the hardware under the Lattice QCD SciDAC grant. The hardware and software will be used to carry out some of the most challenging large scale simulations undertaken to date.
8. The project will provide the nation's theoretical high energy physics and nuclear physics communities with access to the world-class computational facilities they need to advance their fields.

This project supports the missions of the HEP and NP Programs.

The mission of the HEP Program is to explore and to discover the laws of nature as they apply to the basic constituents of matter, and the forces between them. The core of the mission centers on investigations of elementary particles and their interactions, thereby underpinning and advancing DOE missions and objectives through the development of key cutting-edge technologies and trained manpower that support these missions. The mission of the NP program is to foster fundamental research in nuclear physics that will provide new insights and advance our knowledge on the nature of matter and energy and develop the scientific knowledge, technologies and trained manpower that are needed to underpin the DOE missions for nuclear-related national security, energy, and environmental quality. As part of these challenging missions, the HEP and NP programs plan, construct, and operate major scientific user facilities and fabricate experimental equipment to serve researchers at universities, national laboratories, and industrial laboratories. These successful programs provides world-class, peer-reviewed research results in the scientific disciplines encompassed by the NP and HEP mission areas under the mandate provided in Public Law 95-91 that established the Department, and assigned the NP and HEP programs the lead responsibility for federal support of fundamental research in nuclear physics and high energy physics. The LQCD computing directly supports the Mission of these two Office of Science programs by proposing to achieve results from theoretical calculations that can be compared to the experimental results, thereby demonstrating an understanding of the science producing the experimental results. This understanding will help guide current and future experiments, design next generation instrumentation and facilities and achieve scientific discoveries.

LQCD computing will contribute to the following scientific performance measures of the NP program:

- o Make factor of 5 improvement in theoretical uncertainties for testing the Standard Model via low energy electroweak observables. (2010) [NP-1]
- o Perform lattice calculations in full QCD of nucleon form factors, low moments of nucleon structure functions and low moments of generalized parton distributions including flavor and spin dependence. (2014) [NP-2]
- o Carry out ab-initio microscopic studies of the structure and dynamics of light nuclei based on two-nucleon and many-nucleon forces and lattice QCD calculations of hadron interaction mechanisms relevant to the origin of the nucleon-nucleon interaction. (2014) [NP-3]

LQCD efforts are also included in the HEP and NP Program Plan Strategic Goals in the 2004 Office of Science Strategic Goals:

- o "Provide precise lattice gauge calculations to compare with established nucleon properties" (NP-2017).
- o "Use computer simulations to calculate with high precision strong interactions between particles" (HEP - 2009)
- o "Measure matter/antimatter asymmetry in the quark sector with high precision" (HEP - 2013).

Within the 2004 Office of Science Strategic Plan, LQCD Computing supports three goals:

- o Goal 4, to "Explore the Fundamental Interactions of Energy, Matter, Time and Space" [SC Goal 4]
- o Goal 5, to "Explore Nuclear Matter from Quarks to Stars" [SC Goal 5] and
- o Goal 6, to "Deliver Computing for the Frontiers of Science" [SC Goal 6]

LQCD Computing is also a critical component for successfully implementing several initiatives identified in the Office of Science's "Facilities for the Future of Science, A Twenty Year Outlook". The knowledge and understanding achieved through LQCD calculations will help guide current and future experiments, design next generation instrumentation and facilities. The facility initiatives that will be impacted by LQCD include:

- o The 12 GeV CEBAF Upgrade (NP), which will provide the capability to study the structure of protons and neutrons in the atom with much greater precision than is currently possible.
- o RHIC II (Luminosity Upgrade to the Relativistic Heavy Ion Collider - NP), which will enable scientists to create and study atomic particle collision events that happen only rarely, and to explore states of matter believed to have existed during the first moments after the Big Bang.
- o eRHIC (Electron-heavy ion collider - NP), which will enable scientists to learn about the structure of protons, and the subatomic particles that bind them.

The scientific justification and Mission Need of LQCD computing has been endorsed by both the High Energy Physics Advisory Panel and the Nuclear Science Advisory Committee. The LQCD effort is needed to ensure that the United States maintains its leadership in science and technology. Without investments in new computational capabilities, the U.S. risks falling behind the rest of the world in the numerical study of QCD. For example, British physicists and the Japanese-supported RIKEN BNL Research Center have each obtained a 5 teraflop/s QCDOC computer during the past year. Italian physicists plan to install computers sustaining several teraflop/s in 2005. Japanese physicists, who have already built machines sustaining approximately one teraflop/s, have begun using the Earth Simulator, and have obtained approval to add dedicated machines sustaining 10-20 teraflop/s in 2006 and again in 2007.

How does it support the strategic goals from the President's Management Agenda?

Program Initiative 8 of the President's Management Agenda for 2003 states that "Science and technology are critically important to keeping our nation's economy competitive... As a result, every federal research and development (R&D) dollar must be invested as effectively as possible." A central goal of this project is to identify and make use of the most cost-effective means of providing the computing facilities needed to study QCD. The approach of designing computing hardware for specific scientific problems was pioneered by physicists studying QCD; however, there is a potential for greater applicability. A review of plans for this project stated that they "are of considerable interest from the point of view of computational science, since they could provide convincing models and demonstrations of the use of cost effective special architectures for scientific problems." As described below in the alternatives analysis, the hardware developed in this investment will provide a cost/performance advantage of more than a factor of six over general purpose supercomputers, and a factor of two over any other alternative expected to exist in that timeframe. Thus, this investment supports Program Initiative 8 in its own working, and may provide a useful paradigm for other R&D projects depending on large scale computations.

This Project supports the following government-wide initiatives set forth in the President's Management Agenda:

Initiative 1 - Strategic Management of Human Capital: The performing organizations, BNL, FNAL and TJNAF, are carrying out the effort as partners. This partnership strategically brings to bear a set of highly experienced scientists to the benefit of the investment. The three institutions have formed an integrated management team with clearly-defined responsibilities and management relationships, to carry out the project in the most effective way possible. Manpower forecasting and planning is done jointly, and the human resources of all three institutions are made available to optimally match the skill mix to the needs of the effort as a function of time.

Initiative 2 - Competitive Sourcing: For each of the major component procurements, the investment will qualify at least two suppliers in order to maintain competition for the production program. The selection of suppliers will be based on best value and their firm fixed-price and -schedule proposals. For conventional systems, commercial off-the-shelf hardware, competitively procured, is used wherever possible.

Alternative Sources BY07

Are there any alternative sources in the public or private sectors that could perform this function?

No. Massive amounts of computational resources are required to provide this function. There are no existing resources available at the scale required, and none planned which would be cost effective. While comparable capabilities are being developed in other countries, these resources are heavily subscribed, and so will not be available to U.S. researchers at a level necessary to accomplish the goals of this effort. There are emerging plans to aggregate the results of international efforts to yield higher statistics and hence better science, but for the U.S. to be a participant in this collective effort, it must have resources at the scale contained in this investment.

To be cost-effective, the research computational systems need to be specially architected for LQCD or they cost from four to tens times as much to achieve the same results. There are no existing or planned scientific computational systems in the public or private sector that have the computer architectures or component prices that are cost-effective for LQCD except for those to be funded by this investment.

The investment will be at up to three (BNL, FNAL and TJNAF) of the four DOE laboratories (BNL, FNAL, TJNAF and SLAC) that have the largest research support within the DOE nuclear and particle physics programs. These DOE laboratories have both the infrastructure to support these investments and strong user programs for the university based researchers to make use of the investments.

It is important to note that all of the procurements for this investment are to commercial companies. These companies provide the computational elements that are assembled to form the specialized computer architecture used for the LQCD systems.

In principle these investments could be located at a university or similar other federal research center. However, the investments for these facilities will achieve their highest performance when they are closely connected with the associated experimental programs. The storage and management of the data would also be highly leveraged by the existing lab infrastructure.

If so, explain why your agency did not select one of these alternatives.

As previously stated, there is no alternative in the public or private sector that could perform this function without an investment four to ten times the proposed investment.

Customers/Stakeholders BY07

Who are the customers for this investment?

Customers are the researchers supported by DOE (Office of Science High Energy Program and Nuclear Physics Program) as well as by the National Science Foundation and foreign governments.

Who are the stakeholders of this investment?

Stakeholders are those developing, participating, supporting, and sponsoring the effort, and those benefiting from it, along with the customers. In addition to the DOE, NSF, Congress and the public, stakeholders include the national and international high-energy physics and nuclear physics scientific research communities, including national laboratory and U.S. university scientists, students, and technical personnel as well as their international counterparts.

Multi-Agency BY07

If this is a multi-agency initiative, identify the agencies and organizations affected by this initiative.

This is not a multi-agency initiative.

If this is a multi-agency initiative, discuss the partnering strategies you are implementing with the participating agencies and organizations.

This is not a multi-agency initiative.

Efficiency and Integration BY07

How will this investment reduce costs or improve efficiencies?

This investment will greatly improve the accuracy of current lattice QCD physics calculations, and enable calculations that cannot be undertaken with current computing resources. The calculations will improve the effectiveness of ongoing and planned scientific experimental programs and enable more effective and prompt scientific conclusions and understandings. Among the most important calculations will be ones required in connection with major experiments in progress FNAL, SLAC, RHIC, and TJNAF. The investment will therefore help to maximize the Office of Science's return on the much larger investments it is making in experimental programs in high energy physics and nuclear physics. The LQCD results will also have an impact on the design of next generation experiments, instrumentation and facilities. As previously pointed out, this investment will substantially reduce the costs of lattice QCD physics calculations, while accelerating the rate at which they will be completed.

List all other assets that interface with this asset.

The LQCD investment substantially leverages off of the existing storage and networking infrastructure, as well as computing expertise at the involved laboratories.

Have these assets been reengineered as part of this investment? No

I.C PERFORMANCE GOALS AND MEASURES BY07

Performance Goals and Measures BY07

Performance Goals and Measures

Fiscal Year	Strategic Goals (s) Supported	Existing Baseline	Planned Performance Improvement Goal	Actual Performance Improvement Results	Planned Performance Metric	Actual Performance Metric Results
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FEA Performance Reference Model (PRM) BY07

FEA PRM

Fiscal Year	Measurement Area	Measurement Category	Measurement Indicator	Baseline	Planned Improvement to the Baseline	Actual Results
2006	Mission and Business Results	General Science and Innovation	Improved staggered configurations generated for studies of CKM matrix and hadron structure [SC Goals 4, 6] [NP-1]	40 ³ x 96 lattices generation 1/3 completed	40 ³ x 96 completed, 48 ³ x 144 50% completed at one quark mass, 25% completed at a second (1.0 TF-Yrs)	
2006	Mission and Business Results	General Science and Innovation	Calculation of CKM matrix elements with improved staggered quarks [SC Goals 4, 6] [NP-1]	Baseline calculation with 28 ³ x 96 lattices completed (< 0.5 teraflops-yr)	Calculation with 40 ³ x 96 lattices completed (1.0 teraflops-yr)	
2006	Mission and Business Results	General Science and Innovation	Hybrid calculation of quark structure of nucleon in chiral regime, including GPDs [SC Goals 4, 6]	< 0.5 TF-Yrs baseline calculation completed	0.8 TF-yrs completed	
2006	Mission and Business Results	General Science and Innovation	Calculation of properties of hot hadronic and quark matter in chiral regime [SC Goals 5, 6]	< 0.5 TF-Yrs baseline calculation completed	1.0 TF-Yrs calculation completed	
2006	Mission and Business Results	Planning and Resource Allocation	Resources are being used in accordance with allocation committee decisions	80% of time used by approved projects	90% of time used by approved projects	
2006	Processes and Activities	Productivity and Efficiency	Meta-facility achieves high uptime and	Average machine uptime of	Average machine uptime of 88%	

			efficiency	80%		
2006	Technology	Effectiveness	Aggregate resource sustained teraflops for Asqtad + DWF (1:1)	5.9 TF This capability allows the completion of the physics program planned for 2006.	+ 2.7 = 8.6 TF This would establish sufficient capability for the planned 2007 physics program.	
2006	Mission and Business Results	General Science and Innovation	Domain wall lattice generations [SC Goals 4,6]	16 ³ x 32 generation completed , 0.5 TF-years	24 ³ x 64 at generation one quark mass completed (1.0 TF - years)	
2006	Customer Results	Timeliness and Responsiveness	Response to service requests	80% of tickets closed within 48 hours	85% of tickets closed within 48 hours	
2007	Mission and Business Results	General Science and Innovation	Improved staggered configurations generated for studies of CKM matrix and hadron structure [SC Goals 4, 6] [NP-1]	40 ³ x 96 lattices completed 48 ³ x 144 lattices in progress (1.75 TF-Years)	48 ³ x 144 lattices completed (1.65 TF-Yrs)	
2007	Mission and Business Results	General Science and Innovation	Calculation of CKM matrix elements with improved staggered quarks [SC Goals 4, 6]	Baseline calculations with 40 ³ x 96 lattices completed (1.0 TF-Yrs)	Calculation with 48 ³ x 144 lattices completed (1.5 TF-Yrs)	
2007	Mission and Business Results	General Science and Innovation	Hybrid calculation of quark structure of nucleon in chiral regime, including GPDs [SC Goals 4, 6]	0.8 teraflops-year calculation completed	1.8 teraflops-year calculation (total) completed	
2007	Mission and Business Results	General Science and Innovation	Pentaquark and N* spectroscopy in the chiral regime [SC Goals 4, 6]	0.5 teraflops-year baseline calculation completed	1.25 teraflops-year calculation (total) completed	
2007	Mission and Business Results	General Science and Innovation	Calculation of properties of hot hadronic and quark matter in chiral regime [SC Goals 5, 6]	1.0 teraflops-year calculation completed	2.25 teraflops-year calculation (total) completed	
2007	Technology	Reliability and Availability	Meta-facility achieves high uptime and efficiency	Average machine uptime of 88%	Average machine uptime of 92%	
2007	Technology	Effectiveness	Aggregate resource sustained teraflops for Asqtad + DWF (1:1)	8.6 TF This capability allows the completion of the physics program planned for 2007.	+ 3.3 (new) – 0.2 (retired) = 11.7 TF This would establish sufficient capability for the planned 2008 physics program.	
2007	Mission and Business Results	General Science and Innovation	Domain wall lattice generation [SC Goals 4,6]	24 ³ x 64 generation at one quark	24 ³ x 64 generation at a second quark mass	

				mass completed (1.0 TF-Yrs)	completed 32 ³ x 64 generation at one quark mass 25% completed (3.0 TF-Yrs)	
2007	Customer Results	Service Coverage	Number of users running jobs each month	30	40	
2007	Customer Results	Timeliness and Responsiveness	Response to service requests	85% of tickets closed within 48 hours	90% of tickets closed within 48 hours	
2007	Customer Results	Customer Benefit	Customer satisfaction survey (Customers rate satisfaction with the service provided on a scale of 1 to 10)	Average score of 8.0	Average score of 9.0	

I.D PROJECT MANAGEMENT (INVESTMENT MANAGEMENT) BY07

Project (Investment) Manager BY07

Is there a project (investment) manager assigned to the investment? Yes

If so, what is his/her name?

Jehanne Simon-Gillo

Identify the members, roles, qualifications, and contact information of the in-house and contract project (investment) managers for this project (investment).

Jehanne Simon-Gillo, Federal Project Manager, Phone: 301.903.1455, E-mail: Jehanne.Simon-Gillo@science.doe.gov. Dr. Jehanne Simon-Gillo holds a B.S. in Chemistry (Juniata College) and a Ph.D. in Nuclear Science (Texas A&M University). She is the Federal Program Manager for all Nuclear Physics Major Items of Equipment and the majority of the NP Line Item Construction Projects, providing scientific, technical and managerial leadership to the project team to optimize the success of the project. Today, she is managing twelve capital initiatives, all of which report their cost performance to her on a regular basis. She works with the project team to formulate realistic cost estimates with contingency analyses. She performs Technical, Cost, Schedule and Management reviews to verify proposed baselines and assess the effectiveness of proposed management structures. She peer reviews and generates necessary documentation for new initiatives such as acquisition strategies and project management plans. She is currently the Federal Program Manager for the CEBAF 12 GeV Upgrade, a \$225M initiative that has obtained Critical Decision -0. As Acting Director of the Facilities and Project Management Division, she is responsible for the funding of operations of the NP facilities. She implements rigorous merit evaluation using independent peer review for all new and ongoing activities supported by the Division in accordance with the requirements of 10 CFR 605 for the grant program and NP, SC and DOE guidelines for the DOE laboratory programs, facilities and projects. She has extensive experience of the Congressional budget process and has played a major role in the formulation of the ~\$400M budget of the NP program, of which ~\$270M is currently her responsibility. She is responsible for the generation of all Exhibit 300's and Project Data Sheets for the Congressional Budget.

The DOE OCIO has classified this project as requiring Level 1 project management. Jehanne Simon-Gillo is in the process of being validated, and will become Level I certified by October 21, 2005. The timing of the validation process has been completely dictated by course availability.

Don Holmgren (FNAL), Contract Project Manager, Phone: 630.840.2745, E-mail: djholm@fnal.gov. Dr. Holmgren holds a B.S. in Physics (Harvey Mudd College) and a Ph.D. in Experimental Condensed Matter Physics (University of Illinois at Urbana-Champaign). He has worked in the Computing Division of Fermilab for 10 years; prior to this he worked in industry (Amoco Technology Company) for 7 years. At Fermilab he has managed the development of tightly coupled computing clusters for lattice QCD calculations for over six years; this work has included the preparation of budgets and schedules, the design, specification, procurement, and integration of computer hardware, as well as the operational responsibility for delivering computing resources to lattice QCD theorists located at Fermilab and at various universities and other laboratories. The project described in this submission is an extension of these efforts.

Bakul Banerjee (FNAL), Associate Contract Project Manager, Phone: 630.840.5251, E-mail: bakulb@fnal.gov. Dr. Banerjee holds a B.A. (hons.) in Mathematics (Presidency College), a M.Sc. in Mathematics (Indian Institute

of Technology, Kanpur, India), and a Ph.D. in Geophysics (Johns Hopkins University). She has worked at Fermilab in the Computing Division for 4 years; prior to this, she worked at Argonne National Laboratory for 10 years, and for 12 years in industry (Rockwell International, Goodyear Atomic Corporation, and Phoenix Corporation). At Fermilab, she has served as the project engineer responsible for managing tasks, resources, and financial coordination within collaborations for the US Compact Muon Solenoid (CMS) Software and Computing project (multiyear, \$72M budget), and for the Tevatron Beam Position Monitor Upgrade project (20 months, \$4M budget). As a member of the IEEE Software Engineering Standards Working Groups, Bakul co-authored six international IEEE standards, including ANSI/IEEE Std. 1058.1 (1990 Standard for Software Project Management Plans) and ANSI/IEEE Std. 828 (1990 Software Configuration Management Plans).

Robert Sugar, Chair of the LQCD Executive Committee, Phone: 805.893.3469, E-mail: sugar@physics.ucsb.edu
Guidance is provided by the LQCD Executive Committee. The Project Manager, Contract Project Manager, and Associate Contract Project Manager, and LQCD Executive Committee work with the Integrated Project Team to set the investment goals, draw up plans for meeting these goals, and oversee progress towards meeting them. The Chair of the Executive Committee, Robert Sugar, serves as spokesperson of the executive committee and together with the Contract Manager, are the principal contacts with the Department of Energy.

The LQCD Executive Committee members are:

R. Brower, (Boston U.) N. Christ (Columbia U.), M. Creutz (BNL), P. Mackenzie (FNAL), J. Negele (MIT), C. Rebbi (Boston U.), S. Sharpe (U. Washington), R. Sugar (UCSB, Chair) and W. Watson, III (TJNAF)

Project Management Qualification Status	1 - The project manager assigned for this investment has been validated as qualified in accordance with OMB PM Guidance
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Contracting Officer BY07

Is there a contracting officer assigned to the project (investment)?	Yes
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If so, what is his/her name?

Don Holmgren

Integrated Project Team BY07

Is there an Integrated Project Team?	Yes
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If so, list the skill set represented.

The current membership of the Integrated Project Team is shown below.

NAME, ROLE, Organization, Description

Jehanne Simon-Gillo, DOE Federal Project Manager, DOE-NP

Dr. Simon-Gillo provides programmatic direction for this project, and functions as the point of contact at DOE headquarters on all project matters. She is responsible for overseeing project progress, organizing reviews as necessary. She is responsible for budgeting funds to execute the project. She will become Level I certified by the start of the project. Dr. Simon-Gillo chairs the meetings of the IPT.

Jeff Mandula, DOE HEP Program Manager, DOE-HEP

Sid Coon, DOE NP Program Manager, DOE-NP

This project is funded through the DOE Office of High Energy Physics (OHEP) and Office of Nuclear Physics (ONP). Jeff Mandula and Sid Coon, the DOE Program Managers for HEP and NP respectively, are the points of contact within OHEP and ONP.

David Goodwin, DOE ASCR Consultant, DOE-ASCR

This project will procure and operate high performance commodity computing equipment, as well as operate the QCDOC supercomputer at BNL. David Goodwin serves as the project's point of contact with ASCR. ASCR contributed to the funding of the QCDOC and has been a source of important computer expertise during the SciDAC Lattice QCD Project. In this project ASCR provides computing expertise, for example, during project and procurement reviews.

Robert Gordon, DOE BNL Site Office, DOE-BNL-SO

Dennis Wilson, DOE FNAL Site Office, DOE-FNAL-SO

Andre Bethea, DOE TJNAF Site Office, DOE-TJNAF-SO

This project operates computing systems housed at BNL, FNAL, and TJNAF, and procures major commodity computing hardware at FNAL and TJNAF. These individuals represent the DOE BNL, FNAL, and TJNAF Site Offices.

Don Holmgren, Contract Project Manager, FNAL

Dr. Holmgren is responsible for the overall project management of this project. He is responsible for the development of project planning documents, including the work breakdown structure and project milestones. He

prepares project budgets, and is responsible for all periodic reporting to the DOE (via the DOE Federal Project Manager) of project status and progress. He interacts with the US Lattice QCD Executive Committee to formulate project plans meeting the scientific objectives established by that committee.

Bakul Banerjee, Associate Contract Project Manager, FNAL

Dr. Banerjee assists Don Holmgren with the overall project management of this project. She is responsible for the maintenance of the project WBS and other project management documents. She maintains the project schedule. She assists in the preparation of project budgets. She serves as the point of contact for the project with the project site managers. She is responsible for gathering budget and performance data for periodic project status and progress reports.

Tom Schlagel, BNL Site Manager, BNL

Chip Watson, TJNAF Site Manager, TJNAF

Amitoj Singh, FNAL Site Manager, FNAL

These individuals serve as the site managers for the projects. They are responsible for the procurement, deployment, and operations of all hardware purchased by the project, as well as the high performance lattice computing hardware present at the start of the project (the QCDOC at BNL, and the various SciDAC clusters at FNAL and TJNAF). These managers allocate the project resources at their respective sites. They are responsible for site operations and user support. They assist in the preparation of project planning documents, and prepare site budgets consistent with these plans. They prepare periodic site status and progress reports. They are responsible for the deployment of software consistent with the project plan.

Robert Sugar, Chair, US LQCD Executive Committee, University of California, Santa Barbara

The US LQCD Executive Committee provides the overall scientific leadership for the project. This committee represents the US Lattice QCD community. This committee determines the membership of the Scientific Program Committee, the body responsible for allocating the resources provided by the high performance computers operated by this project to individual scientists in the US community.

Sponsor/Owner BY07

Is there a sponsor/owner for this investment? Yes

If so, identify the sponsor/process owner by name.

Robin Staffin

If so, provide the sponsor/process contact information.

Robin Staffin: Associate Director for High Energy Physics, 301-903-3624, robin.staffin@science.doe.gov

Dennis Kovar: Associate Director for Nuclear Physics, 301-903-3613, dennis.kovar@science.doe.gov

I.E ALTERNATIVE ANALYSIS BY07

Alternative Solutions BY07

Describe the alternative solutions you considered for accomplishing the agency strategic goals or for closing the performance gap that this investment was expected to address. Describe the results of the feasibility/performance/benefits analysis. Provide comparisons of the returns (financial and other) for each alternative.

Send to OMB	Alternative Name	Alternative Description
True	1	Procure the required 3.3 Tflops computational resources in FY2007, 4.5 Tflops in FY2008, and 3.2 Tflops in FY2009, minimizing costs by taking into account the special features of QCD calculations cited above. Continue to operate the machines integrated in 2006 as part of the 3-site facility (clusters at Fermilab and Jefferson Lab deployed in FY2006, SciDAC prototype clusters deployed in 2004 and 2005, and the HEP/NP QCDOC deployed in 2005). Two approaches have been identified to developing optimized hardware for QCD. One is to design compute nodes that incorporate CPU, memory and inter-node communications on a single chip with components balanced for LQCD calculations. The other is to assemble clusters entirely out of commodity parts with the specific components chosen to optimize performance for QCD. The first approach is represented by the QCD on a Chip (QCDOC), which was developed at Columbia University in partnership with IBM. The commodity clusters are being specially optimized for lattice QCD at FNAL and TJNAF under R&D funding from SciDAC. This two-track approach enables an exploitation of future technological advances, reduces risk and retains the flexibility to invest in the

		<p>hardware that will maximize the scientific output at each stage of the project. Furthermore, it ensures a robust national research effort in the face of unforeseeable circumstances in either track. The proposed objective for FY2007 is to assemble new computational resources based on clusters that sustain a total of 3.3 (average of double precision DWF and single precision improved staggered actions) teraflop/s for production calculations with an average price/performance of \$0.5 per sustained megaflop/s. Thereafter, the objective is to take advantage of the improvements in technology implied by Moore's law, as well as the specific nature of QCD calculations to deploy a series of increasingly powerful capabilities for science. Over the four-year plan for this project, hardware investments will total \$6M (FY2006-FY2009) for 13.7 TFlops. In table I.E.2 below, the Contracts entry is zero because the maintenance is included in the operations line and there is no separate maintenance contracted to the original hardware vendor as there is in Alternative 2. With a 3.5 year operating lifetime for clusters and a 10% of investment per year annual operating cost, then the operating costs would be approximately 35% of the of the total hardware costs, plus \$1.1M estimated fixed cost for integration and operation of the pre-existing machines.</p>
True	2	<p>Expand the major DOE Supercomputer Centers, National Energy Research Scientific Computing Center (NERSC, Lawrence Berkeley Lab) and the Center for Computational Sciences (CCS, Oak Ridge National Lab), to meet the needs of the QCD physics calculations. To estimate the price/performance of general use commercial supercomputers information from the most recent upgrade of the NERSC IBM SP, Seaborg, and from the Japanese Earth Simulator are used. Also, integrate the SciDAC prototype clusters and QCDOC into the operational resource (\$1.1M, all alternatives). In the winter of 2002-2003 NERSC upgraded its IBM SP, Seaborg, from 3,000 to 6,000 processors at a cost of \$30,000,000, or \$10,000 per processor. The LQCD code sustains approximately 240 megaflop/s per processor on Seaborg, which yields a price/performance of \$42 per sustained megaflop/s. Assuming Moore's law will apply, so that performance will double every 1.5 years, the price/performance for a machine of this architecture would drop to \$6 per sustained megaflop/s for 2007. The cost of the Earth Simulator has been stated to be \$350M with a peak speed of 40 teraflop/s. A group of Japanese theoretical physicists who are involved in porting QCD code to the Earth Simulator reported at the 2003 International Symposium on Lattice Field Theory that they obtained 30% of peak speed for formulations of QCD similar to domain wall, which corresponds to a price/performance of \$30 per sustained megaflop/s. The Earth Simulator became operation in March 2002. Again using Moore's law, one can estimate that a computer of this architecture will also have a price/performance of \$6 per sustained megaflop/s for FY 2007. However, the Earth Simulator was a custom machine, not a commercial offering, and is not being refreshed to track technology evolution each year, and a refreshed version is unlikely to be available at this price performance level in FY 2007. This analysis makes Alternative 2 eight times as expensive as Alternative 1. In table I.E.2 below, the Contracts entry assumes 10% per year contracted maintenance to the vendor for the vendor portion of the maintenance for 3.5 years of operating the systems. Operations costs beyond these hardware and software maintenance costs would be minimal (support of users, data management), estimated at 2% for 3.5 years (plus the \$1.1M fixed cost for integration of existing prototypes).</p>
True	3	<p>Purchase commercial supercomputers, locate them at the labs doing the experiments, and dedicate them to LQCD physics calculations. Also, integrate the SciDAC prototype clusters and QCDOC into the operational resource. Commercial supercomputers could be procured that come closest to meeting the requirements for LQCD, e.g. the architecture, I/O, memory, disk space, etc. would be optimized for LQCD. Because of the special architecture of the BlueGene/L system, it will run LQCD much more cost-effectively than typical general purpose supercomputers. The BlueGene/L pricing will be fixed for several years at which time a Moore's Law upgrade can be anticipated. The current systems are estimated to run LQCD at \$2 per megaflop/s. As indicated, this will likely be their price performance for 2007, but suppose for the sake of analysis that an aggressive processor upgrade of the BlueGene/L machine is assumed to exist in early 2007 which has 2.5 times the price/performance (2 years of Moore's Law gain). Thus, in 2007 such a machine might yield \$0.8/Mflops (1.6 times as expensive as clusters). In FY2006 and FY2008 it would be 4 times as expensive as clusters. On average, hardware costs would be approximately twice as expensive as the Alternative 1 approach. This result makes Alternative 3 almost twice as expensive as Alternative 1 for 2007. Note, in table</p>

		I.E.2 below, the Contracts entry is assumed to be 6%/year for the second generation BlueGene/L based on market data in 2005. Operations costs beyond these hardware and software maintenance costs would be minimal (support of users, data management), estimated at 2% for 3.5 years (plus the \$1.1M fixed cost for integration of existing prototypes).
False	4	Operate the existing systems only. This option is included only for completeness, and would not be capable of providing the necessary computational capacity to achieve the scientific goals of this project. The cost of this alternative is \$1.3M to operate the existing facilities as a coherent resource.

Discuss the market research that was conducted to identify innovative solutions for this investment (e.g., used an RFI to obtain four different solutions to evaluate, held open meetings with contractors to discuss investment scope, etc.). Also describe what data was used to make estimates such as, past or current contract prices for similar work, contractor provided estimates from RFIs or meetings, general market publications, etc.

As part of the LQCD SciDAC investment, staff at FNAL and TJNAF have been evaluating relevant commercial technology for cluster based solutions. Surveys of recent and emerging technologies (such as the BlueGene/L) are done at the annual SuperComputing conference (and similar venues), and as information appears in the press and online, and vendors of relevant technology are asked to provide non-disclosure information on near term technology releases. Latest generation technology which is judged to be suitable for LQCD is next evaluated for key performance metrics, and the strongest components are then acquired in a competitive bid process, and integrated into prototype clusters for evaluation under production scenarios. These analyses are repeated each year to chose the best systems that are available at that time.

Information on supercomputing offerings is gained through the operational running experience of researchers around the world on various commercial supercomputing offerings. This performance data is accumulated and used for additional price/performance comparisons.

Custom alternatives (as in the QCDOC) are evaluated for future competitiveness through similar evaluations of commercial offerings (chip fabrication, accessible intellectual property), and through technical discussions and/or collaborations with commercial vendors to arrive at an optimal solution for available technology.

Life Cycle Cost Analysis BY07

Summarize the results of your life-cycle cost analysis performed for each investment and the underlying assumptions.

Element	Alternative 1	Alternative 2	Alternative 3
Government FTE	250	250	250
Hardware/Software	6000	54000	12000
Contracts	0	18900	2500
Other (Facilities, Printing, Maintenance)	3200	2200	2000
Total	\$9,450.000	\$75,350.000	\$16,750.000

Alternative Selected BY07

Which alternative was selected and why was it selected?

Alternative 1 was selected because it meets the scientific goals in the most cost effective manner. Compared to Alternatives 2 and 3, 1 is significantly less expensive because the systems in this alternative are specially architected to optimally perform LQCD calculations. Alternative 1 (Planned Solution) is chosen because it optimizes performance, cost and coupling to the user communities.

Three criteria are used for choosing the best alternative:

1. Achievement of the performance goals of the project
2. Lowest cost
3. Most effective collaboration between the experimental and theoretical collaborators and the systems developers

Each of the first three alternatives are scoped to achieve the scientific goals. The fourth alternative is included only for completeness, and does not meet the goals of the project. Based upon criteria 1, alternative 1, 2, or 3 is preferred.

The three alternatives have very different costs as the performance of any given supercomputer varies dramatically depending on application. Consequently the actual application is used to verify the performance. The performance depends almost exclusively on the floating point performance for the project's specific LQCD applications, measured in terms of \$ per sustained megaflop/s (dollars per sustained million floating point operations per second). Note, sustained refers to the value actually delivered to the application, not the

theoretical peak performance of a given processor.

Staffing needs will be approximately the same for commercial machines as for the proposed system assembled from commercial components. Maintenance contracts for commercial supercomputers typically run to 10% of the initial cost of the hardware per year. The favored plan would stock spare parts, which would be less expensive, and would minimize downtime. The maintenance costs are included in the contract line in the table above for the commercial supercomputer solutions (Alternatives 2) and they are included in the hardware line for Alternative 1 where components are commercially procured and for Alternative 2 where IBM is including maintenance in the base offering.

The price/performance during this period can be estimated with minimal risk based on the research and development effort carried out under the LQCD SciDAC grant and NP and HEP R&D funds. Two formulations of QCD on the lattice are considered that are expected to dominate the research over the next five years, the improved staggered action (ASQ), and the domain wall action (DW). As discussed in section I.A.1, they run at different megaflop/s rates on the same hardware because they have different ratios of floating point operations to data movements. Typically, the megaflop/s rate for the ASQ action is 70% of that for the DW action, so that percentage is used when benchmarks with both actions are not available.

Alternatives 1 and 3 would locate scientific computational facilities at laboratories where the experiments are taking place. This means that the theoretical and experimental users most interested in the performance of the systems and the results would have the maximum assurance that the computational results are closely linked to the experimental results and planning. While modern networking and collaboration tools will be used to integrate the systems at the several labs with the largely university based community, close physical proximity of the computational hardware, the systems developers, the experimentalists and theorists has been observed by the community to enhance the focus on total performance. Based on criteria 1, Alternative 1 or 3 is preferred.

Summary: Alternative 1 is the most cost effective way of meeting the scientific objectives, and the most effective solution for community collaboration.

Quantitative Benefits BY07

Will any quantitative benefits be achieved through this investment (e.g., systems savings, cost avoidance, stakeholder benefits, etc)? Define the Return on Investment (ROI).

This investment will provide quantitative benefits by directly impacting the HEP and NP experimental physics programs. As indicated in section I.A.1, 60% of the \$750M HEP program and 50% of the \$400M NP program for a total of \$850M are impacted by these LQCD calculations.

There are three significant ways in which this project will yield a return on investment: (1) reduced running time for given science goals, (2) improved selection of experiments, (3) new discoveries.

The scientific output of roughly 10% of these experiments is influenced by the accuracy of the theoretical numbers which go into the analysis of the experimental results. The proposed computing capabilities (including those coming online in FY2005, and those being added in FY2006) will improve the accuracy of these numbers by anywhere from 10% to a factor of 1.5, depending upon the number. These improvements will then improve the accuracy of the experimental results by an amount roughly equivalent to increasing the running time of the experiments by 5% (experiment dependent). In other words, this investment increases the output of the \$850M investment by 5% of 10%, or 0.5%, a \$4.2M ROI. Half of this benefit will be realized in the first year of the investment (FY2006) due to QCDOC and cluster calculations which will begin in late FY05. The remainder will be delayed in time by about 1.5 years from investment start (the time needed for sufficient computational statistics to be accrued to improve data analysis). The full benefit will be realized beginning in FY 2007 and will continue for the life of the project, and for an additional year and a half beyond, albeit at a reduced rate as less new capacity is procured in the final year of the project, and since machines will be de-commissioned.

One of the LQCD investment impacts comes from the process used to select the experiments in the HEP and NP experimental programs. In this process individual experiments are proposed to Program Advisory Committees for inclusion in the program. One of the key criteria for an experiment to be approved is that it has an adequate theoretical foundation. Proposed experiments that have justifications based on a solid theoretical analysis have a significantly better chance of being approved. As a result of expanding possible theoretical analysis to include the LQCD calculations from this investment, better experiments will be performed, optimizing the scientific output of investments made in the experimental programs. Potential savings are expected to accrue from scientific discoveries, which influence the design or selection of future major facilities, thereby potentially significantly enhancing the scientific output of very large investments.

Net Present Value BY07

For alternative selected, provide financial summary, including Net Present Value by Year and Payback Period Calculations:

The table below shows the net present value by year for the alternative chosen. The payback period for the investment is less than two years starting in FY2006. A risk adjusted net present value analysis is also presented.

The risk analysis in Section I.F states that the risks to this project are all low. The project is also fixed cost; the most likely risk is a failure to achieve the desired performance. In the worst case anticipated the benefit would decrease by 10% each year of the project resulting in the data in the second part of the table. (That is, the computing capacity delivered will fall short by 10%, or the physics impact will fall short by 10% compared with the analysis given above). The net present value of the investment will decrease to \$3.025M in the worst case but the payback period will still be shorter than two years.

Description	FY1	FY2	FY3	FY4	FY5	FY6	FY7	FY8	FY9
Investment	2500	2500	2500	1700	9200	0	0	0	0
Investment Present Value (4.5% DR)	2500	2392	2289	1490	8691	0	0	0	0
Risk Adjusted Cost Avoidance/Benefit	1800	3600	3600	3600	12600	0	0	0	0
Risk Adjusted Cost Avoidance Present Value (4.5% DR)	1800	3445	3297	3155	11696	0	0	0	0
Risk Adjusted Net Present Value	-700	1053	1007	1665	3025	0	0	0	0

Cost Benefit Analysis BY07

What is the date of your cost benefit analysis? 5/20/2005

I.F RISK INVENTORY AND ASSESSMENT BY07

Risk Assessment Results BY07

Risk Assessment Results

Date Identified	Area of Risk	Description	Probability of Occurrence	Strategy for Mitigation	Current Status as of the date of this exhibit
7/1/2004	1 - Schedule	The schedule for achieving investment milestones might slip for the following reasons: a) Vendors may take longer than anticipated to bring new cpu's, memory systems, and/or interconnect systems to market. b) It may take longer than expected to bring new systems on line for production use. c) Funding may be lower than anticipated.	Basic	An ongoing research and development program is currently in its third year and is expected to continue as the LQCD investment begins in FY 2006. It will continue throughout the lifetime of the project. Experienced professional staff are following the commodity market carefully, and gaining insight by building prototype hardware of increasing size and capability. Project members frequently meet with vendors under non-disclosure agreement and are briefed on roadmaps for components such as processors, chipsets, motherboards, network interface cards and switches. In addition, working closely with manufacturers and system integrators has allowed testing of prerelease components. This has	In place. Annual reviews will be completed by June 30 of each year of the investment to validate planned modifications to the project baseline in response to schedule slips due to the various factors listed. This milestone for BY07 will be complete by June 30, 2006. The DOE held a cost and schedule review for CY06 on May 24-25, 2005; the reviewers supported and recommended the project's strategy and schedule.

				both allowed the manufacturers to be informed of deficiencies in their products, and the LQCD investment team to determine whether some new capability will actually provide any advantage in future systems. As with any investment, a successful implementation of the schedule assumes the approved Budget Authority profile.	
7/1/2004	2 - Initial Costs	Although cost projections for current budget year appear to be reasonably reliable, projections for subsequent years become progressively uncertain.	Basic	Market information will be gathered and prototypes built throughout the lifetime of the project. Open procurements of commodity components will provide competitive prices. All hardware is modular in nature, so if prices exceed expectations in any given year, it is possible to deploy smaller machines.	In place. In each year of the investment we will review the cost and performance projections for the next year and will present an acquisition plan to a review panel for that coming year's purchases. In FY05, such a review for CY06 was held on May 24-25, 2005. The next review is milestone #1 in our BY07 baseline, to be completed 6/30/2006.
7/1/2004	3 - Life-Cycle Costs	Unexpected increases in life-cycle costs arise after systems are acquired.	Basic	Hardware maintenance costs are included in procurement of components for each new system procured (each year). Operations costs are well understood based on years of similar operational experience.	In place. The DOE held a cost and schedule review of the project on May 24-25, 2005, and found that the cost projections for the hardware were reasonable. Operations costs will be monitored and reported quarterly; the investment begins Oct 1 2005 and the first quarterly report will cover Oct 1 – Dec 31 2005.
7/1/2004	4 - Technical Obsolescence	Systems are held too long and become ineffective, increasing cost and using facility space.	Basic	The approach taken is that clusters will be replaced every three and a half years, consistent with historical life cycles. Some components, such as cluster	In place. In December 2005, a 128-node SciDAC cluster which will have reached three years of operation will be retired at Fermilab to free

				interconnects, have longer lifetimes, and will be reused. This strategy is already in operation for the prototype clusters and will continue throughout the project.	facility space. By 6/30/2006 we will determine which of the other existing lattice QCD SciDAC clusters operated by this investment will remain in operation for the next 12 months.
7/1/2004	5 - Feasibility	The performance of hardware components may not improve or its price may not drop as rapidly as anticipated.	Basic	This risk is low for current budget year, but increases in succeeding years. The strategy is to follow the market carefully, and build prototypes before developing large production machines. The two track approach further reduces risk. Components of clusters are carefully selected for cost effectiveness. Thus, if the network performance does not improve as expected, money can be saved on nodes by selecting slower, more cost effective CPUs whose speed will not be wasted because the network limits overall performance. This savings on each node will enable purchasing a larger number of nodes. Performance goals are set more conservatively for the later years in the project to account for market evolution uncertainty.	In place. In May 2005, Fermilab brought online an Infiniband based cluster whose price /performance was better than planned in this document. The performance milestones in the baseline as well as the technical goals were modified accordingly.
7/1/2004	6 - Reliability of Systems	Complex multi-processor systems fail more frequently as they grow in size.	Basic	Clusters of size 500-1000 processors are planned. Experience gained during the SciDAC Lattice Gauge Computing Project with machines of 128 to 256 processors indicates that proposed machines of this size will run reliably.	In place. By November 2005, Fermilab will have completed purchase and integration of a 520 node Infiniband cluster. Operational experience with this cluster will confirm that the 1000-processor cluster planned for Spring 2006 will be reliable.
7/1/2004	7 - Dependencies and	Host institutions will provide space, power, network	Basic	The required space is available. Only a small fraction of the	In place. At the DOE May24-25 2005 project

	Interoperability Between This and Other Investments	connectivity, and mass storage.		Internet bandwidth and mass storage of the laboratories will be used. The experiments that are the main users of these facilities are a high priority for the laboratories, and the computer space, and network and mass storage resources will continue to evolve to support these experiments in a way that will also meet the needs of this investment.	review, the space and power requirements and plans were presented. The reviewers approved of these plans.
7/1/2004	8 - Surety (Asset Protection) Considerations	Natural disaster and/or major electrical failure	Basic	The planned host institutions (BNL, FNAL and TJNAF) will write a continuity of operations plan.	To be completed 10/1/2005
7/1/2004	9 - Risk of Creating a Monopoly For Future Procurements	The lattice QCD community becomes such a large purchaser of components that it effects the market for them.	Basic	Given the small size of this effort compared to the commodity market, this is a very low risk. No mitigation would appear to be necessary.	In place. To be reviewed annually by June 30 of each fiscal year.
7/1/2004	10 - Capability of Agency to Manage the Investment	Agency personnel changes limiting continuity and support.	Basic	DOE staff has knowledge of the investment, and have been providing support for over five years. As the investment spans multiple programs, this expertise is not limited to a single individual, and so the impact of a single change is minimal. The existence of an Integrated Project Team, whose composition is about half federal, will also mitigate risks due to agency personnel changes. A rigorous review process will be established to mitigate risks, including monthly and quarterly reports and annual reviews.	In place. Quarterly project reports will begin at the start of the investment, Oct 1 2005. Annual reviews will be completed by June 30 of each year of the investment.
7/1/2004	11 - Overall Risk of Investment Failure	A major system simply fails to work.	Basic	Continue to install prototype machines before installing production ones (annually). Build appropriate	Ongoing (since new systems are purchased and brought online during each year of the investment).

				acceptance criteria into major purchases.	Plans for each year of the investment will be altered according to the results of prototyping and operational experience; annual reviews will be completed by June 30 of each year of the investment.
7/1/2004	12 - Organizational and Change Management	Changes in technology and staff can have adverse effects on the project.	Basic	Continue to study and understand changes in technology that impact the investment (ongoing, each year). Maintain broad expertise within the staff working on the investment.	In place. In August 2005 plans for systems to be built in the first year of the investment were revised to ensure that Infiniband expertise at FNAL was passed on to TJNAF staff. The project will perform integrated procurements across the three labs, ensuring distribution of expertise among the three sites. This approach was presented at the DOE's May 24-25 project reviews and was endorsed by the review committee.
7/1/2004	13 - Business	Changes in funding, due to alteration in administration policy, or legislative directives.	Basic	The investment will allocate resources and build new computing capabilities on a yearly basis, so it will be possible to adjust to changing funding levels. This is particularly so because the systems are modular, so reductions in funding can be adjusted for by reducing the size of the systems. Such reductions will delay reaching computational and scientific milestones.	In place. The project will adjust procurements and allocations annually according to available resources. These adjustments will be one of the subjects of the annual project reviews that will be completed by June 30 of each year.
7/1/2004	14 - Data/Info	Loss of stored data.	Basic	Important data sets will be backed up to tape. Essential output is stored at multiple sites.	In place. In FY05 the project established procedures for users to move files between the three sites, and implemented mass

					storage areas at FNAL and TJNAF. Data storage and replication will be monitored as part of monthly and quarterly project reports.
7/1/2004	15 - Technology	Technology does not fulfill expectations.	Basic	Test individual components, build prototypes, and perform acceptance tests.	Ongoing (since new systems are built in each year of the investment). Prototype clusters were built at FNAL and TJNAF in 2005; the results of this prototype work drove the formation of plans for procurements in the first year of the investment (FY06). Further prototyping will be done in Fall and early Winter 2005 to refine the components to be purchased in the Spring FY06 procurement. BY07 plans, including projected performance of cost of the available technology, will be reviewed by June 30 2006.
7/1/2004	16 - Strategic	Changes in the mission and plans of the Office of Science	Basic	LQCD systems will have a broad range of applicability in other areas of science.	Completed
7/1/2004	17 - Security	Inappropriate use by unauthorized personnel	Basic	Strong authentication is required for access to the system. Computer resources are on private networks behind secure systems. The project will coordinate security with the host laboratories. Usage is carefully monitored and controlled by batch systems. Performance is also carefully monitored, so any unauthorized usage would be very quickly noticed and terminated. On clusters, batch systems	In place. System specific security plans for each of the three sites will be completed by Oct 1, 2005.

				automatically terminate user processes at the end of each job and before each new job starts up. Thus, any unauthorized process would be terminated.	
7/1/2004	18 - Privacy	Unauthorized access can disclose private information	Basic	No classified information, sensitive data, or personally identifiable information are stored on the systems.	Completed.
7/1/2004	19 - Project Resources	Resources insufficient to meet the needs of the entire community	Basic	Availability of funding will impact schedule milestones and delay achievement of computing capabilities, putting U.S. leadership in QCD computation at risk and decreasing scientific productivity.	Ongoing risk throughout the project lifecycle. Project plans will be adjusted according to available funding resources; BY07 plans will be formally reviewed by June 30, 2006.
6/1/2005	14 – Data/Info	Slow internet data transfer rates between the three labs inhibits productivity	Basic	FNAL, BNL, and TJNAF network staff will tune parameters to optimize transfers. Scientific allocations of time on the LQCD clusters will take into account the quantity of data which must be transferred between sites; if network performance would limit productivity, allocations will be made such that analysis jobs would run at the same site as data are stored (i.e., to minimize transfers).	In place. Transfer rates and their impact on data movement will be monitored as part of monthly and quarterly project reports.
6/1/2005	14 – Data/Info	Differing authentication schemes among the three labs makes data transfers difficult and limits productivity	Basic	BNL and TJNAF use ssh firewalls to secure LQCD systems, whereas FNAL uses Kerberos authentication. The SciDAC Lattice Gauge Computing project will be asked to design, implement, and maintain scripts and other tools to assist users.	In place and on-going (security policies have and continue to evolve which will inevitably result in software and configuration changes at the three laboratories). Status as of Aug 2005: tools are in place and tested which allow facile movement of data by users while continuing to fulfill the computer security

					requirements (strong authentication) at each lab. The SciDAC Lattice Gauge Computing project's Software Committee will monitor and report on this issue at each collaboration meeting; the next meeting will be in February 2006.
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Risk Management Plan BY07

What is the date of your risk management plan?	5/1/2005
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I.G ACQUISITION STRATEGY BY07

Contracts BY07

Will you use a single contract or several contracts to accomplish this project?	Several
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What is the type of contract/task order if a single contract is used?

The LQCD effort will be executed by the three existing Managing and Operating (M&O) contractors for TJNAF, BNL and FNAL. The M&O contractors will use subcontracts for the system procurements.

This will not be a single contract.

If multiple contract/task orders will be used, discuss the type, how they relate to each other to reach the project outcomes, and how much each contributes to the achievement of the investment cost, schedule and performance goals. Also discuss the contract/task order solicitation or contract provisions that allow the contractor to provide innovative, transformational solutions.

The Managing and Operating (M&O) contractors for the three labs will be responsible for accomplishing the LQCD effort under the terms of its performance based contract with the Department of Energy. Procurement of components will be accomplished by fixed-price subcontracts awarded on the basis of competitive bidding. Procurements will occur at one or more labs in each year, coordinated by the Project Office according to the acquisition plan. Inspection, coordination, tie-ins, testing and checkout witnessing, and acceptance will be performed by the Laboratory M&O contractors. The DOE federal program manager will work closely with the Integrated Project Team and Laboratories' Federal Site Offices to monitor progress.

The vendors who will bid on the fixed-price subcontracts of this investment have the latitude to propose alternative components. For example, the Requests for Proposals for the COTS computers used in this investment will specify suggested processors, chipsets, motherboards, and networks; however, these RFP's will also specify that the vendors may propose other components which will give equivalent or superior price/performance. Further, both the laboratories involved in this investment (BNL, FNAL, TJNAF) and the various vendors involved in bidding on contracts are in frequent contact with the principal manufacturers of LQCD system components (for example, Intel, AMD, Mellanox, Myricom). Historically, based on the on-going R&D program for LQCD systems since 2000 (the DOE SciDAC Lattice Gauge Computing Project), these manufacturers and vendors have proactively suggested components and technologies that will optimize price/performance for the computer codes that are used on these types of systems. Thus, the vendors and manufacturers involved in this investment have many opportunities to provide innovative, transformational solutions.

The Offices of Nuclear Physics and High Energy Physics held a panel review on May 24-25, 2005 to assess the proposed management plan, scientific technical approach and subsequent cost and schedule of the investment. In the written report, the panel commented that the "computing resource acquisition plan will meet the overall project scientific objectives, within the budget limitations."

Progress reviews with a panel of experts will be held on an annual basis to monitor progress and to validate the acquisition plan for the next fiscal year. Quarterly progress reports will be submitted to the headquarters office to monitor progress.

For other than firm-fixed price, performance-based contracts, define the risk not sufficiently mitigated in the risk mitigation plan, for that contract/task order, that requires the Government to assume the risk of contract achievement of cost, schedule and performance goals. Explain the amount of risk the government will assume.

The contracts used at the three labs during the investment to procure computing systems will be firm-fixed price contracts.

Competition / Incentives BY07

Will you use financial incentives to motivate contractor performance (e.g. incentive fee, award fee)?

The Office of Science (SC) annually reviews its laboratories' performance under a performance-based management approach that uses negotiated performance plans, laboratory self-assessments, DOE review and validation, and performance fee/incentives. Based on SC guidance, each of the SC laboratory performance plans must have a section on the science and technology (S&T) performance of the laboratory. In addition, this section must be weighted at 50% or more in determining the overall rating and score for the laboratory. Under the S&T portion of the plan, the Department evaluates the DOE funded program activities conducted by the laboratory and provides an overall rating and score for the laboratory's performance in this area. The Department also evaluates and provides ratings and scores for the business/operational functions performed by the laboratory (e.g., ES&H, financial management, procurement). Based on the fee arrangement negotiated for the laboratory, DOE calculates the fee award based on the performance scores and ratings provided by the Department for the S&T and business/operational performance of laboratory.

Discuss the competition process used for each contract/task order, including the use of RFP's, schedules or other multiple agency contracts, etc?

Based on annual reviews, and discussions with the LQCD management and the Integrated Project Team, the Offices of Nuclear Physics and High Energy Physics will make decisions each year as to how to distribute the available funds in the most optimum manner.

The M&O contractors for BNL, TJNAF and FNAL will use subcontracts for the procurement of components such as COTS computers, networking hardware, and disk arrays. These procurements will be awarded on the basis of competitive bidding. At FNAL, procedures for such purchases are documented in the Commercial Procurements Procedure manual. To ensure adequate price competition, independently priced offers are solicited from two or more offerors for all purchases above \$2500.00. For large purchases, these solicitations take the form of RFP's. FNAL procurement terms and conditions documents, including RFP instructions to offerors (FL-15) are available at <http://www-bss.fnal.gov/procurement/index.html>. During prior acquisitions at FNAL of similar equipment for LQCD, RFP responses were received from at least 6 vendors. BNL and TJNAF have similar procurement procedures which are documented at <https://sbms.bnl.gov/SBMSearch/LD/ld02/ld02t011.htm> and <HTTP://WWW.Jlab.org/business.html>, respectively.

COTS Products BY07

Will you use commercially available COTS products for this investment? Yes

To what extent will these items be modified to meet the unique requirements of this investment?

Commercially available components will be used as appropriate. Each year, evaluations of current off the shelf offerings will be performed, and compared with the potential of achieving higher performance using a custom solution, which in turn is based upon commercially available intellectual property (IP).

For the COTS clusters acquired by this investment, the components will be procured with options specified to optimize the science for LQCD. No modifications to these COTS components will be necessary.

What prevented the use of COTS without modification?

For FY2007, un-modified COTS will be used, with options specified to meet LQCD requirements.

Acquisition Plan and Section 508 Compliance BY07

What is the date of your acquisition plan? 8/8/2005

How will you ensure Section 508 compliance?

The Contracting Officer (CO) and the Contracting Officer's Technical Representative (COTR), share responsibilities for ensuring the procured Information Technology best meets the Section 508 standard while satisfying the technical and functional requirements.

The CO and COTRs ensure that statements of work include Section 508 technical standards and ensure that all information technology acquisitions provide the greatest possible degree of Section 508 compliance while satisfying other functional requirements. The Project Manager ensures that procured information systems comply with Section 508 technical standards (36 CFR 1194.21 - 1194.26) and is ultimately responsible for Section 508 compliance of the total information technology solution.

***** The following text supplements the acquisition plan date:

The Offices of Nuclear Physics and High Energy Physics held a panel review on May 24-25, 2005 to assess the proposed management plan, acquisition plan, scientific technical approach and subsequent cost and schedule of the investment. In the written report, the panel commented that the "computing resource acquisition plan will meet the overall project scientific objectives, within the budget limitations." Modifications to the acquisition plan were made as a result of some of the findings and recommendations of the review committee; the revised plan was presented to the Federal Project Manager and the chairman of the May 24-25 review at a meeting on August

8, 2005. The revisions were approved.

Acquisition Costs BY07

For budget year, what percentage of the total investment is for hardware acquisition?	72
For budget year, what percentage of the total investment is for software acquisition?	0
For budget year, what percentage of the total investment is for services acquisition?	28

I.H. PROJECT (INVESTMENT) AND FUNDING PLAN BY07

Performance-Based Management System (PBMS) BY07

Is this project an existing baseline?	No
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Explain the methodology used by the agency to analyze and use the earned value performance data to manage performance. Describe the process you will use or used to verify that the contractor's project management system follows the ANSI/EIA Standard 748-A. If the investment is operational (steady state), define the operational analysis system that will be used. If this is a mixed life cycle investment with both operational and development/modernization/enhancement (DME) system improvement aspects, EVMS must be used on the system improvement aspects of the investment and operational analysis on the operations aspects. Using information consistent with the work breakdown structure (WBS), provide the information requested in all parts of this section.

Don Holmgren from FNAL has been selected as the Contract Project Manager for this endeavor. Members of the Integrated Project Team, led by the Contract Project Manager, will implement a PBMS to manage the project. Each site, FNAL, BNL and TJNAF, will have a Site Manager dedicated to this project. The Contract Project Manager will be assisted by Bakul Banerjee, Associate Contract Project Manager. The Contract Project Manager will coordinate all project management activities with the Site Managers and be responsible for reporting status to DOE. The investment scope, schedule performance, and cost will be evaluated at pre-established intervals (no less than quarterly) using the industry-standard project management tools currently in place at FNAL. The Project Manager will identify, monitor, and assess accomplishments or deviations from baseline goals. The Integrated Project Team, led by the project manager, will periodically review, assess, update and improve the project management plan to ensure that all key milestones and project cost estimates have been adequately adjusted for risk. In addition, operational analysis will be utilized to ensure that the investment is performing within baseline cost, schedule and performance goals. The Contract Project Manager, Associate Contract Project Manager and key site managers each have more than 7 years experience in large scale IT project management.

The PBMS for the investment will be designed according to the guidance from the DOE M 413.3 and Project Management Institute (PMI) Guide to the Project Management Body of Knowledge (PMBOK). Overall performance at all three laboratories, namely, FNAL, BNL and TJNAF, is managed under the terms of the performance-based management contract with the DOE to implement PBMS, which specifies the development of an annual Performance Evaluation Plan that includes performance expectations for business operations. Under the terms of the contract, laboratories are expected to integrate contract work scope, budget, and schedule to achieve realistic, executable performance plans. Following existing processes at FNAL, BNL and TJNAF, a set of key performance measures, both financial and operational, will be established. Methods of collecting and analyzing data measured will be established and the data will be used to improve performance and reduce risks. Additionally, annual self-assessments will be used at the investment level to assess and evaluate results and to improve performance. The Contract Project Manager will work with BNL and TJNAF financial and technical contacts to obtain necessary data from those sites.

A detailed WBS, including WBS dictionary, will be developed for the work to be done for the investment using MS Project with basis of estimates derived from past purchase records and effort reports. Laboratories will prepare Memoranda of Understanding (MOU) along with the Statement of Work. After the WBS is defined to certain degree of certainty, it will be baselined and monthly status reporting process against the baseline will be initiated. Budgeted cost and % Completed will be tracked through MS Project. FNAL uses Oracle based Project Accounting system to capture actual costs for WBS items at certain predetermined level. Data on the Actual Cost of Work Performed will be calculated from this system. Similar data will be collected from other laboratories and consolidated. This data will be used to create cost and schedule performance reports as well as necessary change requests and exception reports. FNAL has deployed various software tools, such as WelcomCobra, appropriate for comprehensive Performance Based Management Systems. This investment project will utilize these tools as deemed necessary. The budget planning and resource allocation process will be based on the financial management systems of the respective laboratories that are based on DOE's general guidance. Details of fund management for the investment that includes both DOE's High Energy Physics and Nuclear Physics organizations will be established. The information pertinent to the investment will be detailed in the MOUs.

I.H.2 Original baseline BY07

Identify the phase or segment/module that corresponds to the data in the I.H.2 table.	Proposed
<p>What are the cost and schedule goals for this phase or segment/module of the project e.g. what are the major project milestones or events; when will each occur; and what is the estimated cost to accomplish each one? Also identify the funding agency for each milestone or event if this is a multi-agency project. If this is a multi-agency project or one of the Presidents E-Gov initiatives, use the detailed project plan with milestones on the critical path, to identify agency funding for each module or milestone. This baseline must be included in all subsequent reports, even when there are OMB approved baseline changes shown in I.H.3.</p>	

Description	Planned					
	Schedule		Duration		Plan Cost	Funding Agency
	Start Date	End Date	Days	Hours		
1 Procurement and deployment of 1.8 teraflops (sustained) system at either FNAL or TJNAF	10/01/2005	03/30/2006	181	0.00	\$1,000.000	DOE
2 7 Teraflops-years computing delivered	10/01/2005	09/30/2006	365	0.00	\$1,000.000	DOE
3 Procurement and deployment of 2.2 teraflops (sustained) system at either FNAL or TJNAF	10/01/2006	03/30/2007	181	0.00	\$900.000	DOE
4 Additional 9 Teraflops-years computing delivered	10/01/2006	09/30/2007	364	0.00	\$1,100.000	DOE
5 Procurement and deployment of 3 teraflops (sustained) system at either FNAL or TJNAF	10/01/2007	03/30/2008	182	0.00	\$800.000	DOE
6 Additional 12 Teraflops-years computing delivered	10/01/2007	09/30/2008	365	0.00	\$1,200.000	DOE
7 Procurement and deployment of 4.5 teraflops (sustained) system at BNL, FNAL or Thomas Jefferson Lab	10/01/2008	09/30/2009	365	0.00	\$800.000	DOE
8 Additional 15 Teraflops-years computing delivered	10/01/2008	09/30/2009	364	0.00	\$1,200.000	DOE
9 Additional 12 Teraflops-years computing delivered	10/01/2009	09/30/2010	364	0.00	\$1,200.000	DOE
Project Totals	10/01/2005	09/30/2010	1826	0.00	\$9,200.000	

I.H.3 Proposed/Current Baseline BY07

Identify the phase or segment/module that corresponds to the data in the I.H.3 table.	
Indicate whether table I.H.3 represents the Proposed or Current (OMB Approved) baseline for this Phase/Segment/Module of the Project.	Current (OMB-Approved)
Cost and Schedule Goals: Proposed or Current (OMB Approved) Baseline for a Phase/Segment/Module of Project	

Description	Planned					
	Schedule		Duration		Plan Cost	Funding Agency
	Start Date	End Date	Days	Hours		
1. FY07 computer architecture planning complete and reviewed	01/01/2006	06/30/2006	181	0.00	\$23,000	DOE
2. Procurement and deployment of systems totaling 2.0 teraflops (sustained)	01/01/2006	09/30/2006	273	0.00	\$1,850,000	DOE
3. 6 Teraflops-years computing delivered	10/01/2005	09/30/2006	365	0.00	\$627,000	DOE

4. FY08 computer architecture planning complete and reviewed	01/01/2007	06/30/2007	181	0.00	\$24,000	DOE
5. Procurement and deployment of systems totaling 3.1 teraflops (sustained)	01/01/2007	06/30/2007	181	0.00	\$1,694,000	DOE
6. Additional 9 Teraflops-years computing delivered	10/01/2006	09/30/2007	365	0.00	\$782,000	DOE
7. FY09 computer architecture planning complete and reviewed	01/01/2008	06/30/2008	182	0.00	\$25,000	DOE
8. Procurement and deployment of systems totaling 4.2 teraflops (sustained)	01/01/2008	06/30/2008	182	0.00	\$1,598,000	DOE
9. Additional 12 Teraflops-years computing delivered	10/01/2007	09/30/2008	366	0.00	\$877,000	DOE
10. Procurement and deployment of systems totaling 3.0 teraflops (sustained)	01/01/2009	06/30/2009	181	0.00	\$798,000	DOE
11. Additional 15 Teraflops-years computing delivered	10/01/2008	09/30/2009	365	0.00	\$902,000	DOE
Project Totals	10/01/2005	09/30/2009	1461	0.00	\$9,200,000	

I.H.4 OMB Approved Baseline and Actuals BY07

Identify the phase or segment/module that corresponds to the data in the I.H.4 table.

Comparison of OMB-Approved Baseline and Actual Outcome for Phase/Segment/Module of a Project (Investment)

Description	Planned					Actual				
	Schedule		Duration		Plan Cost	Funding Agency	Schedule		% Complete	Actual Cost
	Start Date	End Date	Days	Hours			Start Date	End Date		
Project Totals					\$0.000					\$0.000

Project Summary (EVMS) BY07

Provide a performance curve graph plotting BCWS, BCWP and ACWP on a monthly basis from inception of this phase or segment/module through the latest report. In addition, plot the ACWP curve to the estimated cost at completion (EAC) value, and provide the following EVMS variance analysis

Project (Investment) Summary Cumulative

Provide the following investment summary information from your EVMS software as of:

12/23/2004

Show the budgeted (planned) cost of work scheduled (BCWS):

Show budgeted (planned) cost of work performed (BCWP):

Show the actual cost of work performed (ACWP):

Cost Variance (CV) = (BCWP-ACWP):

Cost Variance Percent (CV%) = ((CV/BCWP) x 100%):

Cost Performance Index (CPI) = (BCWP/ACWP):

Schedule Variance (SV) = (BCWP-BCWS):

Schedule Variance Percent (SV%) = ((SV/BCWS) x 100%):

Schedule Performance Index (SPI) = (BCWP/BCWS):

Budget at Completion (BAC):

Performance Factor 1 (1/CPI)

Estimate at Completion (EAC) = (((BAC-BCWP)/(CPI)) +

ACWP):

Variance at Completion (VAC) = (BAC - EAC):

Variance at Completion Percent (VAC%) = ((VAC/BAC)*100%)

:

Estimated Cost to Complete (ETC):

Performance Factor 2 (1/CPI *SPI)	
Estimate at Completion 2 (EAC2) = (((BAC-BCWP)/(CPI *SPI))	
+ ACWP):	
Variance at Completion 2 (VAC2) = (BAC - EAC2):	
Variance at Completion Percent 2 (VAC%2) = ((VAC2/BAC)x	
100%):	
Estimated Cost to Complete 2 (ETC2):	
Expected Completion Date:	
Cost/Schedule Variance BY07	
If cost and/or schedule variance are a negative 10 percent or more at the time of this report or EAC is projected to be 10 percent or more, explain the reason(s) for the variance(s).	
Performance Variance BY07	
Provide performance variance. Explain based on work accomplished to date, whether or not you still expect to achieve your performance goals. If not, explain the reasons for the variance. For steady state projects, in addition to a discussion on whether or not the system is meeting the program objectives, discuss whether the needs of the owners and users are still being met.	
Estimates at Completion BY07	
For investments using EVMS, discuss the contractor, government, and at least the two EAC index formulas in I.H.4.B, current estimates at completion. Explain the differences and the IPT's selected EAC for budgeting purposes. This paragraph is not applicable to operations/steady state investments.	
Corrective Actions / Continuance BY07	
Discuss the corrective actions that will be taken to correct the variances, the risk associated with the actions, and how close the planned actions will bring the investment to the original baseline. Define proposed baseline changes, if necessary.	
If the investment cost, schedule or performance variances are 10% or greater, has the Agency Head concurred in the need to continue the program at the new baseline?	
ENTERPRISE ARCHITECTURE: BUSINESS BY07	
Agency Enterprise Architecture BY07	
Is this investment identified in your agency's enterprise architecture? If not, why?	
No, this is a new investment and so is not yet specifically listed in the DOE Enterprise Architecture. However, this investment is one of a class of systems covered in section 6.5.1, High Performance Computing for the Office of Science. It would complement those systems by providing more cost effective platforms for Lattice QCD.	
Will this investment be consistent with your agency's target architecture?	
Yes, this project will be consistent with DOE's "to be" modernization blueprint.	
Was this investment approved through the EA Review committee at your agency?	Yes
Major Process Modifications BY07	
What are the major process simplification/reengineering/design projects that are required as part of this IT investment?	
This investment supports leading edge science and process simplification/reengineering will be driven by the science and not by the project.	
Restructuring, Training, Change Management BY07	
What are the major organization restructuring, training, and change management projects that are required?	
The three host laboratories (BNL, FNAL, TJNAF) have in place training and change management processes appropriate to support this project, and no restructuring will be necessary as a result of this project.	

FEA BRM BY07

FEA BRM

BRM FEA Code	Line Of Business	BRM FEA Code	Sub Function	Primary Mapping to BRM	Send To OMB
202	Knowledge Creation and Management	202069	Research and Development	False	True
404	Information and Technology Management	404139	IT Infrastructure Maintenance	False	True
404	Information and Technology Management	404138	System Maintenance	False	True
109	General Science and Innovation	109026	Scientific and Technological Research and Innovation	True	True

BRM Mode of Delivery

202069

ENTERPRISE ARCHITECTURE: DATA BY07**Data Types BY07**

What types of data will be used in this investment? Examples of data types are health data, geospatial data, natural resource data, etc.

Physics data. Approximately half of the computing resources procured and deployed under this project will be used to generate lattice vacuum configurations using one or more formulations of Quantum Chromodynamics (QCD). These data sets (simulation data) are then used in an analysis phase to measure (again, a simulation) properties of quarks and gluons embedded in the sea of vacuum quarks and anti-quarks. The analyses, collectively, will use the remaining computing resources. In addition to the simulation data, additional data will be generated to track these simulations (data provenance).

Access to Existing Data BY07

Does the data needed for this investment already exist at the Federal, State, or Local level? If so, what are your plans to gain access to that data?

No. The data is generated as part of the physics theory simulation.

Are there legal reasons why this data cannot be transferred?

There are no legal reasons or restrictions on transferring this data.

Federal Geographic Data Committee Compliance BY07

If this initiative processes spatial data, identify planned investments for spatial data and demonstrate how the agency ensures compliance with the Federal Geographic Data Committee standards required by OMB Circular A-16.

This initiative does not process spatial data.

Information Quality and Management BY07

If this activity involves the acquisition, handling or storage of information that will be disseminated to the public or used to support information that will be disseminated to the public, explain how it will comply with your agency's Information Quality guidelines (Section 515 requirements)?

This activity does not involve the acquisition, handling or storage of information that will be disseminated to the public or used to support information that will be disseminated to the public. All of the data is associated with basic scientific research related to quarks and gluons and how they interact to form matter. The generated configurations and other analysis data products will be archived at one or more of the three primary sites in the project. This data will be used by researchers in the U.S., and under exchange agreements, by researchers in other countries. Data quality will be maintained by embedded provenance information (a copy of which will be held in a meta-data catalog for rapid queries), as well as by checksums on each constituent data set to protect against data replication errors.

Managing business information means maintaining its authenticity, reliability, integrity, and usability and providing for its appropriate disposition. Address how the system will manage the business information (records) that it will contain throughout the information life cycle.

In addition to the simulation data described above, it will be necessary to keep accounting records of the usage of the computational facilities. These records will be kept as standard output files of the batch systems at each site,

and digests of this information will also be held in standard SQL databases for a variety of purposes. Standard access controls will protect this data, restricting it to valid users. All accounting records will be backed up periodically. Procurement records for the computational resources will be kept following normal procedures of the host laboratories.

ENTERPRISE ARCHITECTURE: APPLICATION, COMPONENTS, AND TECHNOLOGY BY07

FEA Service Component Reference Model (SRM) BY07

Discuss this major investment in relationship to the Service Component Reference Model Section of the FEA. Include a discussion of the components included in this major IT investment (e.g., Knowledge Management, Content Management, Customer Relationship Management, etc). For detailed guidance regarding components, please refer to <http://www.feapmo.gov> and the SRM Release Document.

Relation to SRM (i.e., Component Description)	Service Domain	Service Type	Component	New Component
Defines the set of capabilities that support document and data warehousing and archiving.	Digital Asset Services	Document Management	Library / Storage	No
Defines the set of capabilities that allow access to data and information for use by an organization and its stakeholders.	Digital Asset Services	Knowledge Management	Information Retrieval	No
Defines the set of capabilities that support the use of documents and data in a multi-user environment for use by an organization and its stakeholders.	Digital Asset Services	Knowledge Management	Information Sharing	No
Defines the set of capabilities that support the transfer of knowledge to the end customer.	Digital Asset Services	Knowledge Management	Knowledge Distribution and Delivery	No
Defines the set of capabilities that utilize models to mimic real-world processes.	Business Analytical Services	Knowledge Discovery	Simulation	No
Defines the set of capabilities that develop descriptions to adequately explain relevant data for the purpose of prediction, pattern detection, exploration or general organization of data.	Business Analytical Services	Knowledge Discovery	Modeling	No
Defines the set of capabilities that support the formulation and mathematical analysis of probabilistic models for random phenomena and the development and investigation of methods and principles for statistical inference.	Business Analytical Services	Analysis and Statistics	Mathematical	No
Defines the set of capabilities that support the interchange of information between multiple systems or applications; includes verification that transmitted data was received unaltered.	Back Office Services	Data Management	Data Exchange	No
Defines the set of capabilities that allow the classification of data.	Back Office Services	Data Management	Data Classification	No
Defines the set of capabilities that support the monitoring, administration and usage of applications and enterprise systems from locations outside of the immediate system environment.	Support Services	Systems Management	Remote Systems Control	No
Defines the set of capabilities that support the balance and allocation of memory, usage, disk space and performance on computers and their applications.	Support Services	Systems Management	System Resource Monitoring	No

Agency EA Technical Reference Model BY07

Are all of the hardware, applications, components, and web technology requirements for this investment included in the Agency EA Technical Reference Model? If not, please explain.

Yes. Standard compliant service access and delivery, component framework, and service interface and integration are all completely standard. Compute servers anticipated in the first several years are included in the DOE TRM service platform and infrastructure. The proposed next generation QCDOC machine, while more unusual in architecture, is a variant of a mainframe or enterprise server composed of embedded microprocessors, both covered in the TRM.

FEA Technical Reference Model (TRM) BY07

Discuss this major IT investment in relationship to the Technical Reference Model Section of the FEA. Identify each Service Area, Service Category, Service Standard, and Service Specification that collectively describes the technology supporting the major IT investment. For detailed guidance regarding the FEA TRM, please refer to <http://www.feapmo.gov>.

Relation To SRM	Service Area	Service Category	Service Standard	Service Specification (i.e., vendor and product name)
Library / Storage	Service Platform and Infrastructure	Database / Storage	Storage	Anacapa "XTORE" NAS (network attached storage)
Library / Storage	Service Platform and Infrastructure	Database / Storage	Storage	StorageTek Tape Silos ("Powderhorn") and Tape Drives (T9940A, T9940B)
Information Retrieval	Service Access and Delivery	Delivery Channels	Internet	ESNET
Information Sharing	Service Access and Delivery	Service Transport	Supporting Network Services	SSH (OpenSSH)
Information Sharing	Service Access and Delivery	Service Transport	Supporting Network Services	Kerberos (MIT krb5)
Knowledge Distribution and Delivery	Service Access and Delivery	Service Transport	Service Transport	SFTP (OpenSSH)
Knowledge Distribution and Delivery	Service Access and Delivery	Service Transport	Service Transport	SCP (OpenSSH)
Knowledge Distribution and Delivery	Service Access and Delivery	Service Transport	Service Transport	Hyper Text Transfer Protocol (HTTP)
Knowledge Distribution and Delivery	Service Platform and Infrastructure	Delivery Servers	Web Servers	Apache (www.apache.org)
Simulation	Service Platform and Infrastructure	Hardware / Infrastructure	Servers / Computers	Custom QCDOC Supercomputer
Simulation	Service Platform and Infrastructure	Hardware / Infrastructure	Servers / Computers	Intel Processor-based Clusters (Xeon, Pentium 4)
Simulation	Service Platform and Infrastructure	Hardware / Infrastructure	Local Area Network (LAN)	Ethernet
Simulation	Service Platform and Infrastructure	Hardware / Infrastructure	Local Area Network (LAN)	Myricom Myrinet 2000
Simulation	Service Platform and Infrastructure	Hardware / Infrastructure	Local Area Network (LAN)	Mellanox Infiniband Switches and Host Channel Adapters
Simulation	Service Platform and Infrastructure	Supporting Platforms	Platform Independent	Linux (Scientific Linux)
Simulation	Service Platform and Infrastructure	Supporting Platforms	Platform Dependent	Custom QOS Operating System
Simulation	Component Framework	Business Logic	Platform Independent	C/C++ (GNU compilers, Intel C/C++ compilers, Portland Group C/C++ compilers)
Simulation	Component Framework	Business Logic	Platform Independent	Perl
Simulation	Component	Business Logic	Platform	Python

	Framework		Independent	
Data Exchange	Service Interface and Integration	Interoperability	Data Format / Classification	XML (World Wide Web Consortium, w3.org)
Data Classification	Component Framework	Data Interchange	Data Exchange	XQuery (World Wide Web Consortium, w3.org)
Remote System Control	Component Framework	Business Logic	Platform Independent	IPMI (Intelligent Platform Management Interface)
System Resource Monitoring	Component Framework	Presentation / Interface	Dynamic Server-Side Display	MRTG
System Resource Monitoring	Component Framework	Presentation / Interface	Dynamic Server-Side Display	Ganglia (sourceforge.ganglia.net)

Existing Components BY07

Will the application leverage existing components and/or applications across the Government (i.e., FirstGov, Pay.Gov, etc). If so, please describe.

No. This investment is specifically an Office of Science basic science research investment.

***** The following text applies precedes the TRM table:

The scientific activity supported by this investment is by nature highly distributed. Thus, this investment must utilize a number of technologies related to remote access. Networking and distributed computing standards and standard technology are used throughout the investment. In addition, the software developed under the related SciDAC R&D activity is intended to be platform independent, and so is constructed using standard methods and languages. Key standards for this investment are listed below.

Systems Inventory BY07

Financial Management Systems and Projects, as indicated in Part One, must be mapped to the agency's financial management system inventory provided annually to OMB. Please identify the system name(s) and system acronym(s) as reported in the most recent systems inventory update required by Circular A-11 Section 52.4.

SECURITY AND PRIVACY BY07

Funding BY07

How is security provided and funded for this investment (e.g., by program office or by the CIO through the general support system/network)?

The DOE Office of the Chief Information Officer (CIO) provides the directives, i.e. policies, orders, manuals and guidelines, for cyber security across the DOE enterprise. Under these directives, the DOE Office of Science provides a Program Cyber Security Plan. DOE Order 205.1 requires each of the laboratories to document their security controls in a Cyber Security Program Plan (CSPP), and update this document at least every two years. This order also specifies the guidelines of the CSPP, which is consistent with NIST SP 800-18. The laboratory CSPPs are approved by DOE. In the case of the three laboratories (BNL, FNAL and TJNAF) involved in this investment, the CSPPs also include the LQCD specific cyber security plans. All of these documents meet the security requirements from FISMA, OMB policy, and NIST guidelines, as well as the current DOE timeline for HSPD-12 implementation.

This investment spans three laboratories (BNL, FNAL and TJNAF) and two Office of Science program offices, HEP and NP. The computers at each of the laboratories are covered by the site's CSPP. The "front end" computers that will provide access to the three lattice gauge computing systems use strong authentication (ssh for BNL and TJNAF, Kerberos for FNAL). Although the three sites will operate independently in CY06 and BY07, users will also need to transfer data files between the sites. These file transfers will use the same authentication protocols (ssh, kerberos), which will evolve according to the current DOE timeline for HSPD-12 implementation. Over the next three years all three labs will migrate their identify verification systems to be compliant with HSPD-12 requirements, which include interlab operability. The three sites will exchange data across the ESnet backbone. Coordination of security efforts among the laboratories for these systems will be required; the three lattice gauge computing Facility Managers are responsible for security planning and implementation at their laboratories. The Contract Project Manager is responsible for the integrated LQCD cyber security program between the laboratories. The three laboratories CSPPs will be updated to include the LQCD specific cyber security plan prior to the start of this investment at the beginning of FY2006.

The FY05 funding in preparation for the three lab LQCD systems is coming from the DOE Office of Science HEP, NP and SciDAC programs.

Funding for the cyber security for this new investment starting in FY06 and continuing in BY07 comes in two parts:

- + A portion of the direct funding for security functions in the DOE is for cyber security. A portion of this funding in the Office of Science goes to run the cyber security program the Office of Science and a portion of this funding goes to the laboratories to fund the central support level for cyber security at the individual laboratories. This investment at BNL, FNAL and TJNAF will receive support from the central cyber security support groups at each of the three labs.
- + The cyber security specific to the LQCD systems is included in the operating funds for this investment, provided by the HEP and NP programs of the DOE Office of Science.

What is the total dollar amount allocated to IT security for this investment in this budget year? Please indicate whether an increase in IT security funding is requested to remediate IT security weaknesses, specifying the amount and a general description of the weakness.

For FY2007, a total of \$80K of the operating funds of this investment will go towards cyber security. This accounts for security activities by LQCD system administrators, and preparation of security plans by the site managers.

In addition, this investment will receive support from the laboratories' central cyber security services as indicated in II.B.1. The amount of this funding is in the proportion of the LQCD funding to the total IT funding at the three laboratories. The aggregate funding in FY2007 from the three laboratories is estimated at \$200K.

This funding will support the following activities:

- System patching
- Development of firewall and Intrusion Detection System (IDS) rule sets
- Implementation of secure access methods (SSH and Kerberos)
- Retrofitting existing authentication schemes to include HSPD-12

No increase in IT security funding is requested.

Security Plan BY07

Please describe how the investment (system/application) meets the following security requirements of the Federal Information Security Management Act, OMB policy, and NIST guidelines:

The investment will purchase and operate LQCD systems at three sites, Fermilab (FNAL), Jefferson Lab (TJNAF), and Brookhaven (BNL). At each of these sites, the LQCD system will be part of existing cyber enclaves. An integrated project security team (LQCD Security Team) consists of representatives from the cyber security staffs of each of the three laboratories.

FNAL, TJNAF, and BNL each meet the FISMA, OMB and NIST requirements through the following controls:

- * Cyber-security roles and responsibilities are included in position descriptions and performance standards, updated on a yearly basis.
- * The FNAL, TJNAF, and BNL Security Teams provide additional resources to continuously assess risks and adapt site methods and practices to effectively respond to the changing environments.
- * FNAL, TJNAF, and BNL Management review security controls and changes to calibrate the potential risk and magnitude of harm.
- * The LQCD systems are unclassified and open systems that contain data only related to scientific research and do not contain "personally identifiable information" and therefore are considered a low level of risk by the DOE.
- * Security requirements are included in appropriate procurements and documents. The requirements are developed in concert with the LQCD Security Team and reviewed and approved by project management.
- * Security specifications are periodically reviewed and updated. Specifications and methods are updated as new threats and vulnerabilities are detected or whenever there is an identified benefit.
- * New systems are integrated in the FNAL, TJNAF, and BNL computing centers with testing and integration processes. When appropriate and feasible, systems are built, configured and tested before being made available to the general network.
- * FNAL, TJNAF, and BNL perform annual risk assessments and self-assessments. All lab systems including LQCD systems are tested at least quarterly, with interim ad hoc tests performed monthly or as needed. All systems are monitored continuously. Threats, countermeasures, and incident handling are reviewed weekly with the FNAL, TJNAF, and BNL Security Teams, by the FNAL, TJNAF, and BNL Computer Protection Program Managers (CPPMs), and by the site Systems and Network Security (SNS) teams.

DOE Notice 205.1 UNCLASSIFIED CYBER SECURITY PROGRAM requires FNAL, TJNAF, and BNL to develop Cyber Security Program Plans (CSPP), which are updated biannually or as necessary. OMB and NIST requirements and guidance are incorporated into DOE policy and directives. These policies and directives are addressed as requirements in the FNAL, TJNAF, and BNL Contracts with DOE. The labs adhere to the following DOE security directives in their contracts:

- * DOE M 200.1-1 TELECOMMUNICATIONS SECURITY MANUAL
- * DOE O 205.1 DEPARTMENT OF ENERGY CYBER SECURITY MANAGEMENT PROGRAM
- * DOE P 205.1 DEPARTMENTAL CYBER SECURITY MANAGEMENT POLICY
- * DOE N 205.2 FOREIGN NATIONAL ACCESS TO DOE CYBER SYSTEMS

<ul style="list-style-type: none"> * DOE N 205.3 PASSWORD GENERATION, PROTECTION, AND USE * DOE N 205.4 HANDLING CYBER SECURITY ALERTS AND ADVISORIES AND REPORTING CYBER SECURITY INCIDENTS * DOE O 241.1A SCIENTIFIC AND TECHNICAL INFORMATION MANAGEMENT * DOE O 470.1, Chg 1 SAFEGUARDS AND SECURITY PROGRAM (Chapters I, VII, and IX) * DOE P 470.1 INTEGRATED SAFEGUARDS AND SECURITY MANAGEMENT (ISSM) POLICY * DOE O 471.3 IDENTIFYING AND PROTECTING OUO INFORMATION * DOE M 471.3-1 MANUAL FOR IDENTIFYING AND PROTECTING OUO INFORMATION * DOE O 473.1 PHYSICAL PROTECTION PROGRAM * DOE M 473.1 PHYSICAL PROTECTION PROGRAM MANUAL <p>This investment implements and maintains a security program, as documented in the FNAL, TJNAF, and BNL Cyber Security Program Plans and as required by DOE Order 205.1, by ensuring the systems and applications operate effectively and provide appropriate confidentiality, integrity, and availability; and protecting information commensurate with the level of risk and magnitude of harm resulting from loss, misuse, unauthorized access, or modification. The investment meets FISMA security in the following ways:</p> <ul style="list-style-type: none"> * Ensuring security policies are founded on a continuous risk management life-cycle; * Implementing security controls that adequately assess information risks; * Promoting continuing security awareness of information risks; * Continually monitoring and evaluating information security policy; * Controlling effectiveness of information security practices; * Identify additional security controls that are necessary to minimize risk to and potential loss from those systems that promote or permit public access; * Ensure that the handling of personal information is consistent with relevant government-wide agency policies; * Update strategies that identifies and mitigates risks associated with each information system. <p>In addition, the requirements of the Cyber Security Program and its corollary in the Office of Science require that CSPPs be updated and self-assessments (NIST 800-26) against CSPP goals be performed every 2 years. This evaluation includes a threat and risk assessment (NIST 800-30), vulnerability analysis, and follow-up action plan. Specifically the goals of this process are as follows.</p> <ul style="list-style-type: none"> * Ensure that security is commensurate with sensitivity, criticality, etc.; * Ensure that security is cost-effective based on a cost versus risk ratio, or that is necessary to meet with applicable mandates; * Ensure appropriate support for the security of data in each functional area; * Ensure individual accountability for data, information, and other computing resources; * Ensure audit ability; * Provide sufficient guidance to users for the discharge of responsibilities regarding automated information security; * Ensure that all critical functions have contingency or disaster recovery plans to provide continuity of operation; * Ensure that all applicable Federal department and organizational policies, mandates, etc. are applied and followed; * Deploy effective security controls and authentication tools consistent with the protection of privacy, such as public-key based digital signatures, for those systems that promote or permit public access; * Ensure that information systems are monitored for any security weaknesses, and are continually assessed; and effectively ensure that controls are implemented effectively and remain effective over time; * Ensure users receive awareness and training; * Ensure certification and accreditation is performed within the life-cycle.
<p>Does the investment (system/application) have an up-to-date security plan that meets the requirements of OMB policy and NIST guidelines? What is the date of the plan?</p>
<p>Three LQCD systems will be operated as part of this investment, consisting of one system at each of the DOE laboratories Fermilab (FNAL), Brookhaven (BNL), and Jefferson Lab (TJNAF). These LQCD systems will be part of existing cyber enclaves at FNAL, BNL, and TJNAF.</p> <p>As mandated by DOE Order 205.1, each of the three laboratories maintains a Cyber Security Program Plan (CSPP) that defines cyber security processes, strategy, roles, incident response, and the duties and responsibilities of staff members and users. These CSPP's are prepared in accordance with the guidelines presented in NIST SP 800-18 and under the guidance in the PCSP for the DOE Office of Science. The current and all planned updated versions of the three labs' CSPP's incorporate by reference the system specific security plans for the LQCD systems. These system specific security plans, written according to NIST SP 800-18, will be completed at FNAL and TJNAF by the start of the investment, October 1, 2005, and at BNL by October 30, 2005. The system categorization for the LQCD systems has been determined to be Low using FIPS 199.</p>
<p>Certification and Accreditation BY07</p>
<p>Has the investment been certified and accredited (C&A)? Note: Certification and accreditation refers to a full C&A and does not mean interim authority to operate. Additionally, specify the C&A methodology used (e.g., NIST guidelines) and the date of the last review.</p>
<p>The LQCD systems acquired by this investment will be part of existing cyber enclaves at their respective laboratories (BNL, FNAL, TJNAF). The cyber enclaves at each of the three labs (BNL, FNAL, TJNAF) have been C&A. The certification reviews were performed utilizing information and checklists from NIST SP 800-18 (Security Plans), NIST SP 800-26 (Self Assessments), NIST SP 800-37 (Certification and Accreditation), NIST SP 800-53</p>

(Recommended Security Controls), FIPS 199, and published interim OMB guidance to review the system security plan and to determine the sensitivity, confidentiality, integrity, and availability levels for this application. Based on this self-assessment certification documentation, they received authority to operate (i.e. accreditation) from senior management. The current C&As based on this process are: FNAL's last C&A was issued in September, 2004, and the FNAL Authority to Operate (ATO) is valid until October 2006. TJNAF's last C&A was issued on July 1, 2005, and TJNAF has an ATO until July 2008. BNL is revising its C&A package based on input from an internal DOE review. The updated package will be completed by October 30, 2005. BNL's current ATO is valid until Sept 30, 2005; the BNL site office will extend this ATO by up to two months during the period that the updated C&A package is being put into place and accredited.

Investment C&A Status	55 - All of the systems within this investment have been through a C&A Process and have been granted Full Authority to Operate
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Testing and Training BY07

Have the management, operational, and technical security controls been tested for effectiveness? When were most recent tests performed?

The LQCD systems of this investment are unclassified, open systems that contain data only related to scientific research and do not contain "personally identifiable information." Following DOE directive Order 205.1, each site conducts periodic peer reviews. The latest peer reviews were conducted in [BNL: November 2002, FNAL: March, 2005, TJNAF: April 2002].

Each laboratory performs an annual risk assessment and self-assessment. All lab systems, including the LQCD systems of this investment, are tested at least quarterly by the laboratories, with interim ad hoc tests performed monthly or as needed. All systems are monitored continuously. At each of the three sites (BNL, FNAL, TJNAF), threats, countermeasures, and incident handling are reviewed weekly with the site security team, by the site CPPM (Computer Protection Program Manager), and the SNS (Systems and Network Security) team.

When the LQCD systems of this investment become operational, testing of security controls in compliance with NIST 800-53A will begin. The results of these tests will be used during the self assessment process described in NIST 800-26 to determine whether any modifications to the controls are necessary.

Have all system users been appropriately trained in the past year, including rules of behavior and consequences for violating the rules?

In order to obtain computing accounts on the LQCD systems at each lab, all users are required to read and sign an acceptable use policy that includes cyber security policies and the consequences for violating the policies. All users of the BNL and TJNAF systems were required in 2005 to take a web-based computer security course that included coverage of the local acceptable use and cyber security policies, and the consequences for violating the policies. All users of the FNAL LQCD systems will be required to take a similar web based course by the start of the investment (October 1, 2005). All users of the LQCD systems will be required to repeat these web-based computer security courses on an annual basis.

The web-based security courses cover the requirements for reporting suspected computer security incidents, provide guidelines on avoiding phishing and identity hijacking activities, cover password selection and security, and discuss the responsibilities for maintaining data integrity.

Incident Handling BY07

How has incident handling capability been incorporated into the system or investment, including intrusion detection monitoring and audit log reviews? Are incidents reported to DHS FedCIRC?

At each site, all network activity originating internally or externally is monitored. The detection of inappropriate activity triggers an incident investigation by each site's CIRT (Computer security Incident Response Team). Response and reporting of incidents will follow the procedures outlined in the host site's CSPP. Further, the Facility Manager of the affected site will notify the Facility Managers and CIRTs of the other sites so that immediate scrutiny of the other lattice gauge computing facilities and coordination of responses can occur. Following the DOE CSPP, computer incidents are reported to the DOE Computer Incident Advisory Capability (CIAC), which is sponsored by the DOE CIO. CIAC handles the reporting of all incidents to DOE and to FedCIRC, as well as providing analysis and alerts to the DOE community. In each month in which there are no incidents to report, in accordance to DOE policy each site submits negative reports.

Contractor Security Procedures BY07

Is the system operated by contractors either on-site or at a contractor facility? If yes, does any such contract include specific security requirements required by law and policy? How are contractor security procedures monitored, verified and validated by the agency?

The lattice gauge computing systems are managed at BNL, FNAL, and TJNAF, each of which is a government-owned, contractor-operated facility. 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, Universities Research Association (URA) for FNAL, and Southeastern Universities Research Association (SURA) for TJNAF). These contracts include requirements for compliance with pertinent government 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) annual site reviews by the Office of Science, 4) the DOE-IG, and 5) external reviews.

Public Access and Privacy BY07

How does the agency ensure the effective use of security controls and authentication tools to protect privacy for those systems that promote or permit public access?

DOE has issued directives and policy that implement OMB guidance to ensure the effective use of security controls and authentication tools (up-to-date security patches, "out-of-band" console access, access logging, firewalls, restricted physical access, access control lists, intrusion monitoring, Virtual Private Network access) in the area of privacy and public access. DOE monitors FNAL, TJNAF, and BNL adherence to these policies.

The lattice gauge computing facilities at these three DOE laboratories are open and unclassified, containing data only related to scientific research and no "personally identifiable information". The LQCD systems at FNAL, TJNAF, and BNL post and comply with the "Privacy and Security Policy" of their host laboratory, and post the DOE Security Warning Banner, which is linked from public ingress points.

How does the agency ensure that the handling of personal information is consistent with relevant government-wide and agency policies.

The lattice gauge computing facilities at these three DOE laboratories are open and unclassified, containing data only related to scientific research and no "personally identifiable information". DOE has issued directives and policy that implement OMB guidance in this area. The DOE monitors adherence to these policies at these three sites. The LQCD systems do not meet any of the conditions under which a Privacy Impact Assessment is required. Specifically, they do not collect, store, process or transmit identifiable data; they do not establish electronic collections of identifiable data on ten or more people; and they do not create new privacy risks, such as the conversion of paper-based systems to automated systems.

The DOE requires a Privacy Manager at each laboratory who is responsible for ensuring compliance with privacy requirements. The Privacy Manager reviews privacy impact assessments, evaluates whether personally identifiable information is contained on systems, and determines whether a privacy impact assessment is required.

If this is a new or significantly altered investment involving information in identifiable form collected from or about members of the public, has a Privacy Impact Assessment (PIA) for this investment been provided to OMB at PIA@omb.eop.gov with the investment's unique project (investment) identifier?

N/A

GPEA BY07

GPEA Plan BY07

If this investment supports electronic transactions or record-keeping that is covered by GPEA, briefly describe the transaction or record-keeping functions and how this investment relates to your agency's GPEA plan.

This project does not support items covered by the GPEA.

What is the date of electronic conversion from your GPEA plan?

OMB PRA BY07

Identify any OMB Paperwork Reduction Act (PRA) control numbers from information collections that are tied to this investment.

This investment does include any PRA control numbers.

ADDITIONAL BUSINESS CASE COMMENTS

Additional Business Case Comments

Additional Comments