Advanced Scientific Computing Research
Funding Profile by Subprogram and Activity

(Dollars in Thousands)

	FY 2011 Current	FY 2012 Enacted	FY 2013 Request
Mathematical, Computational, and Computer Sciences Research			
Applied Mathematics	45,604	45,604	49,500
Computer Science	47,301	47,400	54,580
Computational Partnerships	52,813	44,250	56,776
Next Generation Networking for Science	12,313	12,751	16,194
SBIR/STTR	0	4,560	5,570
Total, Mathematical, Computational, and Computer Sciences Research	158,031	154,565	182,620
High Performance Computing and Network Facilities			
High Performance Production Computing	59,514	57,800	65,605
Leadership Computing Facilities	158,020	156,000	145,000
Research and Evaluation Prototypes	4,301	30,000	22,500
High Performance Network Facilities and Testbeds	30,451	34,500	32,000
SBIR/STTR	0	8,003	7,868
Total, High Performance Computing and Network Facilities	252,286	286,303	272,973
Total, Advanced Scientific Computing Research	410,317[a]	440,868[b]	455,593

[a] Total is reduced by $11,680,000: $10,428,000 of which was transferred to the Small Business Innovation Research (SBIR) program and $1,252,000 of which was transferred to the Small Business Technology Transfer (STTR) program.
[b] The FY 2012 appropriation is reduced by $1,132,000 for the Advanced Scientific Computing Research share of the DOE-wide $73,300,000 rescission for contractor pay freeze savings. The FY 2013 budget request reflects the FY 2013 impact of the contractor pay freeze.

Public Law Authorizations

Public Law 95-91, "Department of Energy Organization Act", 1977
Public Law 108-423, "Department of Energy High-End Computing Revitalization Act of 2004"
Public Law 109-58, "Energy Policy Act of 2005"
Public Law 110-69, "America COMPETES Act of 2007"

Program Overview and Benefits

The Advanced Scientific Computing Research (ASCR) program's mission is to advance applied mathematics and computer science; deliver, in partnership with disciplinary science, the most advanced computational scientific applications; advance computing and networking capabilities; and develop, in partnership with U.S. industry, future generations of computing hardware and tools for science. A particular challenge of this program is fulfilling the science potential of emerging computing systems and other novel computing architectures, which will require numerous and significant modifications to today's tools and techniques to deliver on the promise of exascale science.

ASCR efforts support the Department's goal to maintain a vibrant U.S. effort in science and engineering as a cornerstone of our economic prosperity with clear leadership in strategic areas. As a direct result of DOE investments over the past decade, the U.S. currently holds clear leadership in high performance computational science and engineering. To continue U.S.

leadership in this area, ASCR must address two significant challenges: advancing the Department's science and engineering missions by effectively utilizing our existing hardware and software, and supporting research to extend these capabilities and take on even more complex challenges. Through our regular requirements gathering efforts, it is clear that Department of Energy (DOE) simulation and data analysis needs exceed petascale capabilities and are driving us toward exascale computing. However, computer industry roadmaps reveal a period of significant change and several critical technology challenges on the path to exascale that will impact both data-intensive and compute-intensive applications. These changes will require a fundamental shift in both hardware and software development to deliver increased application performance while limiting growth in system power requirements. In addition, new algorithms will be required that optimize management of data movement.

According to the National Research Council of the National Academies' 2011 report *The Future of Computing Performance, Game Over or Next Level?* [a], "Virtually every sector of society—manufacturing, financial services, education, science, government, the military, entertainment, and so on—has become dependent on continued growth in computing performance to drive new efficiencies and innovation." The report found "The growth in the performance of computing systems . . . will become limited by power consumption within a decade" and "There are opportunities for major changes in system architectures, and extensive investment in whole-system research is needed to lay the foundation of the computing environment for the next generation."

Informed by analyses of future computational needs including this report, ASCR is supporting long-term, coordinated investments across the ASCR research portfolio including Research and Evaluation Prototypes investments fund breakthrough technologies that minimize the technical risk associated with the next generation of supercomputing hardware.

ASCR is also supporting new and redirected efforts in Applied Math and Computer Science to develop new tools and techniques that address the challenges of current and future data-intensive science and the coming generation of high performance computing (HPC) designs. Co-design partnerships between applications and vendors are supported to create feedback loops in the design of the emerging HPC architectures to ensure science and engineering applications are ready and able to use commercial offerings that have been made more competitive and more resilient through input from their most challenging users. To achieve all of this, ASCR is working closely with the National Nuclear Security Administration (NNSA), which is addressing these same challenges for the Department's national security applications. In April 2011, a Memorandum of Understanding was signed between the Office of Science (SC) and the NNSA's Office of Defense Programs regarding collaboration and coordination of exascale activities across the two organizations. The ten year goal for these efforts is the delivery of energy-efficient exascale computing systems (computing systems capable of 10^{18} (a quintillion) floating point operations per second—1,000 times current capabilities—while using only twice as much electricity) for the advancement of DOE science and engineering. However, this effort will also deliver, along the path to the exascale goal, solutions to the software and hardware challenges of future computing at all scales. In this way, DOE's investment in exascale research will impact the entire computing and scientific research enterprise in the United States.

Today, ASCR is actively engaged in sharing our expertise to further broaden the benefits of our past and current investments. The National Energy Research Scientific Computing Center (NERSC) is available for scientists supported by SC programs for mission-related research, ASCR Leadership Computing Facilities (LCFs) are available to all researchers—including industry and academia—for scientific discovery and to address critical engineering challenges. These partnerships, and planned exascale partnerships, benefit many sectors of the economy from high-tech industry and academic research to software development and engineering. ASCR's support of researchers and students (the next generation of researchers) is a benefit to the national research and development workforce.

ASCR has long-established expertise in delivering forefront computational capabilities in a way that involves and prepares the research communities for advancing science. ASCR-supported high-performance computing systems are the culmination of a decade-long effort to build computing architectures with unprecedented speed and capability. At the same time,

[a] http://www.nap.edu/openbook.php?record_id=12980

ASCR-supported development of new mathematical theories and algorithms increases the speed at which difficult scientific problems can be solved as much or more than the increased computational power of supercomputers. Finally, to ensure that the Department's science and engineering communities were ready to use Leadership Computing Facilities, ASCR fostered collaborations encompassing applied mathematics, computer science, physics, biology, chemistry, and others.

These investments extend our knowledge of the natural world and have direct benefit to science and society at large. For example, Scientific Discovery through Advanced Computing (SciDAC) efforts include:

- Computational chemistry and simulation of nanomaterials relevant to energy applications in partnership with the Basic Energy Sciences program.
- Next generation integrated earth system models with uncertainty quantification to dramatically improve our ability to characterize variables in global climate and quantify the impact of energy production and use on the environment and human health in partnership with the Biological and Environmental Research program.
- Computer modeling of nuclear structure with relevance for science, nuclear energy, and nuclear weapons in partnership with the Nuclear Physics program and the National Nuclear Security Administration.

ASCR is working to broaden the impact of our research efforts through outreach, workshops and program manager interactions with the DOE applied programs. For example, ASCR is taking a new approach to our small business investments to help commercialize our software and middleware. The Leadership Computing Facilities also regularly transfer ASCR developed tools and techniques to academic and industrial users through user support. ASCR-supported researchers are also focusing on the mathematical and computational challenges of the electricity grid and nuclear reactor modeling. ASCR research in the mathematics of complex natural and engineered systems and uncertainty quantification is relevant to DOE efforts in carbon sequestration, wind energy, next generation nuclear reactors, Smart Grid, cyber security, and fuels from sunlight.

In many areas of research, computation is an essential tool for discovery. SciDAC accelerates scientific progress by breaking down the barriers between disciplines and fostering more dynamic partnerships between applications (materials, chemistry, fusion, bioenergy, climate, accelerator R&D, nuclear structure, etc.) and computer scientists and mathematicians. These partnerships have been spectacularly successful, with documented improvements in code performance in excess of 10,000 percent.

Advances in mathematics and computing are the foundation for models, simulations, and data analysis, which permit scientists and engineers to gain new insights into problems ranging from bioenergy and climate change to optimizing complex engineered systems such as nuclear reactors and the electricity grid. ASCR and its predecessor programs have led these advances for more than thirty years by supporting the best applied math and computer science research, delivering world-class scientific simulation facilities, and working with discipline scientists to deliver exceptional science.

Science is increasingly collaborative, requiring researchers not only to communicate with each other, but also to move, share and exchange large scientific data sets. Scientists also need to run complex calculations and experiments in locations remote from where the original data is collected or generated. ASCR has played a leading role in driving development of the high-fidelity, high-bandwidth networks connecting researchers to each other and their data.

Looking forward, ASCR will continue to be guided by science needs and engineering challenges as it develops tools, techniques, computers and networks at the leading edge of technology. ASCR has the experience and know-how to deliver exascale computing. Like the path to petascale computing, the path to exascale is driven by the requirements of applications that are critical to DOE and the Nation. In addition, this path will result in not only exascale computing capability but also new tools and techniques for data-intensive science, and affordable, energy efficient petascale systems to drive scientific and engineering discovery across the country. With this integrated approach, ASCR will continue to deliver scientific insight to address national problems in energy and the environment.

Basic and Applied R&D Coordination

Coordination across disciplines and programs is an ASCR cornerstone. Partnerships within SC are mature and continue to advance the use of high performance computing and scientific networks for science. In addition, ASCR continues to have a strong partnership with the National Nuclear Security Administration in areas of mutual interest including exascale research, workforce development, and best practices for management of high performance computing facilities. In April 2011, ASCR and NNSA strengthened this partnership by signing a Memorandum of Understanding for collaboration and coordination of exascale research within the Department. Through the National Information Technology Research and Development (NITRD) subcommittee, an interagency networking and information technology R&D collaboration effort, ASCR also coordinates with similar programs across the Federal Government and directly partners with the Department of Defense on developing High Productivity Computing Systems and software.

Key areas of mutual interest with the DOE technology programs continue to be applied mathematics for the optimization of complex systems, control theory, and risk assessment. A March 2009 workshop, in partnership with the Office of Electricity Delivery and Energy Reliability (OE), focused on the challenges of grid modernization efforts. This workshop was part of a series of workshops on basic research needs in applied R&D areas. Other workshops have covered advanced nuclear energy systems (with the Office of Nuclear Energy), subsurface science (with the Offices of Environmental Management and Fossil Energy), cyber security (with OE), alternative and renewable energy (with the Office of Energy Efficiency and Renewable Energy), and the scientific challenges of exascale computing for national security (with the National Nuclear Security Administration). These workshops facilitate a dialogue between the ASCR research community and a specific applied R&D community to identify opportunities for new research. This research becomes part of the ASCR program through investigator-driven research proposals and is coordinated with the applied efforts through program manager interactions and joint principal investigator meetings.

ASCR and OE significantly increased interactions during FY 2011 through the Grid Tech Team meetings and other activities. ASCR and OE program managers meet weekly to enhance communication and collaboration on the electric grid. In addition, ASCR researchers had a significant role in the OE-sponsored workshop on Computational Needs for the Next Generation Electric Grid held at Cornell University in April 2011. OE was represented at an ASCR-sponsored workshop for Mathematics for the Analysis, Simulation, and Optimization of Complex Systems in September 2011 and the ASCR Applied Mathematics program meeting in October 2011.

Program Accomplishments and Milestones

Minimizing Data Movement to Speed Computations. On modern, high-performance computers, data computations can occur 100 times faster than data movement to the processor. ASCR researchers have developed a new approach (message driven computation) to take advantage of hardware innovations by arranging algorithms to minimize data movement and speed computation up to 30-fold[a].

Novel Designs Save Energy, Accelerate Networks. ASCR computer scientists, focusing on the energy demands of data movement, are using simulators to explore novel memory systems and interconnects that have the potential to provide power savings of up to $13 billion annually, while sharply reducing network latency—making data flow faster. Their initial studies show 63–98% reduction in energy usage and a factor of 10 improvement in effective network bandwidth. These efforts will inform the new vendor partnerships to develop critical technologies that realize those potentials.

High Performance Computations Save DOE Time and Money. A SciDAC partnership with NNSA focused on nuclear structure provided a quantitative description of neutron-tritium scattering that was precise enough for designers at the National Ignition Facility (NIF) to make critical fuel assembly decisions that could not have been achieved using physical testing within the NIF cost and schedule baselines.

Crash Site Investigation for Networks: The complex structure of modern networks means that faults on any single link in the network can impact multiple users across the network. These faults can cause data traffic to slow-down in other parts of the network, misleading operators as they attempt to find the faulty link. DOE

[a] http://lightwave.ee.columbia.edu/files/Bergman2011.pdf

researchers have developed analysis algorithms that can quickly sort through measurement data to separate real faults from these secondary effects. Once fully deployed, network operators will be able to track down infrastructure faults more quickly and efficiently.

Simulations Explain LED-based Light Bulb Performance Issues. Light-emitting diodes (LEDs) hold enormous potential as energy-efficient, nontoxic, long-lasting replacements for incandescent bulbs and compact florescent lights. However, LED lighting is expensive because of a dramatic drop in efficiency, known as droop, at the intensities needed for full room illumination. A simulation using NERSC computers allowed researchers to discover the dominant contributors to LED droop, as well as hints to how it might be overcome leading to better LED-based light bulbs.

Understanding the Complex Behavior of Oil in the Gulf of Mexico. Researchers running simulations at the Argonne Leadership Computing Facility were able to do the first ever simulations of a buoyant oil plume in a stratified and rotating ocean environment. These results helped in understanding the behavior of the Deepwater Horizon oil spill in the Gulf of Mexico and informed planning for future emergencies.

Partnering with Industry to Save Energy and Improve Competitiveness. GE Global Research used the Oak Ridge Leadership Computing Facility to study, for the first time, unsteady airflows in the blade rows of turbo machines used in modern jet engines. Simulations of unsteady airflow are orders of magnitude more complex than simulations of steady flows and beyond the capabilities of GE's in-house systems. The insights gained will impact aircraft engine design and could lead to substantial reductions in energy consumption and substantial cost savings. GE Global Research recently purchased a substantial upgrade to its in-house computing capabilities to continue this work, based largely on the results of this project.

First Nation-wide 100 gigabit per second Network. In September 2011, ESnet turned on to the world's first nation-wide 100 gigabit per second optical network testbed. The demonstration network is designed in part to help accelerate the commercial deployment of emerging networking technologies, and ensure America's global leadership in the development of ultra-high broadband networking, by demonstrating the technology and providing a research testbed at scale. The network uses special optical equipment to transmit more than ten times more data via already existing fiber optic cable and will immediately provide greater connectivity among ASCR supercomputing centers to meet the ever growing requirements of scientific research and collaboration.

Milestone	**Date**
Develop joint plan for exascale R&D with NNSA.	Q2 FY 2012
Award at least two new SciDAC science application partnerships.	Q4 FY 2012

Explanation of Changes

The market for computer hardware is driven by the demands of consumer electronics, commercial data farms, and business computing. The demands of DOE science and engineering applications and data-intensive science are significantly different from these high-volume customers yet progress is dependent on the availability of usable commercial hardware. The challenges of developing high performance scientific computing systems on the path to exascale and the demands of some critical DOE facilities and applications require us to look ahead and make long-term, coordinated investments across the ASCR research portfolio. The FY 2013 budget increases investments across the ASCR research portfolio with a focus on the linked challenges of data-intensive science and exascale computing. These investments will span the entire enterprise from hardware to applications and will advance critical technologies, mathematical methods, software, tools, middleware, and science applications. In FY 2013, exascale relevant investments total $68,500,000 and data-intensive science investments total $21,000,000.

New research efforts will be supported across the ASCR portfolio with a focus on addressing the challenges of data-intensive science and the massive data expected from DOE mission research, including research at current and planned scientific user facilities. There are two broad categories in which DOE's missions lead to unique data-centric computing challenges that span the portfolios of ASCR and the other research programs:

- DOE researchers routinely compute detailed models of time dependent, three dimensional systems on some of the world's largest computers. These simulations generate enormous data sets that are difficult to extract and archive, let alone analyze.

More comprehensive analysis of the data will help in the discovery and identification of unanticipated phenomena, and also help expose shortcomings in the simulation methodologies and software.

- DOE manages the Nation's most advanced experimental resources, and these facilities generate tremendous amounts of data. Data sets generated at DOE's scientific facilities today significantly outstrip the current analysis capability. Basic research in Applied Mathematics and Computer Science, coupled to expertise from the facilities, is required to realize the significant potential that exists in DOE facilities data.

Investments in Research and Evaluation Prototypes will focus on long-lead time critical technologies for exascale and are reduced to support research for data-intensive science. In FY 2013, these efforts will focus on R&D in breakthrough technologies that will enable novel hardware designs for Exascale computing with priority given to early-stage technology development. These investments seek to minimize technical risk associated with exascale computing systems. By actively participating in the development of next-generation machines, ASCR can accelerate the development of technologies that enable exascale and ultimately accelerate and influence the development of architectures more appropriate for science. Also, researchers using the hardware will gain a better understanding of the inherent challenges of the hardware, both for leadership applications and data-intensive science, and begin to work on overcoming them.

In FY 2013, increased funding for Production Computing will support site preparations for a planned relocation of NERSC to a new computing facility. Both the Argonne and Oak Ridge Leadership Computing facilities will be upgraded to 10 petaflops in 2013 with reduced funding for infrastructure in FY 2013 to support the NERSC move. ESnet will begin production operation of a 100 gigabit per second optical network to select sites.

<u>Program Planning and Management</u>

ASCR planning and priority setting strongly benefits from input by outside experts. ASCR peer review and oversight processes are designed to regularly assess the quality, relevance, and performance of the ASCR portfolio.

The Advanced Scientific Computing Advisory Committee (ASCAC) provides input to ASCR by responding to charges from the Office of Science. For example, ASCAC organizes regular Committees of Visitors (COVs) to review ASCR research management, reviews of progress and bottlenecks in specific areas of research, reviews of the impact of ASCR scientific user facilities, and progress toward the long-term goals of the program. In addition, ASCAC identifies scientific challenges and opportunities, including specific bottlenecks to progress in areas such as climate change or computational biology. In FY 2011, ASCAC delivered a report on the opportunities and challenges associated with exascale computing. Also in 2011, a COV reviewed the Next Generation Networking for Science elements of the ASCR program. ASCAC provided input on the data policies of ASCR relevant communities, facilities, and publications, and an ASCAC subcommittee reviewed the management and impact of the Computational Sciences Graduate Fellowship.

The pace of progress in the computing industry requires ASCR to make more frequent and more dramatic changes in our portfolio than in other areas of basic research. However, this is not uniform across activities. For example, the development of robust, yet novel, applied mathematics for high performance computing can take sustained efforts over a decade or more while computer science changes dramatically in relatively short periods of time and networking research naturally progresses into production ready middleware and tools that are delivered via ESnet or program partners. ASCR goals for exascale computing require that the portfolio is continuously assessed and shifted to support critical new research efforts. In FY 2011, the Applied Mathematics activity redirected nearly $2,000,000 of effort toward new projects to develop algorithms and solvers for emerging architectures, the Computer Science activity renewed only 3 of 42 projects eligible for renewal in FY 2011 to make room for new efforts to address data movement and effective energy management in high performance computing systems, the Next Generation Networking for Science activity successfully completed projects representing more than half of the portfolio and is supporting new efforts to address the challenges of optical switches and high speed data flows, and the SciDAC portfolio was recompeted and streamlined to support petascale scientific discovery with application partners and the new exascale relevant co-design efforts in combustion, nuclear engineering and advanced materials.

Critical tools for managing ASCR scientific user facilities include tailored project management principles, annual operational reviews, and regular requirements gathering workshops. For example, ESnet and NERSC conduct requirements workshops with at least two SC program offices every year in order to accurately characterize their near-term, medium-term, and long-term network and computing requirements.

Other planning and management tools include community-driven workshops, the National Science and Technology Council's (NSTC) subcommittee on Networking and Information Technology Research and Development (NITRD), and studies by outside groups such as the National Research Council and the U.S. Council on Competitiveness.

Program Goals and Funding

Office of Science performance expectations (and therefore funding requests) are focused on four areas:

- *Research*: Enable high performance computational science and engineering to increase our understanding of and enable predictive control of phenomena in the physical and biological sciences.
- *Facility Operations*: Maximize the performance, usability, and capacity of the SC scientific computing user facilities and connect Office of Science researchers, labs and facilities via an ultra-reliable, high performance scientific network.
- *Future Facilities*: Build future and upgrade existing facilities and capabilities to get the best value from investments and advance continued U.S. leadership in computational science and engineering.
- *Scientific Workforce*: Continue to support graduate students and Post-Doc on research projects to ensure a sustained pipeline of highly skilled, computationally savvy, and diverse science, technology, engineering, and mathematics (STEM) workers.

Goal Areas by Subprogram

	Research	Facility Operations	Future Facilities	Workforce
Mathematical, Computational, and Computer Sciences Research	98%	0%	0%	2%
High Performance Computing and Network Facilities	10%	90%	0%	0%
Total, Advanced Scientific Computing Research	49%	50%	0%	1%

Explanation of Funding and Program Changes

(Dollars in Thousands)

	FY 2012 Enacted	FY 2013 Request	FY 2013 vs. FY 2012
Mathematical, Computational, and Computer Sciences Research	154,565	182,620	+28,055

New research will address the challenges of data-intensive science and the massive data expected from current and next generation scientific user facilities including new core research efforts in Applied Mathematics, Computer Science, and Next Generation Networking for Science that will address the full spectrum of data challenges from hardware to applications and new Computational Partnership investments focused on specific challenges of program partners.

	(Dollars in Thousands)		
	FY 2012 Enacted	FY 2013 Request	FY 2013 vs. FY 2012
High Performance Computing and Network Facilities	286,303	272,973	-13,330
Increased funding for NERSC will support site preparations for relocation to a new computing facility. ESnet begins production use of 100Gbps optical ring. Both the Argonne and Oak Ridge LCFs will be upgraded to 10 petaflops with reduced funding for infrastructure investments.			
Research and Evaluation Prototypes is reduced to support research in data-intensive science and will focus on long-lead time R&D in breakthrough technologies that will enable novel hardware designs for Exascale computing with priority given to early-stage technology development.			
Total, Advanced Scientific Computing Research	440,868	455,593	+14,725

Mathematical, Computational, and Computer Sciences Research
Funding Profile by Activity

	(Dollars in Thousands)		
	FY 2011 Current	FY 2012 Enacted	FY 2013 Request
Applied Mathematics	45,604	45,604	49,500
Computer Science	47,301	47,400	54,580
Computational Partnerships	52,813	44,250	56,776
Next Generation Networking for Science	12,313	12,751	16,194
SBIR/STTR	0[a]	4,560	5,570
Total, Mathematical, Computational, and Computer Sciences Research	158,031	154,565	182,620

[a] In FY 2011, $4,128,000 was transferred to the Small Business Innovation Research (SBIR) program and $496,000 was transferred to the Small Business Technology Transfer (STTR) program.

Overview

The Mathematical, Computational, and Computer Sciences Research subprogram supports activities aimed at effectively utilizing the Department's forefront computational and networking capabilities to advance DOE missions. Computational science is increasingly central to progress at the frontiers of science and to our most challenging engineering problems. Accordingly, the subprogram must be positioned to address scientifically challenging questions, to deliver:

- new mathematics required to more accurately model systems involving processes taking place on vastly different time and length scales such as the earth's climate and the behavior of living cells;
- software, tools and middleware to efficiently and effectively harness the potential of today's high performance computing systems and advanced networks for DOE science and engineering applications;
- operating systems, data management, analyses, representation model development, user interfaces, and other tools are required to make effective use of future-generation supercomputers and the data sets from current and future scientific user facilities;
- computer science and algorithm innovations that increase the energy efficiency of future-generation supercomputers; and
- networking and collaboration tools to make scientific resources readily available to scientists, regardless of whether they are in a university, national laboratory, or industrial setting.

Explanation of Funding Changes

The challenges of high performance computing systems on the path to exascale, the demands of DOE's data-intensive research, and the need for future collaborations and scientific user facilities require us to look ahead and make long-term, coordinated investments across the ASCR research portfolio with continuous monitoring of relevance and performance. For example, basic research in Applied Mathematics and Computer Science, coupled to expertise from the facilities, is required to realize the significant potential that exists in data produced by DOE research and facilities. Research in Computational Partnerships addresses application specific challenges, end user tools for data management and visualization, and challenges from emerging hardware. Next Generation Networking for Science provides the tools and middleware that enables moving and sharing facilities and collaboration data.

	(Dollars in Thousands)		
	FY 2012 Enacted	FY 2013 Request	FY 2013 vs. FY 2012
Applied Mathematics	45,604	49,500	+3,896
New research efforts will be supported to address the mathematical challenges of the massive quantities of high throughput data at scientific user facilities. These efforts will focus on novel mathematical analysis techniques necessary to understand and extract meaning from these massive datasets.			
Computer Science	47,400	54,580	+7,180
New research efforts will be supported to develop tools and software to address the challenges of data-intensive science and of capturing, storing, visualizing, and analyzing massive, high throughput data from scientific user facilities. These efforts will look at the full spectrum of computer science data challenges—from hardware to user interfaces and tools.			
Computational Partnerships	44,250	56,776	+12,526
New research efforts across this activity will engage partners across the Office of Science to address data challenges at the application level. One new Co-Design Center will be supported with a focus on the challenges to data-intensive science from emerging hardware. New Science Application partnerships will be added to focus on data challenges from the scientific user facilities, and a dedicated SciDAC Institute for Scientific Data Management Analysis and Visualization will also be supported.			
Next Generation Networking for Science	12,751	16,194	+3,443
New research efforts will be supported to address the challenges of moving, sharing, and validating massive quantities of data from DOE scientific user facilities and large scale collaborations. This includes the challenges in building, operating, and maintaining the network infrastructure over which these data pass.			
SBIR/STTR	4,560	5,570	+1,010
In FY 2011, $4,128,000 and $496,000 were transferred to the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs, respectively. SBIR/STTR funding is set at 2.95% of non-capital funding in FY 2012 and 3.05% in FY 2013.			
Total, Mathematical, Computational, and Computer Sciences Research	154,565	182,620	+28,055

Applied Mathematics

Overview

The Applied Mathematics activity supports the research and development of applied mathematical models, methods, and algorithms for understanding complex natural and engineered systems related to DOE's mission. These mathematical models, methods, and algorithms are the fundamental building blocks for describing physical and biological systems computationally. Applied Mathematics research underpins all of DOE's modeling and simulation efforts.

This activity supports the development of

- numerical methods related to problems such as fluid flow, magneto-hydrodynamics, wave propagation, and other natural or physical processes;
- computational meshing tools for developing ways in which physical domains can be efficiently partitioned into smaller, possibly geometrically complex, regions as part of a larger-scale simulation;
- advanced linear algebra libraries for fast and efficient numerical solutions of linear algebraic equations that often arise when simulating physical processes;
- optimization of mathematical methods for minimizing energy or cost, finding the most efficient solutions to engineering problems, or discovering physical properties and biological configurations;
- multiscale mathematics and multiphysics computations for connecting the very large with the very small, the very long with the very short, and multiple physical models in a single simulation;
- uncertainty quantification methodology and techniques to improve our overall understanding of complex scientific and engineering problems and allow us to make quantitative predictions about the behavior of these systems;
- efficient new mathematical models, algorithms, libraries, and tools for next generation computers that blur the boundary between applied mathematics and computer science;
- mathematics for the analysis of extremely large datasets for identifying key features, determining relationships between the key features, and extracting scientific insights from large, complex data sets; and
- mathematical optimization and risk assessment in complex systems such as cyber security or the electric grid that address anomalies in existing engineered systems, modeling of large-scale systems, and understanding dynamics and emergent behavior in these systems.

Funding and Activity Schedule

Fiscal Year	Activity	Funding ($000)
2011 Current	Basic research activities continue for fundamental mathematical advances and computational breakthroughs across DOE and Office of Science missions—including model formulation and algorithm development to realize the potential from the ultra-low power, multicore-computing future. The Computational Science Graduate Fellowship (CSGF) program is funded at $6,000,000 within this activity.	45,604
2012 Enacted	The recompetition of mathematics of large datasets is delayed until 2013 to allow more workshops to focus these efforts on emerging challenges. This allows for increased support for Uncertainty Quantification in 2012. Uncertainty Quantification is important to understanding the results from petascale simulations and has been deemed critical to realizing the potential of exascale computing for predictive science. For many problems in the fields of natural sciences and engineering, incomplete descriptions, measurements, and data for these problems introduce uncertainties as	45,604

Fiscal Year	Activity	Funding ($000)
	researchers attempt to understand complex phenomena through computer modeling and simulation. As we increase the use of computing to study such problems, the development of more sophisticated techniques for the incorporation and quantification of uncertainties becomes key to our success. New efforts in the research and development of uncertainty quantification methodology and techniques will improve our overall understanding of complex scientific and engineering problems and allow us to make quantitative predictions about the behavior of these systems. The Computational Science Graduate Fellowship (CSGF) program is funded at $6,000,000.	
2013 Request	FY 2013 supports new and redirected research efforts to develop new algorithms and methods that address the challenges of data-intensive science. There are two broad categories in which DOE's missions lead to unique data-centric computing needs: advanced computing to simulate complex physical and engineering systems and DOE's advanced experimental resources. DOE researchers routinely compute detailed simulations of time-dependent 3D systems on the world's largest computers. These simulations generate enormous datasets that are difficult to extract and archive, let alone analyze. As leadership-class computers continue to grow in size, the data analysis problems will be a major scientific challenge. In addition, current DOE facilities and collaborations generate petabytes of data per year. Planned facilities will generate as much data each day. These trends present many challenges to the facilities and to the scientific user communities. Advancing data-intensive science is critical for understanding simulations of combustion, global climate modeling and cosmology, as well as understanding data from neutron scattering facilities, x-ray observatories, systems biology, and complex engineered systems such as the power grid. The increasing size and complexity of data related to DOE simulations, collaborations, and experimental facilities requires the development of novel mathematical analysis techniques to understand and extract meaning from these massive datasets. New methods are also necessary for analyzing and understanding uncertainty, especially in the face of noisy and incomplete data, and near real-time identification of anomalies in streaming and evolving data to detect and respond to phenomena that are either short-lived or urgent. New research efforts will focus on understanding, representing and learning from these massive DOE datasets. The Computational Science Graduate Fellowship (CSGF) program is funded at $6,000,000. New fellows in FY 2013 will be fully funded.	49,500

Computer Science

Overview

The Computer Science activity supports research to utilize computing at extreme scales and to understand extreme scale data from both simulations and experiments. Industry reports indicate that because of power constraints, data movement, rather than computational operations, will be the limiting factor for future systems. Memory per core is expected to decline sharply while the performance of storage systems will lag even further behind the computational capability of the systems. Multi-level storage architectures that span multiple types of hardware are anticipated and will require the Activity to support research that develops new approaches to run-time data management and analysis.

A fundamental challenge for researchers supported by this activity is enabling science applications to harness computer systems with increasing scale and increasing complexity that take advantage of technology advances such as multicore chips and specialized “accelerator” processors. This will require developing system software (operating systems, file systems, compilers, and performance tools) with more dynamic behavior than historically developed to deal with time varying power and resilience requirements. Substantial innovation is needed to provide essential system software functionality in a timeframe consistent with the anticipated availability of hardware.

This activity supports the development of: operating and file systems for extreme scale computers with many thousands of multi-core processors and complicated interconnection networks; performance and productivity tools for extreme scale systems that enable users to diagnose and monitor the performance of software and scientific application codes to enable users to improve performance and get scientific results faster; programming models that enable today’s computations and discover new models that scale to hundreds of thousands of processors to simplify application code development for petascale computing; approaches to simulate and understand the impact of advanced computer architectures on scientific applications critical to the Department; data management and visualization tools to transform extreme scale data into scientific insight through investments in visualization tools that scale to multi-petabyte datasets and innovative approaches to indexing and querying data; and efficient new mathematical models, algorithms, libraries, and tools for next generation computers that blur the boundary between applied mathematics and computer science.

Funding and Activity Schedule

Fiscal Year	Activity	Funding ($000)
2011 Current	Basic research activities continue to enable critical DOE applications to utilize computing at extreme scales and to understand data from both simulations and experiments. This focus of efforts was critical to realizing the potential of ultra-low power, high performance multicore computing.	47,301
2012 Enacted	In FY 2012, the Computer Science activity focuses on the challenges of emerging extreme scale architectures containing as many as a billion cores and hybrid processors (such as mixed Central Processing Unit/Graphical Accelerator nodes). Research efforts continue in advanced architectures and related technologies for exascale computing including the associated software with significant investments in simulators for future systems.	47,400

Fiscal Year	Activity	Funding ($000)
2013 Request	FY 2013 supports new research efforts to address the challenges of data-intensive science with a focus on full data lifecycle management and analysis for the massive data from DOE scientific user facilities. These efforts will look at the full spectrum of the computer science data challenges from hardware to user interfaces and tools. This builds on decades of DOE leadership in this area of computer science and will be informed by recent ASCR workshops and reports including the requirements gathering workshops of NERSC and ESnet and the exascale series of workshops that identified many data challenges across DOE communities and those associated with the complexity of emerging hardware.	54,580

Computational Partnerships

Overview

The Computational Partnerships activity supports the Scientific Discovery through Advanced Computing (SciDAC) program to dramatically accelerate progress in scientific computing that delivers breakthrough scientific results through partnerships between applied mathematicians, computer scientists, and scientists from other disciplines. These efforts apply results from Applied Mathematics and Computer Science core research to scientific applications sponsored by other SC programs. These partnerships enable scientists to conduct complex scientific and engineering computations on leadership-class and high-end computing systems at a level of fidelity needed to simulate real-world conditions. SciDAC applications pursue computational solutions to challenging problems in climate science, fusion research, high energy physics, nuclear physics, astrophysics, material science, chemistry, particle accelerators, biology, and the reactive subsurface flow of contaminants through groundwater.

Over the past decade, SciDAC has influenced and shaped the development of a distinct approach to science and engineering research through high performance computation. Today the SciDAC program is recognized as the leader in accelerating the use of high-performance computing to advance the state of knowledge in science applications.

SciDAC focuses on the very high end of high performance computational science and engineering and faces two distinct challenges: to broaden the community and thus the impact of high performance computing, particularly to address the Department's missions, and to ensure that further progress at the forefront is enhanced rather than curtailed by the emergence of hybrid, multi-core architectures. A decade of effort has enabled this program to simultaneously meet both of these important challenges. SciDAC has also shown U.S. industry new ways to use computing to improve competitiveness.

Looking to the challenges of the future, the SciDAC portfolio was recompeted and streamlined in FY 2011 and FY 2012 to support strategic investments in petascale scientific discovery (Institutes and Science Applications) and Co-Design Centers focused on advancing applications that need exascale computing systems while informing the designs of the emerging hardware.

Funding and Activity Schedule

Fiscal Year	Activity	Funding ($000)
2011 Current	Supported completion of the current SciDAC portfolio and ensured that results were published and tools widely distributed to broaden the impact of these efforts. The ten ASCR-led SciDAC Centers and Institutes awarded in FY 2006 were recompeted and replaced with three tightly integrated SciDAC Institutes in a restructuring of the program. The SciDAC Institutes are multi-institutional teams focused on delivering the applied mathematics and computer science needed for current scientific applications to make effective use of the multi-petaflop computing systems available in the near-term. These smaller, more closely integrated efforts provide a more efficient one-stop-shop for the scientific applications recompeted in FY 2012. Co-Design Centers are multi-institutional teams focused on understanding how to reformulate applications, algorithms and software (applied mathematics and computer science) to address the longer-term challenges of future computing systems with the intent to also influence the design of those systems and address the requirements of science and engineering. Three Co-Design Centers were initiated in FY 2011 with the selection of collaborations comprised of researchers in critical DOE applications (materials, combustion, and nuclear engineering), core Computer Science and Applied Mathematics researchers and hardware vendors. One important factor in the selection of these three particular applications areas was the fact that collectively they use and will advance	52,813

Fiscal Year	Activity	Funding ($000)
	many of the methods (structured and adaptive grids, dense and sparse linear algebra, particle methods, etc.) that span the DOE application space.	
2012 Enacted	In partnership with other Office of Science programs, ASCR is recompeting the Science Applications with a focus on the highest priorities of the partner programs and on development of community codes with sustained multi-petaflop performance. The selected applications will work with the ASCR-led SciDAC Institutes to enhance capabilities and ready codes for the 10 petaflop leadership computing systems available in FY 2013. These efforts will support areas such as nuclear physics, with relevance for basic research, national security, and nuclear engineering; earth system models to understand and quantify the impact of energy production and use on the environment; fusion simulations; accelerator design to make more effective use of existing facilities and inform plans for future facilities; combustion to improve the efficiency of fossil energy sources; and advanced materials for energy and national security applications. In addition, ASCR will establish a SciDAC Institute for Scientific Data Management, Analysis and Visualization to provide a single point of contact for scientists participating in the Science Applications to leverage ASCR expertise to more efficiently and effectively manage, analyze, visualize and understand their scientific data. The materials, combustion, and nuclear engineering Co-Design Centers will continue.	44,250
2013 Request	New research efforts will engage partners across the Office of Science to address the data-intensive science challenges at the science application level. ASCR will support an additional Co-Design Center with a focus on the challenges to data-intensive science from emerging hardware. This effort will engage SC scientific user facilities at forefront of the data challenge that are also dependant on leveraging commercially available hardware. In addition, new Science Applications will be added, in partnership with the other programs, to focus on the unique data challenges from their scientific user facilities. These efforts will be informed through a series of workshops such as the joint ASCR-BES workshop "*Data and Communications in Basic Energy Sciences: Creating a Pathway for Scientific Discovery***"** held in early FY 2012. The dedicated SciDAC Institute for Scientific Data Management, Analysis and Visualization will continue to be supported as well as the other projects selected in FY 2011 and FY 2012.	56,776

Next Generation Networking for Science

Overview

To facilitate scientific collaborations, ASCR has played a leading role in driving development of the high-bandwidth networks connecting researchers to facilities, data, and each other. The invisible glue that binds today's networks—passing trillions of bits across the world—has roots in ASCR-supported research. For example, ASCR-supported researchers helped establish critical protocols on which the Internet is based. Next Generation Networking for Science research makes possible international collaborations such as the Large Hadron Collider and underpins virtual meeting and other commercial collaboration tools. These research efforts build upon results from Computer Science and Applied Mathematics to develop integrated software tools and advanced network services to utilize new capabilities in ESnet to advance DOE missions. These efforts broaden opportunities for other government agencies, U.S. industry, and the American people.

Funding and Activity Schedule

Fiscal Year	Activity	Funding ($000)
2011 Current	Basic research activities continue to address advanced network technologies, high-performance software stacks, and distributed systems software to facilitate the distribution and sharing of scientific data generated by large-scale scientific collaborations. All networking research projects have a limited life span—research continues until tools and middleware are considered robust enough to be put into production on ESnet or in program-sponsored grid efforts such as the Open Science Grid. In FY 2011, 15 university and 16 national laboratory projects totaling $9,800,000 successfully completed their work, which was put into production. The successful completion of these projects enabled support of new research activities critical to realizing the potential from the prototype ultra-high throughput optical networks supported by the Advanced Networking Initiative to meet the growing needs large-scale scientific collaborations.	12,313
2012 Enacted	In FY 2012, research will continue to focus on developing networking software, middleware, and hardware that delivers 99.999% reliability while allowing the successful products of prior research to transition into operation. Research in this activity will continue to make critical investments, including new protocols that allow hosts to rapidly and efficiently adapt to network conditions to maximize the available bandwidth, new routing algorithms that can improve the performance of routers and switches, a rich suite of secure collaboration tools and services, and advanced simulation environments that duplicate real networks to ensure that science communities achieve their goals.	12,751
2013 Request	FY 2013 supports new research efforts to address the data-intensive science challenges facing scientific communities using unique DOE facilities and engaging in large-scale collaborations. Currently these user communities generate and share multi-petabyte datasets that pass through ESnet and are stored and shared within program-sponsored grids. These datasets will continue to grow, surpassing exabyte scales in the next few years. This presents many challenges in moving, sharing, analyzing, and validating such massive quantities of data. It also presents new challenges in building, operating, and maintaining the network infrastructure over which data passes. This activity focuses on developing new middleware and networking tools for moving, sharing, and verifying such massive datasets and on innovative analysis tools and services.	16,194

High Performance Computing and Network Facilities
Funding Profile by Activity

	(Dollars in Thousands)		
	FY 2011 Current	FY 2012 Enacted	FY 2013 Request
High Performance Production Computing	59,514	57,800	65,605
Leadership Computing Facilities	158,020	156,000	145,000
Research and Evaluation Prototypes	4,301	30,000	22,500
High Performance Network Facilities and Testbeds	30,451	34,500	32,000
SBIR/STTR	0[a]	8,003	7,868
Total, High Performance Computing and Network Facilities	252,286	286,303	272,973

[a] In FY 2011, $6,300,000 was transferred to the Small Business Innovation Research (SBIR) program and $756,000 was transferred to the Small Business Technology Transfer (STTR) program.

Overview

The High Performance Computing and Network Facilities subprogram delivers forefront computational and networking capabilities to scientists nationwide. These include high performance production computing at the National Energy Research Scientific Computing Center (NERSC) facility at LBNL and Leadership Computing Facilities (LCFs) at Oak Ridge and Argonne National Laboratories. These computers, and the other SC research facilities, generate many petabytes of data each year. Moving data to the researchers who need them requires advanced scientific networks and related technologies provided through High Performance Network Facilities and Testbeds, which includes the Energy Science network (ESnet). The Research and Evaluation Prototypes activity invests in long-term needs that will play a critical role in achieving exascale computing.

Computing resources are allocated through competitive processes. Up to 60% of the processor time on the LCFs is allocated through the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program, which is open to all researchers and results in awards to 20–30 large projects per year. The high performance production computing facilities at NERSC are predominately allocated to researchers supported by SC programs. Remaining processor time on the LCFs and NERSC is allocated through the ASCR Leadership Computing Challenge (ALCC). ALCC is open year-round to scientists from the research community in the national labs, academia and industry for special situations of interest to DOE with an emphasis on high-risk, high-payoff simulations in areas directly related to the DOE's energy mission, for national emergencies, or for broadening the community of researchers capable of using leadership computing resources.

Allocations on ASCR facilities provide critical resources for the scientific community following the public access model used by other SC scientific user facilities. In addition, ASCR facilities provide a crucial testbed for U.S. industry to deploy the most advanced hardware and have it tested by the leading scientists across the country in universities, national laboratories, and industry.

Explanation of Funding Changes

The challenges of developing and utilizing the ultra-low power, high performance multicore-computing systems on the path to exascale while meeting the demands of critical DOE applications require sustained, coordinated research and hardware investments across the ASCR research portfolio with innovation and collaboration key to continued progress. New Research and Evaluation prototype investments in critical technologies are central to these efforts.

	(Dollars in Thousands)		
	FY 2012 Enacted	FY 2013 Request	FY 2013 vs. FY 2012
High Performance Production Computing	57,800	65,605	+7,805
Increase support for site preparations for the planned relocation of NERSC to a new computing facility.			
Leadership Computing Facilities	156,000	145,000	-11,000
LCFs upgraded to 10 petaflops with reduced funding for infrastructure investments.			
Research and Evaluation Prototypes	30,000	22,500	-7,500
Funds will support R&D in breakthrough technologies that will enable novel hardware designs for Exascale computing; awards will prioritize early-stage technology development. This activity is reduced to allow for investments in other areas to address the urgent challenges of data-intensive science.			
High Performance Network Facilities and Testbeds	34,500	32,000	-2,500
ESnet completes installation and begins production use of 100 Gbps optical ring.			
SBIR/STTR	8,003	7,868	-135
In FY 2011, $6,300,000 and $756,000 were transferred to the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs, respectively. SBIR/STTR funding is set at 2.95% of non-capital funding in FY 2012 and 3.05% in FY 2013.			
Total, High Performance Computing and Network Facilities	286,303	272,973	-13,330

High Performance Production Computing

Overview

This activity supports the National Energy Research Scientific Computing Center (NERSC) facility located at LBNL. NERSC delivers high-end production computing services for the SC research community. Annually, over 4,000 computational scientists in about 500 projects use NERSC to perform basic scientific research across a wide range of disciplines including astrophysics, chemistry, climate modeling, materials, high energy and nuclear physics, and biology. NERSC enables teams to perform modeling, simulation, and data analysis on some of the most capable computational and storage systems in the world to address some the biggest scientific challenges within the SC mission. NERSC users come from nearly every state in the U.S., with about 65% based in universities, 25% in DOE laboratories, and 10% in other government laboratories and industry. NERSC's large and diverse user base requires an agile support staff to aid users entering the high performance computing arena for the first time as well as those preparing codes to run across the largest machines available at NERSC and other SC computing facilities.

NERSC is a vital resource for the SC research community and it is consistently oversubscribed, with requests exceeding capacity by a factor of 3–10. This gap between demand and capability exists despite regular upgrades to the primary computing systems approximately every 3 years. NERSC regularly gathers requirements from SC programs through a robust process that informs NERSC upgrade plans. These requirements activities are also vital to planning for SciDAC and other ASCR efforts to prioritize research directions and inform the community of new computing trends, especially as the computing industry moves toward heterogeneous, multi-core computing.

Funding and Activity Schedule

Fiscal Year	Activity	Funding ($000)
2011 Current	In FY 2011, this activity supported staff, operations and lease payments for the NERSC high-end capability systems—the 352 teraflop Cray XT4 (NERSC-5) and the newly upgraded over 1 petaflop Cray XE6 (NERSC-6). NERSC also provided users with access to smaller clusters and testbeds and the global storage systems that enable users to easily migrate to any of the available resources.	59,514
2012 Enacted	Support operation of the NERSC high-end capability systems (NERSC-5 and NERSC-6), lease payments, user support, and preparation for future system upgrades.	57,800
2013 Request	Supports staff, maintenance, operations and lease payments for the NERSC high-end capability systems, including an upgrade from NERSC-5 to a planned NERSC-7, while NERSC-6 remains in production. The NERSC-7 upgrade requires more power and space than available at the current site. NERSC will select a new site in 2012. The funding increase supports site preparations in FY 2013 for the planned relocation of NERSC to a new site.	65,605

Leadership Computing Facilities

Overview

The Leadership Computing Facilities (LCFs) enable open scientific applications, including industry applications, to harness the potential of leadership computing to advance science and engineering. The era of petaflop science opened significant opportunities to dramatically advance research, as simulations more realistically capture complex behavior in natural and engineered systems. The success of this effort is built on the gains made in Research and Evaluation Prototypes and ASCR research efforts. LCF staff operates and maintains forefront computing resources. One LCF strength is the staff support provided to INCITE projects, ASCR Leadership Computing Challenge projects, scaling tests, and tool and library developers. Support staff experience is critical to the success of industry partnerships to address the challenges of next-generation computing.

The Oak Ridge Leadership Computing Facility (OLCF) 2.3 petaflop Cray XT5 system is one of the most powerful computers in the world for scientific research. Through INCITE allocations, several applications, including combustion studies in diesel jet flame stabilization, simulations of neutron transport in fast reactor cores, and groundwater flow in porous media, are running at the petascale. OLCF staff is sharing its expertise with industry to broaden the benefits for the Nation. For example, OLCF worked with Boeing to significantly reduce the need for costly physical prototyping and wind tunnel testing; with Ramgen to advance the development curve of their CO_2 compressor with a next generation rotor, which is scheduled for testing in early 2012; and with BMI trucking to increase fuel efficiency in 18 wheelers. The OLCF will complete its planned upgrade to 10 petaflops in FY 2013.

The Argonne Leadership Computing Facility (ALCF) provides a high performance 556 teraflop peak capability IBM Blue Gene/P with low-electrical power requirements. It will be upgraded in FY 2012 to the next generation system, an IBM Blue Gene/Q, with peak capability of approximately 10 petaflops. The Blue Gene/Q was developed through a joint research project with NNSA, IBM, and ASCR's Research and Evaluation Prototypes activity. The ALCF and OLCF systems are architecturally distinct and this diversity of resources benefits the Nation's HPC user community. ALCF supports many applications, including molecular dynamics and materials, for which it is better suited than OLCF or NERSC. Through INCITE, ALCF also transfers its expertise to industry, including working with Proctor and Gamble to study the complex interactions of billions of atoms to determine how tiny submicroscopic structures impact the characteristics of the ingredients in soaps, detergents, lotions, and shampoos, as well as in fire retardants and foams used in national security applications.

Funding and Activity Schedule

Fiscal Year	Activity	Funding ($000)
2011 Current	In FY 2011, this activity supported staff, operations, and lease payments for the computer systems at the two Leadership Computing Facilities. Funding also supported significant investment in infrastructure equipment including storage arrays, network switches, and disks.	158,020
2012 Enacted	In FY 2012, this activity supports staff, operations, and lease payments. OLCF will complete site preparations and phase 1 of their upgrade of the Cray XT5 to a 10 petaflop Cray XK6 by replacing the processor boards and interconnects, while continuing to support users and managing INCITE allocations. At ALCF, installation and operation of an IBM Blue Gene/Q test and development system in early FY 2012 provides early science access to the Blue Gene/Q architecture, with installation of the full 10 petaflop upgrade completed by the end of FY 2012. The upgrade will be tested and a decision on acceptance made in FY 2013. In addition, the ALCF will support users and manage INCITE allocation of the Blue Gene/P.	156,000

Fiscal Year	Activity	Funding ($000)
2013 Request	In FY 2013, this activity supports staff, operations, and lease payments. OLCF will complete phase 2 of the upgrade with the addition of GPUs to a portion of the Cray XK6 cabinets taking it to 10 petaflops and will provide access to early science applications. Overall funding is reduced in FY 2013 due to reduced funding for infrastructure upgrades. ALCF will support full operation and INCITE allocations of the Blue Gene/Q with associated increased lease and power payments.	145,000

	(Dollars in Thousands)		
	FY 2011 Current	FY 2012 Enacted	FY 2013 Request
Leadership Computing Facility at ANL	62,000	62,000	63,000
Leadership Computing Facility at ORNL	96,020	94,000	82,000
Total, Leadership Computing Facilities	158,020	156,000	145,000

Research and Evaluation Prototypes

Overview

DOE has been at the forefront of leadership computing for science and national security applications for decades. ASCR continues to invest in leadership class systems at Argonne and Oak Ridge, which play a key role in the health of the U.S. high performance computing industry. However, the challenges of the future require long-lead time investments in critical technologies. Research partnerships among ASCR, NNSA, the national laboratories, and researchers, including industry, are critical to ensuring that emerging systems are capable of meeting the demands of DOE mission applications—including our power restrictions. This will require basic research innovation from the underlying components to architectures—and the formulation of scientific applications that are tightly coupled to ASCR and NNSA co-design efforts. In addition to advancing DOE missions, these investments have the potential to dramatically impact the entire computing infrastructure for science, engineering, and industry by the end of the decade.

The Research and Evaluation Prototypes activity addresses the challenges of next generation computing systems. By actively partnering with the research community, including industry, on the development of technology that enables next-generation machines, ASCR research can help accelerate the development of architectures that serve the needs of the scientific community, while application and software researchers can gain a better understanding of future systems to get a head start in developing software and models to take advantage of the new capabilities. Research and Evaluation Prototypes prepares researchers to effectively utilize the next generation of scientific computers and seeks to reduce risk for future major procurements.

Funding and Activity Schedule

Fiscal Year	Activity	Funding ($000)
2011 Current	Completed SC's partnership with the NNSA and the Defense Advanced Research Projects Agency (DARPA) program for High Productivity Computing Systems. Expanded partnership with the NNSA to explore architectures on the path toward exascale computing.	4,301
2012 Enacted	ASCR will partner with NNSA and work with the research community, including industry, to deliver high bandwidth, power efficient memory technology for future computer systems. This activity will support basic research and development to optimize the performance and energy capabilities of emerging hybrid memory technology. These investments are critical because the current commercial roadmaps indicate that memory power requirements will dominate the power budgets for computers targeted at scientific and engineering applications. The goal of these efforts is to deliver low-energy, high performance memory with the 10–100 fold improvement over current commercial offerings that is required for DOE applications. This approach eases the path to broad commercial adoption in this decade—from individual laptops to servers—leading to energy efficiency gains across the information technology (IT) sector. In addition, this activity will support partnerships with NNSA and the research community, including industry, to advance the Department's goals for exascale computing. Significant technical challenges must be faced in meeting the needs of the computational science and engineering community over the next decade, among these are power, performance, concurrency, cost, and resiliency. The system goals are aggressive, and thus tradeoffs will be necessary—for example, reducing memory bandwidth would reduce system power but negatively affect science application performance.	30,000

Fiscal Year	Activity	Funding ($000)
2013 Request	This activity will continue research started in FY 2012 with NNSA and the research community, including industry, to develop critical technologies and low level software architectures that enable the creation of high performance scientific applications for these computers, as well as the smaller scale commercial versions that will be ubiquitous in the scientific infrastructure.	22,500

High Performance Network Facilities and Testbeds

Overview

The Energy Sciences Network (ESnet) provides the national network and networking infrastructure connecting DOE science facilities and SC laboratories with other institutions connected to peer academic or commercial networks. This network allows scientific users to effectively and efficiently access, distribute, and analyze the massive amounts of data produced by these science facilities.

The costs for ESnet are dominated by operations, including refreshing switches and routers on the schedule needed to ensure the 99.999% reliability required for large-scale scientific data transmission. Additional funds are used to support the testing and evaluation of new technologies and services that will be required to keep up with the data volume of new DOE facilities and unique DOE scientific instruments.

Funding and Activity Schedule

Fiscal Year	Activity	Funding ($000)
2011 Current	In FY 2011, ESnet acquired the optical technologies and infrastructure needed to expand ESnet capacity and allow incremental upgrades over several years. The new infrastructure will support both scientific user communities' current production needs and allow for the creation of testbeds to experiment with new technologies and services in a contained environment. This testbed provides unique capabilities for networking and cyber security researchers to test new ideas and concepts at scale without risking disruption to production traffic. ESnet deployed a Nation-wide 100 gigabit-per-second (Gbps) prototype network in FY 2012 connecting the three ASCR computing facilities and the European peering point in New York. This prototype will allow ESnet to verify the operation of emerging 100 Gbps technologies.	30,451
2012 Enacted	ESnet will operate the network infrastructure to support critical DOE science applications and unique SC facilities. Building on 2011 procurements, ESnet will transition the 100 Gbps prototype network to production service replacing the 10 Gbps production link to this first segment of the ESnet backbone. In addition, 100 Gbps production network will be extended to additional SC laboratories by upgrading and connecting the Bay area metropolitan ring.	34,500
2013 Request	ESnet will operate the network infrastructure to support critical DOE science applications and SC facilities. ESnet will continue to extend deployment of 100 Gbps capacity to additional SC laboratories by upgrading additional segments of the backbone network and Metropolitan Area Networks to 100 Gbps speeds.	32,000

Supporting Information

Operating Expenses, Capital Equipment, and Construction Summary

(Dollars in Thousands)

	FY 2011 Current	FY 2012 Enacted	FY 2013 Request
Operating Expenses	390,135	425,868	440,593
Capital Equipment	20,182	15,000	15,000
Total, Advanced Scientific Computing Research	410,317	440,868	455,593

Funding Summary

(Dollars in Thousands)

	FY 2011 Current	FY 2012 Enacted	FY 2013 Request
Research	162,332	180,005	199,550
Scientific User Facility Operations	247,985	248,300	242,605
Other	0	12,563	13,438
Total, Advanced Scientific Computing Research	410,317	440,868	455,593

Scientific User Facility Operations

(Dollars in Thousands)

	FY 2011 Current	FY 2012 Enacted	FY 2013 Request
NERSC	59,514	57,800	65,605
OLCF	96,020	94,000	82,000
ALCF	62,000	62,000	63,000
ESnet	30,451	34,500	32,000
Total, Scientific User Facility Operations	247,985	248,300	242,605

Facilities Users and Hours

	FY 2011 Current	FY 2012 Enacted	FY 2013 Request
NERSC			
Achieved Operating Hours	8,474	N/A	N/A
Planned Operating Hours	8,585	8,585	8,585
Optimal Hours	8,585	8,585	8,585
Percent of Optimal Hours	98.7%	100%	100%
Unscheduled Downtime	1.3%	1%	1%
Number of Users	3,500	4,000	4,200

	FY 2011 Current	FY 2012 Enacted	FY 2013 Request
ESnet			
Achieved Operating Hours	8,760	N/A	N/A
Planned Operating Hours	8,760	8,760	8,760
Optimal Hours	8,760	8,760	8,760
Percent of Optimal Hours	99.999%	99.999%	99.999%
Unscheduled Downtime	0.001%	0.001%	0.001%
Number of Users [a]	N/A	N/A	N/A
OLCF			
Achieved Operating Hours	6,672	N/A	N/A
Planned Operating Hours	7,008	7,008	7,008
Optimal Hours	7,008	7,008	7,008
Percent of Optimal Hours	95.2%	100%	100%
Unscheduled Downtime	4.8%	1%	1%
Number of Users	625	625	700
ALCF			
Achieved Operating Hours	6,854	N/A	N/A
Planned Operating Hours	7,008	7,008	7,008
Optimal Hours	7,008	7,008	7,008
Percent of Optimal Hours	97.8%	100%	100%
Unscheduled Downtime	2.2%	1%	1%
Number of Users	350	350	450
Total			
Achieved Operating Hours	30,760	N/A	N/A
Planned Operating Hours	31,361	31,361	31,361
Optimal Hours	31,361	31,361	31,361
Percent of Optimal Hours	97.3%	100%	100%
Unscheduled Downtime	2.1%	1%	1%
Number of Users	4,475	4,975	5,350

[a] ESnet is a high performance scientific network that connects DOE facilities to researchers around the world and it is therefore not possible to estimate users.

Scientific Employment

	FY 2011 Current	FY 2012 Enacted	FY 2013 Request
# University Grants	210	210	210
Average Size	$232,000	$247,000	$262,000
# Laboratory Projects	180	175	188
# Graduate Students (FTEs)	563	563	614
# Permanent Ph.D.s (FTEs)	772	770	812
# Other (FTEs)	274	270	280