Advanced Scientific Computing Research

Overview

The Advanced Scientific Computing Research (ASCR) program's mission is to advance applied mathematics and computer science; deliver the most advanced computational scientific applications in partnership with disciplinary science; advance computing and networking capabilities; and develop future generations of computing hardware and tools for science, in partnership with the research community, including U.S. industry. The strategy to accomplish this has two thrusts: developing and maintaining world-class computing and network facilities for science; and advancing research in applied mathematics, computer science and advanced networking.

U.S. private- and public-sector organizations are increasingly using supercomputers to achieve breakthroughs of major scientific or economic importance. These achievements have already advanced U. S. competitiveness^a and were, in many cases, accomplished through access to very powerful supercomputers and High Performance Computing (HPC) experts at the Department of Energy (DOE) national laboratories using tools developed with support from ASCR. ASCR has a strong track record of supporting innovative scientific computing. Researchers using ASCR facilities have: made discoveries in functional materials, fundamental studies of turbulence in chemically reacting systems, climate change, and in the understanding of the physical properties of matter, such as the quark-gluon nature of nuclear matter; modeled 3-D full-core reactor neutron transport to predict the behavior of novel nuclear fuels in fission reactors; conducted 3-D turbulent combustion simulations of hydrocarbons to increase fuel efficiency; made U.S. airplane engines quieter, more fuel efficient, and less polluting; made long haul trucks more energy efficient in record time; simulated ice formation in million-molecule water droplets to reduce the wind turbine downtime in cold climates; and are identifying novel materials for use in extreme energy environments.

According to a recent study by the Council on Competitiveness^b, U.S. companies that use high performance computing to deliver a competitive edge, "...are confident their organizations could consume up to 1,000-fold increases in capability and capacity in a relatively short amount of time" but 92% see "scalability of software" as a significant barrier to delivering on that potential followed closely by the cost of the systems, the programmability of the systems, and the availability of expertise.

Numerous reports have documented the challenges of simply scaling existing computer designs to reach exascale. Drawing from these reports and experience, the Advanced Scientific Computing Advisory Committee (ASCAC) identified the top 10 computing technology advancements that are needed to achieve productive, economically viable exascale systems:

- create more energy efficient circuits, power and cooling technologies;
- increase the performance and energy efficiency of data movement through new interconnect technologies;
- integrate advanced memory technologies to dramatically improve capacity and bandwidth;
- develop scalable system software that is power- and resilience- aware;
- invent new programming environments that express massive parallelism, data locality, and resilience;
- create data management software that can handle the volume, velocity and diversity of data that is anticipated;
- reformulate science problems and redesign, or reinvent, their solution algorithms for exascale systems;
- facilitate mathematical optimization and uncertainty quantification for exascale discovery, design, and decision making; ensure correct scientific computation in the face of faults, reproducibility, and algorithm verification challenges; and
- increase the productivity of computational scientists with new software engineering tools and environments.^c

The Office of Science, through ASCR, and the National Nuclear Security Administration (NNSA), have partnered to make strategic investments in hardware, methods, and critical technologies to address the exascale technical challenges and deliver an exascale system. Such a system will help scientists harness the thousand-fold increase in capability to address

^a "Real-World Examples of Supercomputers Used For Economic and Societal Benefits: A Prelude to What the Exascale Era Can Provide", May 2014, International Data Corporation (IDC) #248647

^b "*The Exascale Effect: Benefits of Supercomputing Investment for U.S. Industry*", September 2014, Council on Competitiveness and Intersect360 Research.

^c "Top Ten Exascale Research Challenges", Feb. 10, 2014, Advanced Scientific Computing Advisory Committee (ASCAC).

critical research challenges and will maintain U.S. competitiveness in high performance computing (HPC). These efforts are linked with investments to advance data-intensive science and to effectively use the massive scientific data generated by DOE's unparalleled suite of scientific user facilities and large-scale collaborations. By investing in both next-generation computing and data-intensive science, the ASCR program will enable the community of HPC users to improve and shorten industrial design processes; design advanced materials; better understand dark matter and dark energy; explore possibilities for dramatically increasing fuel efficiency while lowering emissions; design advanced nuclear reactors that are modular, safe, and affordable; improve accuracy of climate predictions; predict and investigate how to control the behavior of fusion plasmas; and calculate the subatomic interactions that determine nuclear structure.

Highlights of the FY 2016 Budget Request

The FY 2016 Budget Request for ASCR makes significant new investments in research and partnerships to advance the Department's goals for capable exascale computing. Capable exascale computing, with a thousand- fold increase in performance over today's systems as measured by science applications important to the DOE mission and HPC scientific community, is the next frontier of development in HPC, extending capability significantly beyond today's petascale computers to address the next generation of scientific, engineering, and large-data problems. The goal of the exascale computing effort in SC is to provide the forefront computing resources needed to meet and advance the Department's science missions into the next decade. This will require major advances in technology, the most important of which are increased parallelism, energy efficiency, and reliability, which are needed for scalable use of these computing systems. Because DOE partners with commercial vendors to accelerate development of commodity parts, its research investments will impact computing at all scales ranging from the largest scientific computers and data farms to department-scale computing to home computers and laptops.

The investment strategy has five components:

- Conduct research, development, and design efforts in hardware, software, and mathematical technologies leading toward capable exascale systems.
- Prepare today's scientific and data-intensive computing applications to exploit fully the capabilities of exascale systems by coordinating their development with the emerging technologies from the research, development, and design efforts.
- Partner with HPC vendors to accelerate the pace of implementation of technologies required for capable exascale computing.
- Acquire and operate increasingly capable computing systems, starting with multi-petaflop machines that incorporate emerging technologies from research investments.
- Collaborate with other Federal agencies to ensure broad applicability of capable exascale computing across the US Government.

Mathematical, Computational, and Computer Sciences Research

To ensure DOE applications can fully exploit an exascale system, this activity will support co-design centers that interact with the vendor partnerships to strengthen feedback loops between DOE applications, research and vendor technologies; research and development of software, tools, and middleware for capable exascale systems; applied mathematics methods that address the challenges from increased parallelism and reliability; software productivity to broaden the impact of capable exascale systems; and data management and advanced storage technologies that are focused on the energy and reliability challenges.

Experiments at several of SC's user facilities, such as the light and neutron sources, and experiments at the Large Hadron Collider (LHC), are migrating towards work flows that need near real-time interaction between instruments and simulations.^a Experiments and simulations are often deeply intertwined as simulations become necessary in the design of large-scale experiments, and data from experiments are analyzed in simulations to inform and guide further experiments. The volume and complexity of data generated have increased such that a focused effort is required to develop theories, tools, and technologies to manage data–from generation through integration, transformation, analysis, and visualization, including collaborative environments; to capture the historic record of the data; and to archive and share it. This request

^a http://science.energy.gov/~/media/ascr/ascac/pdf/reports/2013/ASCAC_Data_Intensive_Computing_report_final.pdf, http://science.energy.gov/~/media/ascr/pdf/research/scidac/ASCR_BES_Data_Report.pdf

supports ASCR efforts in data-intensive science for collaborations with applied mathematicians and computer scientists to address end-to-end data management challenges and develop new scientific workflows.

Software, tools, and methods from core research efforts will be used by the Scientific Discovery through Advanced Computing (SciDAC) partnerships to more effectively use the current and immediate next generation high performance computing facilities.

High Performance Computing and Network Facilities

The Research and Evaluation Prototypes (REP) activity has recently supported R&D partnerships with U.S. vendors to improve the energy efficiency and reliability of critical technologies such as memory, processors, network interfaces, and interconnects for use in next-generation, massively parallel supercomputers. The compute node is the basic building block of a high performance computer where all of these technologies come together. In FY 2016, REP will competitively select R&D partnerships with U.S. computer vendors to initiate the design and development of node and system designs suitable for exascale systems. These efforts will influence the development of prototypes that advance DOE goals and are based on the results of REP investments made in FY 2014-2015. This is an essential component of the Department's exascale computing plan and a key step in the vendor's productization efforts. Industry's full development costs for novel HPC systems are many billions of dollars and cover incorporated technologies that impact commercial offerings across their product line – from laptops and handheld devices to servers and HPC systems. HPC is a small fraction of the overall computing market and direct investment is critical in order to influence the trajectory of technology development. In addition, Industry roadmaps and past experience indicate that vendors will be slow to incorporate novel technologies, such as those developed by REP, in their commercial products. By forging a strong partnership with U.S. vendors with significant direct investment during the design phase, the Department can ensure cohesive development of hardware technologies and applications to deliver exascale capabilities to advance science and engineering.

The Leadership Computing Facilities (LCFs) will continue preparations for planned 75-200 petaflops (pf) upgrades at each site in the 2018-2019 timeframe. Because these upgrades represent technological advances in both hardware and software, funds are included in REP to continue supporting non-recurring engineering efforts for the ASCR facilities that incorporate custom features to meet the Department's mission requirements. REP will also expand efforts in exascale component technology research and development, system engineering, and integration, leading to the design and development of future HPC systems including prototype test beds for demonstrating the feasibility of building exascale systems, and the exascale systems themselves.

The National Energy Research Scientific Computing Center (NERSC) takes delivery of the NERSC-8 supercomputer in FY 2016, which will expand the capacity of the facility by 10-40 pf to address emerging scientific needs.

Experienced computational scientists who assist a wide range of users in taking effective advantage of the advanced computing resources are critical assets at both the LCFs and NERSC. To address this DOE mission need, support continues for a post-doctoral training program for high end computational science and engineering. In addition, the three NERSC sites will continue coordinating efforts to quantify scientist's computational requirements and prepare their users for future architectures.

According to the Advanced Scientific Computing Advisory Committee (ASCAC), the Computational Science Graduate Fellowship (CSGF) has been, according to the Advanced Scientific Computing Advisory Committee (ASCAC), "an exceptionally effective program that has had a significant impact on the national Computational Science infrastructure."^a In July 2014, the ASCAC Workforce Subcommittee found that the CSGF "enables graduates to pursue a multidisciplinary program of education that is coupled with practical experience at the laboratories. The program is highly effective in both its educational goals and in its ability to supply talent to the laboratories. However, its current size and scope are too limited to solve the identified workforce problems. The committee felt strongly that this proven program should be extended to increase its ability to support the DOE mission."^b Both the ASCR facilities and its exascale research efforts rely on the continued availability of highly skilled computational scientists such as those produced by the CSGF and face increasing competition for the limited supply of these workers. Therefore, the FY 2016 budget request includes \$10,000,000 for the

^a http://science.energy.gov/~/media/ascr/ascac/pdf/reports/ASCAC_CSGF_Report_2011-Final.pdf

^b http://science.energy.gov/~/media/ascr/ascac/pdf/charges/ASCAC_Workforce_Letter_Report.pdf

CSGF within the Research and Evaluation Prototypes activity to expand the program and strengthen connections to both the ASCR facilities and to the challenges of exascale computing.

With the 100 gigabit per second (Gbps) expansion to support SC's collaborations in Europe complete, the Energy Science Network (ESnet) will explore, in coordination with the National Science Foundation, next generation optical networking technologies and global networking architectures for future upgrades. The outcomes of these efforts will help ESnet keep pace with the continuing growth of scientific traffic from DOE's scientific user facilities and experiments.

Within the FY 2016 Budget Request, ASCR supports the Department's Exascale Computing Departmental Crosscut. The Exascale Computing Initiative's goal is to significantly accelerate the development of capable exascale computing systems to meet national security needs. Exascale systems are needed to support areas of research that are critical to national security objectives as well as applied research advances in areas such as climate models, combustion systems, and nuclear reactor design that are not within the capacities of today's systems. Exascale systems' computational power are needed for increasing capable data-analytic and data-intense applications across the entire Federal complex. Exascale is a component of long-term collaboration between SC's Advanced Scientific Computing Research (ASCR) program and the National Nuclear Security Administration's (NNSA) Advanced Simulation and Computing Campaign (ASC) program.

FY 2016 Crosscuts (\$K)

Exascale Computing

177,894

177,894

Total

Advanced Scientific Computing Research

Advanced Scientific Computing Research Funding (\$K)

	FY 2014 Enacted	FY 2014 Current ¹	FY 2015 Enacted	FY 2016 Request	FY 2016 vs. FY 2015
Mathematical, Computational, and Computer Sciences Research				·	
Applied Mathematics	47,081	47,081	49,155	49,229	+74
Computer Science	55,835	55,835	55,767	56,842	+1,075
Computational Partnerships	46,261	46,261	46,918	47,918	+1,000
Next Generation Networking for Science	17,852	17,852	19,000	19,000	+0
SBIR/STTR	4,972	0	5,830	6,181	+351
Total, Mathematical, Computational, and Computer Sciences Research	172,001	167,029	176,670	179,170	+2,500
High Performance Computing and Network Facilities					
High Performance Production Computing	67,105	67,105	75,605	76,000	+395
Leadership Computing Facilities	160,000	160,000	184,637	171,000	-13,637
Research and Evaluation Prototypes	36,284	36,284	57,329	141,788	+84,459
High Performance Network Facilities and Testbeds	33,054	33,054	35,000	38,000	+3,000
SBIR/STTR	9,649	0	11,759	15,036	+3,277
Total, High Performance Computing and Network Facilities	306,092	296,443	364,330	441,824	+77,494
Total, Advanced Scientific Computing Research	478,093	463,472	541,000	620,994	+79,994

SBIR/STTR funding:

• FY 2014 transferred: SBIR \$12,722,000 and STTR \$1,899,000 of FY 2014 dollars, plus \$569,000 in unobligated prior years dollars for SBIR

• FY 2015 Enacted: SBIR \$15,457,000 and STTR \$2,132,000

• FY 2016 Request: SBIR \$18,450,000 and STTR \$2,767,000

¹ Funding reflects the transfer of SBIR/STTR to the Office of Science.

Advanced Scientific Computing Research Explanation of Major Changes (\$K)

	FY 2016 vs. FY 2015
Mathematical, Computational, and Computer Sciences Research: Research will continue to focus on the linked challenges of capable exascale and data-intensive science.	+2,500
High Performance Computing and Network Facilities: Increase supports: Research and Development Prototypes, which will significantly expand efforts to support the initiation of R&D partnerships with U.S. vendors for the design and development of exascale node and systems prototypes building on the previous investments in critical technologies and conceptual designs; lease costs; increased power costs; the NERSC upgrade, which will expand the capacity of the facility by 10-40 pf to address emerging scientific needs; ESnet efforts, in coordination with NSF, to develop next generation optical networking and global networking architectures for future upgrades. LCF funding decreases as the majority of site preparations for planned upgrades will be completed in FY 2015.	+77,494
The Computational Sciences Graduate Fellowship is critically important to the ASCR facilities and to our exascale goals. The Research and Evaluation Prototypes activity will support the fellowship at \$10,000,000 in FY 2016. Research and Evaluation Prototypes will also increase to support for non- recurring engineering efforts to ensure user facility upgrades meet the Department's mission requirements.	
Total, Advanced Scientific Computing Research	+79,994

Basic and Applied R&D Coordination

Coordination across disciplines and programs is a cornerstone of the ASCR program. Partnerships within SC are mature and continue to advance the use of high performance computing and scientific networks for science. Growing areas of collaboration will be in the area of data-intensive science and readying applications for exascale. ASCR continues to have a strong partnership with NNSA for achieving the Department's goals for exascale computing. 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. Areas of mutual interest between ASCR and the DOE technology programs, particularly the Office of Electricity Delivery and Energy Reliability (OE) and the Office of Nuclear Energy (NE), are applied mathematics for the optimization of complex systems, control theory, and risk assessment. Through the National Information Technology Research and Development Subcommittee of the National Science and Technology Council's (NSTC) Committee on Technology, the interagency networking and information technology R&D coordination effort, ASCR also coordinates with programs across the Federal Government. In FY 2016, cross-agency interactions and collaborations will continue, fostered by the National Strategic Computing Initiative coordinated by OSTP.

Program Accomplishments

Hydrogen on Demand. As part of an INCITE project on Argonne's Leadership Computing Facility (ALCF), researchers performed a 16,611 atom Quantum Molecular Dynamics (QMD) simulation on Mira to study hydrogen production using the reaction of a lithium-aluminum (Li-Al) alloy particle with water for on-demand hydrogen gas production. Producing hydrogen from aluminum-water reactions has potential for many clean energy applications, including on-board fuel production for hydrogen-powered vehicles. However, the approach has been limited by production scalability issues due to poor yields using aluminum particles. The simulation performed on Mira revealed that alloying Al particles with Li results in orders-of-magnitude acceleration of the reaction rate as well as higher yields.

Advancing Next Generation Nuclear Energy. A team, led by Westinghouse and ORNL, received the International Data Corporation's HPC Excellence Award in June 2014 for their core physics simulations of the Westinghouse AP1000 pressurized water reactor (PWR) core using the Virtual Environment for Reactor Application (VERA) system developed by the Consortium for Advanced Simulation of Light-Water Reactors (CASL), DOE's Nuclear Energy hub. The simulations, performed on the Oak Ridge Leadership Computing Facility (OLCF), produced 3-D, high-fidelity power distributions representing conditions expected to occur during the AP1000 core start-up and used up to 240,000 computational units in parallel. The results included as many as one trillion particle histories per simulation to reduce statistical errors and provide insights that improve understanding of core conditions, helping to ensure safe startup of the AP1000 PWR core. Westinghouse is deploying the AP1000 worldwide with eight plants currently under construction in China and the United States.

Calming the Chaos Keeps Supercomputers Humming. Diagnosis Using the Chaos of Computing Systems, or DUCCS, was developed by ASCR researchers to quickly and nonintrusively detect a variety of hardware faults in processing units, accelerators, memory elements, and interconnects of large-scale high-performance computing systems such as supercomputers, clusters, and server farms. The software combines chaotic map theory with hardware details to detect component faults in systems that handle large computational problems such as scientific computations, weather predictions, and web data processing. DUCCS software provides critical diagnosis information that contributes to the resilience of computing systems in terms of error-free computations and sustained capacity. This work has been recognized as one of the year's top technological innovations with a 2014 "R&D 100 Award" presented by R&D Magazine.

Understanding Mercury Toxicity. Supercomputer simulations run at NERSC show for the first time how mercury, a toxic environmental pollutant, binds preferentially to sulfur-containing molecules rather than those with oxygen and other similar atoms. The simulations revealed that an interaction between mercury and water molecules is important to the process, a finding that establishes a basis for understanding the chemistry of mercury that is impossible from experimentation alone. These results are critical for understanding toxicity, bioavailability, transport, and environmental fate of this major global pollutant.

Advanced Mathematics Bring Nanocrystals Into Focus. X-ray crystallography gives scientists new insights in areas ranging from genomics to photosynthesis to bone disease. As light sources at SC user facilities become more powerful, the emerging technique of X-ray nanocrystallography offers great promise for studying objects that are the size of macromolecules within

the membranes of cell walls. ASCR researchers recently developed an algorithmic framework and new mathematical tools for decoding and combining the diffraction patterns generated by X-ray experiments in order to understand the overall structure of the examined material. The multi-step mathematical process for nanocrystallography involves building up a 3-dimensional structure from 2-dimensional X-ray diffraction patterns from thousands of nanocrystals with different sizes and orientations. This new computational framework is a major development for enabling scientific advances from the analysis of the massive data from the Department's light sources.

Simulations Illuminate Path to Improve Understanding of Type 2 Diabetes. Computing resources at the ALCF have helped researchers determine how proteins misfold to create the tissue-damaging structures that lead to type 2 diabetes. The researchers combined experiments and computation to understand the chemical pathway. The simulations identified a missing intermediate step, in which transient rigid fibrils form, then morph into floppy protein loops, and finally take the form of tough fibrils and stack up to form the damaging amyloid fibril. With the new understanding and access to Mira, future work could target a possible treatment, such as designing an inhibitor to interfere with the harmful pathway. In addition, the research collaboration can apply the method to determine the intermediate steps in similar diseases such as Alzheimer's that are linked to the formation of amyloid fibrils.

Observations Validate SciDAC Supernova Simulations. One of the first terascale accomplishments in 2003 in the SciDAC program was a 3-D simulation that explored the mechanism responsible for the explosion of core-collapse supernovas, phenomena responsible for producing all of the elements in the periodic table. These pioneering simulations produced the theoretical SASI, or standing accretion shock instability, a sloshing of stellar material that destabilizes the expanding shock and helps lead to an explosion. Now, more than a decade later, researchers mapping radiation signatures from the Cassiopeia A supernova with NASA's NuSTAR high-energy x-ray telescope array have published observational evidence that supports the SASI model. During the same period the researchers have improved the initial 3-D simulation so that today, the team is using 85 million core hours and scaling to more than 60,000 cores to simulate a supernova in three dimensions with a fully physics-based model that could generate the most revealing supernova yet.

Beyond Remote Access - New Scientific Workflows. ESnet recently began to support complex scientific workflows requiring access to more than one DOE user facility simultaneously. In these 'coupled facility' experiments, scientific data is streamed at a very high rate from a DOE light source or other data generator, to a high performance computing facility for real-time analysis. The 'coupled facility' architecture was instrumental in facilitating a recent experimental result, in which a team of collaborators from LBNL and SLAC obtained 'snapshots' of photosynthetic water oxidation in Phytosystem-II, using femtosecond X-ray diffraction and spectroscopy.

Advanced Scientific Computing Research Mathematical, Computational, and Computer Sciences Research

Description

The Mathematical, Computational, and Computer Sciences Research subprogram supports research activities that effectively use the current and future generations of DOE's computer and networking capabilities. Computational science is increasingly central to progress at the frontiers of science and to our most challenging engineering problems. Accordingly, the subprogram delivers:

- new mathematics required to more accurately model systems involving processes taking place across a wide range of time and length scales;
- software, tools, and middleware to efficiently and effectively harness the potential of today's high performance computing systems and advanced networks for science and engineering applications;
- operating systems, data management, analyses, representation model development, user interfaces, and other tools
 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;
- networking and collaboration tools to make scientific resources readily available to scientists, in university, national laboratory, and industrial settings.

The research program will develop methods, software, and tools to use HPC systems for data-intensive and computational science at the exascale. This requires a focus on increased parallelism, energy efficiency, and reliability.

Deriving scientific insights from vast amounts of raw data will require a focused research effort to develop the necessary theories, tools, and technologies to manage the full data lifecycle from generation or collection through integration, transformation, analysis, and visualization, to capturing the historic record of the data and archiving, and sharing them.

Applied Mathematics

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. This activity's research underpins all of DOE's modeling and simulation efforts. Significant innovation in applied mathematics is needed to realize the potential of next generation high performance computing systems. High-fidelity modeling and simulation requires a number of new algorithmic techniques and strategies supported by this activity, including: advanced solvers for large linear and nonlinear systems, time integration schemes, multi-physics coupling, methods that use asynchrony or randomness, adaptively, algorithmic resilience, and strategies for reducing global communications.

Computer Science

The Computer Science activity supports research on extreme-scale computing and extreme-scale data. Reports from computer vendors indicate that because of power constraints, data movement, rather than computational operations, will be the constraining factor for future systems. Memory per core is expected to decline sharply due to power requirements and the performance growth of storage systems will continue to lag behind the computational capability of the systems. Multi-level storage architectures that span multiple types of hardware are anticipated and require research within this activity to develop new approaches to run-time data management and analysis.

Significant innovation in computer science is needed to realize the potential of next generation HPC systems and other scientific user facilities in a timeframe consistent with their anticipated availability. There will be continued emphasis on data-intensive science challenges with particular attention to the intersection with exascale computing challenges and the unique needs of DOE scientific user facilities including data management. There will also be significant efforts in tools, user interfaces, the high performance computing software stack that can dynamically deal with time-varying energy efficiency and reliability requirements—including operating systems, file systems, compilers, and performance tools—and visualization

and analytics tools that scale to extremely massive datasets. These efforts are essential to ensure DOE mission applications are able to use commercially available HPC hardware.

Computational Partnerships

The Computational Partnerships activity supports the SciDAC program, which accelerates progress in scientific computing through partnerships among applied mathematicians, computer scientists, and scientists in other disciplines. 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 include climate science, fusion research, high energy physics, nuclear physics, astrophysics, materials science, chemistry, and accelerator physics.

SciDAC focuses on the high-end of high performance computational science and engineering and addresses two challenges: to broaden the community and thus the impact of high performance computing, particularly to address the Department's missions and to ensure that progress at the frontiers of science is enhanced rather than diminished by advances in computational technology, most pressingly, the emergence of hybrid, multi-core architectures.

Next Generation Networking for Science

ASCR has played a leading role in the development of the high-bandwidth networks connecting researchers to facilities, data, and one another. 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 use new capabilities in ESnet to advance DOE missions.

Advanced Scientific Computing Research Mathematical, Computational, and Computer Sciences Research

Activities and Explanation of Changes

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
Mathematical, Computational, and Computer Sciences Research \$176,670,000	\$179,170,000	+\$2,500,000
Applied Mathematics (\$49,155,000)	(\$49,229,000)	(+\$74,000)
Research efforts support the Department's efforts in capable exascale and data-intensive science. These efforts develop scalable mathematical and statistical models, algorithms, and methods for the representation, analysis, and understanding of extreme-scale data from scientific simulations and experiments.	Applied Mathematics will continue efforts to develop new algorithmic techniques and strategies that extract scientific advances and engineering insights from massive data for DOE missions. Applied Mathematics will also address many of the challenges of exascale including: advanced solvers, uncertainty quantification, algorithmic resilience, and strategies for reducing global communications.	The slight increase will support priority research areas in capable exascale and data-intensive science.
Computer Science (\$55,767,000)	(\$56,842,000)	(+\$1,075,000)
To achieve the full potential of exascale computing, a software stack must be developed that includes new programming models and metrics for evaluating system status. This activity supports software efforts that span the spectrum from low-level, operational software to high-level, application development environments. More specifically, it includes operating systems, runtimes for scheduling, memory management, file systems, and performance monitoring. Power management and resilience strategies, computational libraries, compilers, programming models, and application frameworks are also included. Scalability, programmability, resilience, and code portability are emphasized to promote ease of use, reliability, accommodation of legacy code, and	Computer Science will continue efforts to develop an exascale software stack, new programming models and metrics for evaluating system status. This activity is primarily focused on addressing the challenges of exascale and data-intensive science. Emphasis will remain on efforts to promote ease of use; increase parallelism, energy efficiency, and reliability, and will ensure that research efforts are tightly coupled to application requirements and developments in industry, particularly those identified by the co-design centers and developed in partnerships supported by the Research and Evaluation Prototypes activity.	The slight increase will support priority research areas in capable exascale and data-intensive science.

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015
pathways to future development beyond exascale. Research efforts also support the Department's efforts in capable exascale and data-intensive science. These efforts focus on in situ data management, analysis and visualization, new I/O subsystems, and new multi-level storage system software.		
Computational Partnerships (\$46,918,000)	(\$47,918,000)	(+\$1,000,000)
The SciDAC institutes continue to play a key role in assisting DOE mission critical applications to effectively use the ASCR production and leadership computing facilities. The strategic partnerships with the other Office of Science programs continue to address their specific needs as they move toward larger data sets and more complex computing systems. The Scalable Data Management Analysis and Visualization (SDAV) Institute and data-intensive co- design center continue to support the Department's efforts in data-intensive science. The role of this activity is to develop robust tools and software to manage and analyze massive data with SDAV focused on the near term and co-design focused on emerging hardware.	The SciDAC Institutes will be recompeted in FY 2016. These Institutes will continue to provide the bridge between the core research program and the DOE science applications. The development of SciDAC tools and resources by the Institutes is primarily for use on computational systems, such as those existing and planned for at the Oak Ridge and Argonne Leadership Computing Facilities, the National Energy Research Scientific Computing Center, and similar world-class computing facilities over the following 5 years. In addition, the exascale Co-design centers will undergo a comprehensive external peer review in FY 2015 to document progress and impact, and to inform the recompetition of these efforts in FY 2016.	The increase will support a more robust infrastructure in anticipation of the challenges for the SciDAC applications.

scientific user facilities.

This activity focuses on the current set of co-design centers that partner DOE mission applications with forefront researchers and computing vendors. These efforts inform core research efforts in applied mathematics and computer science as well as the computing resources for the next generation of

FY 2015 Enacted	FY 2016 Request	Explanation of Changes FY 2016 vs. FY 2015			
Next Generation Networking for Science (\$19,000,000)	(\$19,000,000)	(\$0)			
With the production deployment of 100 gigabit per second (Gbps) technologies, research continues 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. These investments are increasingly important as ESnet expands production use of very high-throughput and optical technologies. Research focuses on the challenges of moving, sharing, and validating massive quantities of data from DOE scientific user facilities and large scale collaborations via high speed optical networks. This includes the challenges in building, operating, and maintaining the network infrastructure over which these data pass. Research supports the Department's efforts in exascale and data-intensive science. This activity focuses on integrating the SC facilities with computing resources and collaborations.	The Next Generation Networking for Science activity will continue to work closely with SC user facilities and applications, to develop the necessary tools – networking software, middleware and hardware - to address the challenges of moving, sharing and validating massive quantities of data via next generation optical networking technologies. This focus will allow DOE scientists to productively collaborate regardless of the geographical distance between scientists and user facilities or the size of the data.	No change			
SBIR/STTR (\$5,830,000)	(\$6,181,000)	(+\$351,000)			
In FY 2015, SBIR/STTR funding is set at 3.3% of non-	In FY 2016, SBIR/STTR funding is set at 3.45% of non-				

capital funding.

capital funding.

Advanced Scientific Computing Research High Performance Computing and Network Facilities

Description

The High Performance Computing and Network Facilities subprogram delivers forefront computational and networking capabilities. These include high performance production computing at the National Energy Research Scientific Computing Center (NERSC) at LBNL and Leadership Computing Facilities (LCFs) at ORNL and ANL. 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 research and development that will play a critical role in delivering world-leading capabilities and achieving the Department's exascale computing goals.

Allocations of computer time at ASCR facilities provide critical resources for the scientific community, including industry and other agencies, following the peer reviewed, public access model used by other SC scientific user facilities. ASCR facilities provide a testbed for U.S. industry to scale and then validate code performance to optimize in-house HPC investments.

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 technologies that enables next-generation machines, ASCR ensures that commercially available architectures serve the needs of the scientific community. Coupling this activity to the co-design centers ensures that 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. The Research and Evaluation Prototypes activity prepares researchers to effectively use the next generation of scientific computers and seeks to reduce risk for future major procurements.

High Performance Production Computing

This activity supports NERSC, which delivers high-end production computing services for the SC research community. Approximately 5,000 computational scientists in about 500 projects use NERSC annually to perform scientific research across a wide range of disciplines including astrophysics, chemistry, climate modeling, materials, high energy and nuclear physics, fusion, and biology. 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 on the largest machines available at NERSC and other SC computing facilities. In FY 2015, NERSC will complete its move into the new Computational Research and Theory building on the Lawrence Berkeley National Laboratory campus.

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 capacity exists despite upgrades to the primary computing systems approximately every three years. NERSC regularly gathers requirements from SC domain programs through a long-established, robust process and uses these requirements to inform 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 and multi-core computing.

Leadership Computing Facilities

The LCFs enable open scientific applications, including industry applications, to harness the potential of leadership computing to advance science and engineering. The success of this effort is built on the gains made in Research and Evaluation Prototypes and ASCR research efforts. Another LCF strength is the staff, who operate and maintain the forefront computing resources and provide support to Innovative and Novel Computational Impact on Theory and Experiment (INCITE) projects, ASCR Leadership Computing Challenge projects, scaling tests, early science applications, 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's (OLCF) 27 petaflop system is one of the most powerful computers in the world for scientific research, and is ranked number two on the November 2014 Top 500 list^a. Through allocations on the OLCF, several applications, including combustion studies in diesel jet flame stabilization, simulations of neutron transport in fast-fission reactor cores, and earthquake simulations, are running at the multi-pf scale. OLCF staff is sharing its expertise with industry to broaden the benefits of petascale computing for the Nation. For example, OLCF continues to work with industry to significantly reduce the need for costly physical prototypes and physical tests in the development of high-technology products.

The Argonne Leadership Computing Facility (ALCF) operates a 10-pf IBM Blue Gene Q (Mira), developed through a joint research project with support from the NNSA, industry, and ASCR's Research and Evaluation Prototypes activity. This HPC system achieves high performance with relatively lower electrical power consumption than other current petascale computers.

The ALCF and OLCF systems are architecturally distinct, consistent with DOE's strategy to foster a diversity of capabilities that provides the Nation's HPC user community the most effective resources. 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, for example, helping engineers understand the fundamental physics of turbulent mixing to transform product design and to achieve improved performance, lifespan and efficiency.

The demand for 2014 INCITE allocations at the LCFs outpaced the available resources by a factor of three.

Research and Evaluation Prototypes

The next generation of computing hardware will present new challenges for science and engineering applications—most notably increased parallelism, energy efficiency, and reliability. This activity supports research and development partnerships with vendors to influence and accelerate critical technologies for next-generation systems, system integration research, and development and engineering efforts. These partnerships are coupled to application development to ensure Department applications are ready to make effective use of commercial offerings.

Research and Evaluation Prototypes (REP) initiated partnerships with key vendors to accelerate the R&D of critical technologies that advance the Department's exascale goals and reduce the economic and manufacturing barriers to their commercial production. This is an essential component in the Department's Exascale Computing Plan that has been developed during the previous three years. Recent REP efforts were focused on developing conceptual designs and investigating critical technologies. This allowed DOE researchers to work closely with the vendors to better understand requirements and capabilities of the emerging technology. The DOE mission applications, which will execute on exascale systems, force significant requirements on the system design. These requirements will result in systems that have performance and scalability characteristics that exceed those needed in the general commercial sector. Investment in early design and development will allow DOE to strongly influence the eventual products. These efforts will result in computers that will achieve the Department's exascale performance goals and, given current industry roadmaps, without this investment these goals will not be achieved. REP projects require the vendors to cost share at approximately 40% of the cost of each project. The full cost for industry to develop novel HPC systems is multiple billions of dollars per system.

In addition, this activity partners with the NNSA on the Computational Sciences Graduate Fellowship (CSGF) and to support research investments in non-recurring engineering, for near-term technology customization for the ASCR facilities.

High Performance Network Facilities and Testbeds

The Energy Sciences Network (ESnet) provides the national and international network and networking infrastructure connecting DOE science facilities, experiments, and SC laboratories with other institutions connected to peer academic or commercial networks. The costs for ESnet are dominated by operations, including maintaining the fiber optic backbone and 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 growth in science data traffic and for testing and evaluation of new 400 Gbps technologies and software-defined networking services that will be required to keep pace with the expected

^a http://www.top500.org/lists/2014/11/

data volume. In FY14, ESnet achieved 75% completion of its European extension project. This project will increase transatlantic bandwidth available to DOE collaborations—including high-energy physics experiments at CERN—by a factor of ten.

Advanced Scientific Computing Research High Performance Computing and Network Facilities

Activities and Explanation of Changes

FY 2015 Enacted	FY 2016 Request	Explanation of Change FY 2016 vs. FY 2015		
High Performance Computing and Network Facilities \$364,330,000	\$441,824,000	+\$77,494,000		
High Performance Production Computing (\$75,605,000)	(\$76,000,000)	(+\$395,000)		
Funding continues to support operation of the NERSC high-end capability systems (NERSC-7) including power costs, lease payments, and user support and a post-doctoral training program for high-end computational science and engineering.	Will support installation, acceptance and operation of the NERSC high-end capability systems (NERSC-7 and NERSC-8) including increased power costs, lease payments, and user support and continuation of the post-doctoral training program for high-end computational science and engineering.	Additional funds will be provided to support operations of both NERSC-7 and NERSC-8 and to begin planning for NERSC-9 in the FY19-FY20 timeframe.		
Leadership Computing Facilities (\$184,637,000)	(\$171,000,000)	(-\$13,637,000)		
Funding continues to support operation and allocation, through INCITE and ALCC, of the 27 petaflop Titan system at the OLCF and 10 petaflop Mira system at the ALCF. This includes lease payments, power, and user support. Also supports preparations at the LCFs to support 75-200 petaflop upgrades at each facility and a post-doctoral training program for high-end computational science and engineering. Each LCF has achieved Critical Decision -2; established a project baseline and negotiated a contract with the selected vendor.	Will support operation and allocation of the 27 petaflop Titan system at the OLCF and 10 petaflop Mira system at the ALCF through INCITE and ALCC. This includes lease payments, power, and user support. Also supports preparations – such as power, cooling and cabling at the LCFs to support 75-200 petaflop upgrades at each facility and continuation of the post- doctoral training program for high-end computational science and engineering.	Funds continue to support the operation of current resources, preparing applications for the proposed upgrades, and the remaining site preparation work for the upgrade. The decrease in funding for both LCFs reflect that the majority of site preparation will be completed in FY 2015 and they are working with their selected vendor to finalize system specifications.		
Leadership Computing Facility at ANL: \$80,320,000	\$77,000,000	-\$3,320,000		
Leadership Computing Facility at ORNL: \$104,317,000	\$94,000,000	-\$10,317,000		

FY 2015 Enacted	FY 2016 Request	Explanation of Change FY 2016 vs. FY 2015
Research and Evaluation Prototypes (\$57,329,000)	(\$141,788,000)	(+\$84,459,000)
As follow-ons to the previous research efforts in critical technologies and system interconnect, REP will, in FY 2015, competitively select teams to develop system designs suitable for next-generation platforms. In addition, it will fund the development of prototypes based on the results from the <i>Fast Forward</i> program's investments in critical crosscutting technology research in areas such as processors, memory subsystems, network interfaces and the interconnection network. The Computational Science Graduate Fellowships is funded at \$3,000,000.	REP has recently supported efforts to improve the energy efficiency and reliability of critical technologies such as memory, processors, network interfaces and interconnects. The compute node is the basic building block of a high performance computer and all of these technologies come together in the node. Therefore, REP will competitively select R&D partnerships with U.S. vendors to initiate the design and development of node and system designs suitable for exascale systems. These efforts will influence the development of prototypes that advance DOE goals and are based on the results of the <i>Fast Forward and Design Forward</i> investments. This is an essential component of the Department's exascale computing plan and a key step in the vendor's productization efforts. Support will also be provided for non-recurring engineering efforts in support of ASCR facilities. To emphasize the vital importance of the CSGF program to the ASCR facilities and to our exascale goals, Research and Evaluation Prototypes will support the program at \$10,000,000 in FY 2016.	The increase supports the design and development of node and system prototypes. These efforts support the development of four exascale nodes and three system architecture teams. Multiple teams are necessary to adequately explore design options and to mitigate overall project risk. Overall industry investment in this area is significant, with billions of dollars in development costs for next generation HPC systems. To influence the trajectory of technology, the Department must partner early with U.S. vendors and support a significant share of these early design and development efforts. Increased funding is also provided for non-recurring engineering efforts. The Computational Science Graduate Fellowships increases from \$3,000,000 to \$10,000,000.
High Performance Network Facilities and Testbeds (\$35,000,000)	(\$38,000,000)	(+\$3,000,000)
ESnet operates the network infrastructure to support critical DOE science applications, SC facilities and scientific collaborations around the world through 100 Gbps production network and begin research on the 400 Gbps technologies.	ESnet will operate the national and international network infrastructure to support critical DOE science applications, SC facilities and scientific collaborations around the world through 100 Gbps production network and begin upgrade to 400 Gbps testbed for networking testing and research.	The requested increase supports the upgrade of the ESnet 100 Gbps testbed to 400 Gbps to allow researchers to identify technologies needed for production use to support increased data production at DOE scientific user facilities and experiments.

FY 2015 Enacted	FY 2016 Request	Explanation of Change FY 2016 vs. FY 2015
SBIR/STTR (\$11,759,000)	(\$15,036,000)	(+\$3,277,000)
In FY 2015, SBIR/STTR funding is set at 3.3% of non- capital funding.	In FY 2016, SBIR/STTR funding is set at 3.45% of non- capital funding.	

Advanced Scientific Computing Research Performance Measures

In accordance with the GPRA Modernization Act of 2010, the Department sets targets for, and tracks progress toward, achieving performance goals for each program. The following table shows the targets for FY 2014 through 2016.

	FY 2014 FY 2015		FY 2016					
Performance Goal (Measure)	ASCR Facility Operations—Average achieved operation time of ASCR user facilities as a percentage of total scheduled annual operation time							
Target	≥ 90%	≥ 90%	≥ 90%					
Result	Met	TBD	TBD					
Endpoint Target	Many of the research projects that are undertaken at the Office of Science's scientific user facilities take a great deal of time, money, and effort to prepare and regularly have a very short window of opportunity to run. If the facility is not operating as expected the experiment could be ruined or critically setback. In addition, taxpayers have invested millions or even hundreds of millions of dollars in these facilities. The greater the period of reliable operations, the greater the return on the taxpayers' investment.							
Performance Goal (Measure)	ASCR Research—Discovery of new applied mathematics and computer science tools and methods that enable DOE applications to deliver scientific and engineering insights with a significantly higher degree of fidelity and predictive power							
Target	Support at least two new teams to conductConduct an external peer review of the three original co-design centers to document progress, impact, and lessons learned.Fund two teams to develop exascale node designs.Ieast three applied mathematics research teams that address issues of fault tolerance or energy management for next-generation computing systemsConduct an external peer review of the three 							
Result	Met TBD TBD							
Endpoint Target	Develop and deploy high-performance computing hardware and software systems through exascale platforms.							

	Total	Prior Years	FY 2014 Enacted	FY 2014 Current	FY 2015 Enacted	FY 201 Reque	16 FY 2016 vs. est FY 2015
Capital operating expenses							
Capital equipment	n/a	n/a	7,325	7,325	8,000	6,000	0 +2,000
Funding Summary (\$K)							
	FY 2014 Enacted	FY 2014	Current	FY 2015 Enacted	FY 2016 Re	quest	FY 2016 vs. FY 2015
Research	203,313	20	03,313	228,169	314,	777	+86,608
Scientific user facility operations	260,159	26	50,159	295,242	285,	000	-10,242
Other	14,621		0	17,589	21,	217	+3,628
Total, Advanced Scientific Computing Research	478,093	46	53,472	541,000	620,	994	+79,994

Advanced Scientific Computing Research Capital Summary (\$K)

Advanced Scientific Computing Research Scientific User Facility Operations (\$K)

The treatment of user facilities is distinguished between two types: <u>TYPE A</u> facilities that offer users resources dependent on a single, large-scale machine; <u>TYPE B</u> facilities that offer users a suite of resources that is not dependent on a single, large-scale machine.

Definitions:

Achieved Operating Hours – The amount of time (in hours) the facility was available for users.

Planned Operating Hours -

- For Past Fiscal Year (PY), the amount of time (in hours) the facility was planned to be available for users.
- For Current Fiscal Year (CY), the amount of time (in hours) the facility is planned to be available for users.
- For the Budget Fiscal Year (BY), based on the proposed budget request the amount of time (in hours) the facility is anticipated to be available for users.

Optimal Hours – The amount of time (in hours) a facility would be available to satisfy the needs of the user community if unconstrained by funding levels.

Percent of Optimal Hours – An indication of utilization effectiveness in the context of available funding; it is not a direct indication of scientific or facility productivity.

- For BY and CY, Planned Operating Hours divided by Optimal Hours expressed as a percentage.
- For PY, Achieved Operating Hours divided by Optimal Hours.

<u>Unscheduled Downtime Hours</u> - The amount of time (in hours) the facility was unavailable to users due to unscheduled events. NOTE: For type "A" facilities, zero Unscheduled Downtime Hours indicates Achieved Operating Hours equals Planned Operating Hours.

	FY 2014 Enacted	FY 2014 Current	FY 2015 Enacted	FY 2016 Request	FY 2016 vs. FY 2015
TYPE A FACILITIES					II
NERSC	\$67,105	\$67,105	\$75,605	76,000	+395
Number of Users	5,608	5,608	5,608	5,608	0
Achieved operating hours	8,482	8,482	N/A	N/A	N/A
Planned operating hours	8,585	8,585	8,585	8,585	0
Optimal hours	8,585	8,585	8,585	8,585	0
Percent optimal hours	98.8%	98.8%	N/A	N/A	N/A
Unscheduled downtime hours	1.2%	1.2%	N/A	N/A	N/A

	FY 2014 Enacted	FY 2014 Current	FY 2015 Enacted	FY 2016 Request	FY 2016 vs. FY 2015
OLCF	\$93,000	\$93,000	\$104,317	\$94,000	-10,317
Number of Users	1,064	1,064	1,064	1,064	0
Achieved operating hours	6,637	6,637	N/A	N/A	N/A
Planned operating hours	7,008	7,008	7,008	7,008	0
Optimal hours	7,008	7,008	7,008	7,008	0
Percent optimal hours	94.7%	94.7%	N/A	N/A	N/A
Unscheduled downtime hours	5.3%	5.3%	N/A	N/A	N/A
ALCF	\$67,000	\$67,000	\$80,320	\$77,000	-3,320
Number of Users	1,434	1,434	1,434	1,434	0
Achieved operating hours	6,882	6,882	N/A	N/A	N/A
Planned operating hours	7,008	7,008	7,008	7,008	0
Optimal hours	7,008	7,008	7,008	7,008	0
Percent optimal hours	98.2%	98.2%	N/A	N/A	N/A
Unscheduled downtime hours	1.8%	1.8%	N/A	N/A	N/A
ESnet	\$33,054	\$33,054	\$35,000	\$38,000	+3,000
Number of users ^a	N/A	N/A	N/A	N/A	N/A
Achieved operating hours	8,760	8,760	N/A	N/A	N/A
Planned operating hours	8,760	8,760	8,760	8,760	0
Optimal hours	8,760	8,760	8,760	8,760	0
Percent optimal hours	100%	100%	N/A	N/A	N/A
Unscheduled downtime hours	0%	0%	N/A	N/A	N/A

^a ESnet is a high performance scientific network connecting DOE facilities to researchers around the world; user statistics are not collected.

	FY 2014 Enacted	FY 2014 Current	FY 2015 Enacted	FY 2016 Request	FY 2016 vs. FY 2015
Total Facilities	\$260,159	\$260,159	\$295,242	\$285,000	-10,242
Number of Users ^a	8,106	8,106	8,106	8,106	0
Achieved operating hours	30,761	30,761	N/A	N/A	N/A
Planned operating hours	31,361	31,361	31,361	31,361	0
Optimal hours	31,361	31,361	31,361	31,361	0
Percent of optimal hours ^b	97.6%	97.6%	N/A	N/A	N/A
Unscheduled downtime hours	2.4%	2.4%	N/A	N/A	N/A

Scientific Employment

	FY 2014 Enacted	FY 2014 Current	FY 2015 Enacted	FY 2016 Estimate	FY 2016 vs FY 2015
Number of permanent Ph.D.'s (FTEs)	520	520	548	584	+36
Number of postdoctoral associates (FTEs)	130	130	137	146	+9
Number of graduate students (FTEs)	400	400	428	460	+32
Other scientific employment (FTEs) ^c	220	220	234	247	+13

^a Total users only for NERSC, OLCF, and ALCF.

^b For total facilities only, this is a "funding weighted" calculation FOR ONLY TYPE A facilities: $\frac{\sum_{1}^{n}[(\% OH \text{ for facility } n) \times (funding \text{ for facility } n \text{ operations})]}{Total \text{ funding for all facility operations}}$

^c Includes technicians, engineers, computer professionals and other support staff.