Advanced Scientific Computing Research

Funding Profile by Subprogram

	(dollars in thousands)		
	FY 2006 Current Appropriation	FY 2007 Request	FY 2008 Request
Advanced Scientific Computing Research			
Mathematical, Information, and Computational Sciences	228,382[a]	318,654	340,198

Public Law Authorizations:
Public Law 95-91, "Department of Energy Organization Act", 1977
Public Law 103-62, "Government Performance and Results Act of 1993"
Public Law 108-423, "Department of Energy High-End Computing Revitalization Act of 2004"
Public Law 109-58, "Energy Policy Act of 2005"

Mission

The mission of the Advanced Scientific Computing Research (ASCR) program is to deliver forefront computational and networking capabilities to scientists nationwide that enable them to extend the frontiers of science, answering critical questions that range from the function of living cells to the power of fusion energy. In the past two decades, scientific computation has become a cornerstone of the Department of Energy's (DOE) strategy to ensure the security of the nation and succeed in its science, energy, environmental quality, and national security missions.

Benefits

ASCR supports DOE's mission to provide world-class scientific research capacity through peer-reviewed scientific results in mathematics, high performance computing and advanced networks, and through the application of computers capable of many trillions of operations per second (terascale computers) to advanced scientific applications. Computer-based simulation enables us to model the behavior of complex systems that are beyond the reach of our most powerful experimental probes or our most sophisticated theories. Computational modeling has greatly advanced our understanding of fundamental processes of nature, such as fluid flow and turbulence or molecular structure and reactivity. Through modeling and simulation, we can investigate the interior of stars to understand how the chemical elements were created and learn how protein machines work inside living cells, which could enable us to design microbes that address critical waste cleanup problems. We can design novel catalysts and high-efficiency engines that could expand our economy, lower pollution, and reduce our dependence on foreign oil.

Strategic and GPRA Unit Program Goals

The Department's Strategic Plan identifies five Strategic Themes (one each for nuclear, energy, science, management, and environmental aspects of the mission) plus 16 Strategic Goals that tie to the Strategic Themes. The ASCR program supports the following goals:

Strategic Theme 3, Scientific Discovery & Innovation
Strategic Goal 3.1, Scientific Breakthroughs: Achieve the major scientific discoveries that will drive

[a] Total is reduced by $2,371,000 for a rescission in accordance with P.L. 109–148, the Emergency Supplemental Act to Address Hurricanes in the Gulf of Mexico and Pandemic Influenza, 2006; $5,627,000, which was transferred to the SBIR program; and $675,000, which was transferred to the STTR program.

U.S. competitiveness; inspire America; and revolutionize our approaches to the Nation's energy, national security, and environmental quality challenges.

Strategic Goal 3.2, Foundations of Science: Deliver the scientific facilities, train the next generation of scientists and engineers, and provide the laboratory capabilities and infrastructure required for U.S. scientific primacy.

The ASCR program has one GPRA Unit Program goal which contributes to Strategic Goal 3.1 and 3.2 in the "goal cascade":

GPRA Unit Program Goal 3.1/2.51.00: Deliver forefront computational and networking capabilities—Deliver forefront computational and networking capabilities to scientists nationwide that enable them to extend the frontiers of science, answering critical questions that range from the function of living cells to the power of fusion energy.

Contribution to Strategic Goals 3.1, Scientific Breakthroughs and 3.2, Foundations of Science

The ASCR program contributes to Strategic Goals 3.1 and 3.2 by delivering the fundamental mathematical and computer science research that enables the simulation and prediction of complex physical and biological systems, providing the advanced computing capabilities needed by researchers to take advantage of this understanding, and delivering the fundamental networking research and facilities that link scientists across the nation to the computing and experimental facilities and their colleagues to enable scientific discovery. ASCR supports fundamental research in applied mathematics, computer science, computer networks, and tools for electronic collaboration; integrates the results of these basic research efforts into tools and software that can be used by scientists in other disciplines, especially through efforts such as Scientific Discovery through Advanced Computing (SciDAC); and provides the advanced computing and network resources that enable scientists to use these tools for scientific inquiry. Applied Mathematics enables scientists to accurately model physical and natural systems, and provides the algorithms the computer requires to manipulate that representation of the world effectively, exposing the underlying structure. Computer science research provides the link between the mathematics and the actual computer systems. Finally, scientific discovery results from simulations conducted on the advanced computers themselves, including experimental computers with hardware designs optimized to enable particular types of scientific applications, and the largest computing capabilities available to the general scientific community. All of these elements are to advance the frontiers of simulation. Shrinking the distance between scientists and the resources they need is also critical to Office of Science (SC). The challenges that SC faces require teams of scientists distributed across the country, as well as the full national portfolio of experimental and computational tools. High performance networks and network research provide the capability to move the millions of gigabytes that these resources generate to the scientists' desktops.

Therefore, the ASCR program contributes to research programs across SC, as well as other elements of the Department. The following indicators establish specific long term (ten year) goals in Scientific Advancement that the ASCR program is committed to, and progress can be measured against. The Advanced Scientific Computing Advisory Committee (ASCAC) has been charged to review progress toward these long term measures and were reported to the Department in the fall 2006. The long term measures are:

- Develop multiscale mathematics, numerical algorithms, and software that enable more effective models of systems such as the earth's climate, the behavior of materials, or the behavior of living cells that involve the interaction of complex processes taking place on vastly different time and/or length scales.

- Develop, through the Genomics: GTL partnership with the Biological and Environmental Research (BER) program, the computational science capability to model a complete microbe and a simple microbial community. This capability will provide the science base to enable the development of novel clean-up technologies, bio-energy sources, and technologies for carbon sequestration.

Funding by Strategic and GPRA Unit Program Goal

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
Strategic Goals 3.1, Scientific Breakthroughs and 3.2, Foundations of Science			
GPRA Unit Program Goal 3.1/2.51.00, Deliver Forefront Computational and Networking Capabilities			
Advanced Scientific Computing Research	228,382	318,654	340,198

Annual Performance Results and Targets

FY 2003 Results	FY 2004 Results	FY 2005 Results	FY 2006 Results	FY 2007 Targets	FY 2008 Targets
GPRA Unit Program Goal 3.1/2.51.00 (Deliver Forefront Computational and Networking Capabilities)					
Mathematical, Information and Computational Sciences					
Began installation of next generation National Energy Research Scientific Computing Center (NERSC) computer, NERSC-4, that will at least double the capability available in FY 2002 to solve leading edge scientific problems. [Goal Not Met]	Maintained Procurement Baselines. Percentages within (1) original baseline cost for completed procurements of major computer systems or network services, and (2) original performance baseline versus integrated performance over the life of the contracts. [Goal Met]	Maintained Procurement Baselines. Percentages within (1) original baseline cost for completed procurements of major computer systems or network services, and (2) original performance baseline versus integrated performance over the life of the contracts. [Goal Met]			
Initiated at least 5 competitively selected interdisciplinary research teams to provide computational science and applied mathematics advances that will accelerate biological discovery in microbial systems and develop the next generation of computational tools required for nanoscale science based on peer review, in partnership with the Biological and Environmental Research (BER) and Basic Energy Sciences (BES) programs, respectively, of submitted proposals. [Goal Met]	<u>Improved Computational Science Capabilities. Average annual percentage increased in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes within the SciDAC effort. [Goal Met]</u>	<u>Improved Computational Science Capabilities. Average annual percentage increased in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes within the SciDAC effort. [Goal Met]</u>	<u>Improved Computational Science Capabilities. Average annual percentage increased in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes within the SciDAC effort. FY 2006—>50%.</u> [Goal Met]	<u>Improve Computational Science Capabilities. Average annual percentage increase in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes within the SciDAC effort. FY 2007—>100%</u>	<u>Improve Computational Science Capabilities. Average annual percentage increase in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes within the SciDAC effort. FY 2008—>100%</u>
Maintained and operated facilities, including NERSC and ESnet, so the unscheduled downtime on average is less than 10% of the total scheduled operating time. [Goal Met]	Focused usage of the primary supercomputer at the NERSC on capability computing. Percentage of the computing time used was accounted for by computations that required at least 1/8 of the total resource. [Goal Not Met]	Focused usage of the primary supercomputer at the NERSC on capability computing. Percentage of the computing time used that was accounted for by computations that require at least 1/8 of the total resource. [Goal Met]	Focused usage of the primary supercomputer at the NERSC on capability computing. Percentage of the computing time used that was accounted for by computations that require at least 1/8 of the total resource. FY 2006—40%. [Goal Met]	Focus usage of the primary supercomputer at the NERSC on capability computing. Percentage of the computing time used that is accounted for by computations that require at least 1/8 of the total resource. FY 2007—40%	Focus usage of the primary supercomputer at the NERSC on capability computing. Percentage of the computing time used that is accounted for by computations that require at least 1/8 of the total resource. FY 2008—40%

Means and Strategies

The ASCR program will use various means and strategies to achieve its goals. However, various external factors may impact the ability to achieve these goals.

ASCR will support fundamental, innovative, peer-reviewed research to create new knowledge in areas of advanced computing research that are important to DOE. In addition, ASCR will plan, fabricate, assemble, and operate premier supercomputer and networking facilities that serve researchers at national laboratories, universities, and industry, thus enabling new understanding through analysis, modeling, and simulation for complex problems, and effective integration of geographically distributed teams through national laboratories. Finally, the program will continue its role in SC-wide SciDAC initiative with BES and BER in the areas of nanotechnology and Genomics: GTL. All research projects undergo regular peer review and merit evaluation based on procedures outlined in 10 CFR 605 for the extramural grant program, and under a similar process for the laboratory programs and scientific user facilities. All new projects are selected through peer review and merit evaluation.

External factors that affect the programs and performance include: (1) mission needs as described by the DOE and SC mission statements and strategic plans; (2) evolving scientific opportunities, which sometimes emerge in a way that revolutionizes disciplines; (3) results of external program reviews and international benchmarking activities of entire fields or subfields, such as those performed by the National Academy of Sciences (NAS); (4) unanticipated failures, e.g., in the evaluation of new computer architectures for science, that cannot be mitigated in a timely manner; (5) strategic and programmatic decisions made by other (non-DOE) Federal agencies and by international entities; and (6) the evolution of the commercial market for high performance computing and networking hardware and software.

The fundamental research program and facilities supported by ASCR are closely coordinated with the information technology research activities of other Federal Agencies (Defense Advanced Research Projects Agency [DARPA], Environmental Protection Agency [EPA], National Aeronautics and Space Administration [NASA], National Institute of Health [NIH], National Security Agency [NSA], and National Science Foundation [NSF]) through the Networking and Information Technology Research and Development (NITRD) subcommittee of the National Science and Technology Council (NSTC), under the auspices of Office of Science and Technology Policy (OSTP). This coordination is periodically reviewed by the President’s Council of Advisors on Science and Technology (PCAST). In addition to this interagency coordination, ASCR has a number of partnerships with other programs in SC and other parts of the Department, focused on advanced application testbeds to apply the results of ASCR research. Finally, ASCR has a significant ongoing coordination effort with the National Nuclear Security Administration’s (NNSA) Advanced Scientific Computing (ASC) Campaign to ensure maximum effectiveness of both computational science research efforts.

Validation and Verification

Progress against established plans is evaluated by periodic internal and external performance reviews. These reviews provide an opportunity to verify and validate performance. Quarterly, semiannual, and annual reviews consistent with specific program management plans are held to ensure technical progress, cost and schedule adherence, and responsiveness to program requirements.

Program Assessment Rating Tool (PART)

The Department implemented a tool to evaluate selected programs. PART was developed by the Office of Management and Budget (OMB) to provide a standardized way to assess the effectiveness of the Federal Government’s portfolio of programs. The structured framework of the PART provides a means through which programs can assess their activities differently than through traditional reviews. ASCR has incorporated feedback from OMB into the budget request and has taken the necessary steps to continue to improve performance.

In the FY 2005 PART review, OMB gave the ASCR program an overall rating of “Moderately Effective.” The OMB found that: the program supports a supercomputer user facility and targeted research programs in applied math, computer science, and computational application software, many of which have been historically regarded as world class and of high quality; and the program’s performance measures focus on the extent to which unique, large simulations are efficiently enabled by its software development activities and supercomputer user facilities. However, OMB was concerned that the program’s external advisory committee was underutilized. In addition, OMB found that the program supports world-class scientific user facilities, has demonstrated an improved level of interagency communication and cooperation, is in the process of drafting a long-term strategic vision, and has been very successful with a major effort in interdisciplinary software. The assessment found that ASCR has developed a limited number of adequate performance measures which are continued for FY 2008. These measures have been incorporated into this budget request, ASCR grant solicitations, and the performance plans of senior managers. As appropriate, they will be incorporated into the performance-based contracts of Management and Operating (M&O) contractors. To better explain these complex scientific measures, SC has developed a website (http://www.sc.doe.gov/measures/) that answers questions such as “What does this measure mean?” and “Why is it important?” Roadmaps, developed in consultation with the Advanced Scientific Computing Advisory Committee (ASCAC) and also available on the website, will guide reviews every three years by ASCAC of progress toward achieving the long-term Performance Measures. In April 2006, ASCAC was charged to conduct the first such review of progress toward the long-term measures. ASCAC reported to the Department on November 10, 2006, with ratings of good and excellent. The committee reports are available at http://www.sc.doe.gov/ascr/ascac_reports.htm. The Annual Performance Targets are tracked through the Department’s Joule system and reported in the Department’s Annual Performance Report which is available at http://www.cfo.doe.gov/progliaison/part2005.htm.

For FY 2006, there were three PART related actions for Advanced Scientific Computing Research.

- Engaging advisory panel and other outside groups in regular, thorough scientific assessments of the quality, relevance, and performance of its research portfolio and computing/network facilities.
- Engaging advisory panel and other outside groups in assessments of the program’s progress in achieving its long-term goals, and in studies that revisit the strategic priorities for the program.
- Implementing action plans for improving program management in response to past expert reviews.

In response to these previous OMB recommendations ASCR has:

- Established a Committee of Visitors (COVs) to provide outside expert validation of the program’s merit-based review processes for impact on quality, relevance, and performance. ASCR is working on an action plan to respond to the recommendations of the first two COVs, which focused on the research programs and facilities, respectively. ASCR will continue to host COVs and other panels to review the quality, relevance, and performance of the program. Another COV, focused again on the research programs, will be charged in February 2007.
- The Advanced Scientific Computing Research Advisory Committee (ASCAC) reviewed progress toward the long term PART goals of the program in 2006. ASCAC has also been charged to review the ASCR facilities, including ESnet, to evaluate performance measures and scientific accomplishments. ASCAC has also been asked to make recommendations on the networking research programs within ASCR with a view towards meeting the long-term networking needs of

SC. The networking report is expected in November 2007. ASCR published responses to the COV's findings and tracked improvements at http://www.sc.doe.gov/measures/FY06.html.

To improve public access to PART assessments and follow up actions, OMB has created the ExpectMore.gov website. Information concerning ASCR PART assessments and current follow up actions can be found by searching on "Advanced Scientific Computing Research" at http://ExpectMore.gov.

Overview

Computational modeling and simulation are among the most significant developments in the practice of scientific inquiry in the 20th Century. Scientific computing is particularly important for the solution of research problems that are insoluble by traditional theoretical and experimental approaches, hazardous to study in the laboratory, or time-consuming or expensive to solve by traditional means. All of the SC research programs—Basic Energy Sciences, Biological and Environmental Research, Fusion Energy Sciences, High Energy Physics, and Nuclear Physics—have identified major scientific challenges that can only be addressed through advances in scientific computing. The National Academies are currently carrying out a study, which was called for in the Analytical Perspectives of the President's FY 2006 Budget Request, entitled "Toward Better Understanding the Potential Impact of High-End Capability Computing on Science and Technology" to "enable a better understanding of the potential scientific impact of high-end capability computing that identifies and categorizes important scientific questions and technology problems for which an extraordinary advancement in our understanding is difficult or impossible without leading edge scientific simulation capabilities." This study is expected to better inform decision makers about the potential impact of computational science in general and ASCR's approach in particular.

ASCR research underpins the efforts of the other programs in SC. The applied mathematics research activity produces the fundamental mathematical methods to model complex physical and biological systems. The computer science research efforts enable scientists to efficiently perform scientific computations on the highest performance computers available and to store, manage, analyze, and visualize the massive amounts of data that result. The networking research activity provides the techniques to link the data producers (e.g., supercomputers and large experimental facilities) with scientists who need access to the data.

ASCR's other principal responsibility is to provide the high-performance computational and networking resources that are required for world leadership in science. Recent dramatic advances in scientific computation by researchers and computer companies underscore the importance of strengthening our position in computational sciences in strategic areas. The Administration has recognized the importance of high-end computing. The High End Computing Revitalization Task Force (HECRTF) report was published and ASCR is participating in implementing the plan.

How We Work

The program is responsible for planning and prioritizing all aspects of supported research, conducting ongoing assessments to ensure a comprehensive and balanced portfolio, regularly seeking advice from stakeholders, supporting core university and national laboratory programs, and maintaining a strong infrastructure to support research in applied mathematics, network and computer science, and advanced computing software tools. The quality of the research supported by the ASCR program is continuously evaluated through the use of merit-based peer review, scientific advisory committees, and interagency coordinating bodies.

Advisory and Consultative Activities

The Advanced Scientific Computing Advisory Committee (ASCAC) provides valuable, independent advice to DOE on a variety of complex scientific and technical issues related to the ASCR program. The ASCAC is charged with providing advice on promising future directions for advanced scientific computing research; strategies to couple advanced scientific computing research to other disciplines; and the relationship of the DOE program to other Federal investments in information technology (IT) research. ASCAC's recommendations include advice on long-range plans, priorities, and strategies to address more effectively the scientific aspects of advanced scientific computing including the relationship of advanced scientific computing to other scientific disciplines, and maintaining appropriate balance among elements of the program. This advisory committee plays a key role in assessing the scientific and programmatic merit of presently funded activities and in evaluating plans for the future. The Committee formally reports to the SC Director and includes representatives from universities, national laboratories, and industries who are involved in advanced computing research. Particular attention is paid to obtaining a diverse membership with a balance among scientific disciplines, institutions, and geographic regions. ASCAC operates in accordance with the Federal Advisory Committee Act (FACA), Public Law 92–463; and all applicable FACA Amendments, Federal Regulations, and Executive Orders.

The activities funded by the ASCR program are coordinated with other Federal efforts through the NITRD subcommittee of the NSTC. The Federal IT R&D agencies have established over a decade of highly successful collaborative accomplishments in multiagency projects and in partnerships with industry and academic researchers. The multiagency approach leverages the expertise and perspectives of scientists and technology users from many agencies who are working on a broad range of IT research questions across the spectrum of human uses of information technology. DOE has been an active participant in these coordination groups and committees since their inception and the ASCR program will continue to coordinate its activities through these mechanisms including an active role in implementing the Federal IT R&D FY 2002–2006 Strategic Plan under the auspices of the NSTC and OSTP.

In addition, ASCR, both through ASCAC and independently, supported a number of workshops to support its planning. These include the "Federal Plan for High-End Computing, report of the High End-Computing Revitalization Task Force (HECRTF)" which is available at http://www.itrd.gov/pubs/2004_hecrtf/20040702_hecrtf.pdf.

Facility Operations Reviews

The ASCR program has undertaken a series of operations reviews of the National Energy Research Scientific Computing Center (NERSC), the Energy Sciences Network (ESnet), the Advanced Computing Research Testbeds (ACRTs), and the Leadership Computing Facilities (LCFs).

NERSC, operated by the Lawrence Berkeley National Laboratory (LBNL), annually serves about 2,500 scientists throughout the United States as SC's high performance production computing facility. These researchers work at DOE laboratories, universities, industrial laboratories, and other Federal agencies. Proposals for computer time and disk storage are subjected to peer review to evaluate the quality of science, the relevance of the proposed research to SC goals and objectives, and the readiness of the proposed application to fully utilize the computing resources being requested. ASCR conducted a formal cost and schedule review of NERSC, adapting processes used to manage construction projects, in May 2005.

The ESnet, managed and operated by the LBNL, is a high-speed network serving thousands of DOE scientists and collaborators worldwide. ESnet enables researchers at national laboratories, universities, and other institutions to communicate with each other using the leading edge collaborative capabilities, not available in the commercial world, that are needed to address some of the world's most important scientific challenges. To meet the requirements of petascale science to support DOE missions have evolved, ESnet developed a plan for a new network architecture and a partnership with Internet2, the leading provider of advanced networks to U.S. universities, to develop the next generation optical network infrastructure for U.S. science. This plan was peer reviewed by the SC Office of Project Assessment in February 2005.

In FY 2004, ASCR conducted a peer review of the Center for Computational Sciences (CCS) evaluation of the Cray X1 computer. The results from this review validated the effective results of the evaluation and its contributions to the Federal high performance computing effort. Also in FY 2004, ASCR conducted a peer reviewed competition to establish a LCF for Open Science. This competition was won by a partnership of ORNL's CCS with Argonne National Laboratory (ANL) and Pacific Northwest National Laboratory (PNNL) that located the first LCF at the CCS. In March 2005 and in March 2006, the SC Project Assessment group conducted formal Baseline validation reviews of the ORNL LCF.

In FY 2006, ASCAC was charged to review the approach to performance measurement and assessment at the ASCR computing facilities, the appropriateness and comprehensiveness of the measures, the science accomplishments and their effects on Office of Science programs, the evolution of the role of the facilities and their anticipated computational needs for the next three to five years as well as progress towards the ASCR long-term PART measures. The ASCAC report on the PART measures was delivered in November 2006 with ratings of excellent for the goal related to multiscale mathematics and good for the goal related to the partnership with BER.

Program Reviews

In past years, ASCR has reviewed its applied mathematics activity at the National Labs in phases, approximately one-third each year.

In FY 2006, ASCR conducted a peer review of the Numerical Linear Algebra, Optimization, and Predictability Analysis areas at the National Labs. These areas represent 33% of the Applied Mathematics activity. In FY 2007, ASCR plans to review the Differential Equations and Advanced Numerical Methods for High Performance Computing areas within the Applied Mathematics activity, which represents an additional third of the activity.

In FY 2006, ASCR led the SC-wide re-competition of the SciDAC portfolio, with the exception of activities in partnership with the Fusion Energy Sciences program that were initiated in FY 2005. This re-competition included both disciplinary peer review and a cross-cutting panel of peers that evaluated the comprehensiveness, compatibility and impact of the potential portfolio of projects.

Planning and Priority Setting

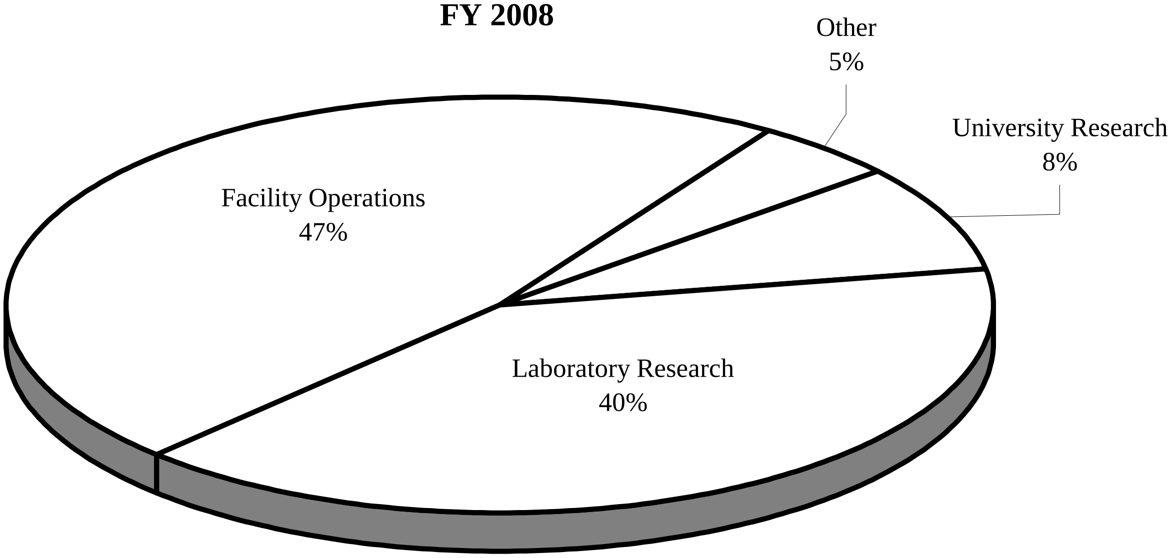
The ASCR program must coordinate and prioritize a large number of goals from agency and interagency strategic plans. One of the most important activities of ASCAC is the development of a framework for the coordinated advancement and application of network and computer science and applied mathematics. This framework must be sufficiently flexible to rapidly respond to developments in a fast paced area of research. The key planning elements for this program are:

- The Department and SC Strategic Plan, as updated through program collaborations and joint advisory committee meetings (http://www.sc.doe.gov/Sub/Mission/mission_strategic.htm); and
- The HECRTF Plan (http://www.itrd.gov/pubs/2004_hecrtf/20040702_hecrtf.pdf).

How We Spend Our Budget

The ASCR program budget has one subprogram: Mathematical, Information and Computational Sciences (MICS). The MICS subprogram has two major components: research and facility operations. The FY 2008 budget request continues the core and SciDAC research efforts and strengthens the research partnerships with other SC offices. Expenses for the operation of ESnet, which are not included in Facility Operations, account for 22% of the national laboratory research.

Advanced Scientific Computing Research Budget Allocation
FY 2008



Research

48 percent of the ASCR program's FY 2008 funding will be provided to scientists at universities and laboratories to conduct research. National laboratory research scientists work together with the other programs of SC to develop the tools and techniques that allow those programs to take advantage of terascale computing for scientific research. The laboratories provide state-of-the-art resources for testbeds and novel applications.

- ***University Research***: University researchers play a critical role in the nation's research effort and in the training of graduate students. During FY 2006, the ASCR program supported over 130 grants to the nation's university researchers and graduate students engaged in civilian applied mathematics, large-scale network, and computer science research. In addition, ASCR supports a Computational Science Graduate Fellowship (CSGF) and an Early Career Principal Investigator (ECPI) activity in Applied Mathematics, Computer Science, and High-Performance Networks. In FY 2006, CSGF activity selected 20 new graduate students representing 16 universities and 12 states. Approximately half of those who received Ph.D.'s in the CSGF program between 1991 and 2001 are pursuing careers outside universities or national labs. ASCR also provides support to other SC research programs. The ECPI activity made 7 new awards to early career principal investigators in FY 2006.

The university grants program is proposal driven, similar to the computer science and applied mathematics programs at the National Science Foundation (NSF). However, ASCR grant solicitation notices are focused on topics that have been identified as important for DOE missions and specifically include the long-term goals of ASCR. ASCR funds the best among the ideas submitted in response to grant solicitation notices that are published at http://www.grants.gov. Proposals are reviewed by external scientific peers and competitively awarded according to the guidelines published in 10 CFR 605 (http://www.science.doe.gov/production/grants/605index.html).

- ***National Laboratory Research***: ASCR supports national laboratory-based research groups at Argonne, Brookhaven, Los Alamos, Lawrence Berkeley, Lawrence Livermore, Oak Ridge, Pacific Northwest, and Sandia National Laboratories and Ames Laboratory. The directions of laboratory research programs are driven by the needs of the Department and the unique capabilities of the laboratories to support large scale, multidisciplinary, collaborative research activities. In addition, laboratory-based research groups are highly tailored to the major scientific programs at the individual laboratories and the computational research needs of SC. Laboratory researchers collaborate with other laboratory and academic researchers, and are important for developing and maintaining testbeds, novel applications of high performance computing, long-term development of software tools, and networking in SC research. At Los Alamos, Livermore, and Sandia, ASCR funding plays an important role in supporting basic research that can improve programs, such as NNSA's Advanced Scientific Computing and Science-Based Stockpile Stewardship programs.

ASCR funds field work proposals from the national laboratories. Proposals are reviewed by external scientific peers and awarded using procedures that are equivalent to the 10 CFR 605 guidelines used for the grants program. Performance of the laboratory groups is reviewed by ASCR staff annually to examine the quality of their research and identify needed changes, corrective actions, or redirection of effort. Individual laboratory groups have special capabilities or access to laboratory resources that can be profitably utilized in the development of the research program.

Significant Program Shifts

The ASCR program has been a leader in the computational sciences for several decades and has been acknowledged for pioneering accomplishments. The FY 2008 ASCR budget is focused in priority areas identified by the joint Office of Management and Budget (OMB) and Office of Science and Technology Policy (OSTP) Research Priorities memorandum.

Major elements of the ASCR portfolio related to SciDAC were recompeted in FY 2006, resulting in support for further enhancements and scaling to petaflop computers of software tools such as mathematical libraries, adaptive mesh refinement software, and scientific data management tools developed in the first 5 years of the effort. Also, efforts initiated in FY 2006 in mathematical methods, computer science and visualization to enable simulations on the path to petascale will be continued. Finally, in FY 2008, ASCR will continue funding the competitively selected SciDAC institutes which can become centers of excellence in high-end computational science in areas that are critical to DOE missions.

The demands of today's facilities, which generate millions of gigabytes per year of data, now far outstrip the capabilities of the public Internet. The evolution of the telecom market, including the availability of direct access to optical fiber at attractive prices and the availability of flexible dense wave division multiplexing (DWDM) products gives SC the opportunity to exploit these technologies to provide scientific data where it is needed at speeds commensurate with the growing data volumes. To take advantage of this opportunity, ESnet has entered into a long term partnership with Internet 2 to build the next generation optical network infrastructure needed for U.S. science.

The ORNL LCF, selected under the Leadership Computing Competition in FY 2004, will continue its evolution into a true leadership facility. The LCF as well as the enhancement of NERSC are aligned with the plan developed by the HECRTF established by OSTP. This area has been identified as a priority within the overall Networking and Information Technology Research and Development (NITRD) priorities of the Administration.

In FY 2007, further diversity of LCF resources will be realized with the acquisition by ANL of a high performance IBM Blue Gene P with low-electrical power requirements and a peak capability of up to 100 teraflops. In FY 2008, the IBM Blue Gene P at ANL LCF will be expanded to 250–500 teraflops. The expansion of the Leadership Computing Facility to include the Blue Gene computer at ANL was an important element of the joint ORNL, ANL, and PNNL proposal selected in 2004. This capability will accelerate scientific understanding in areas that include molecular dynamics, materials science and biology.

Eighty percent of LCF resources are made available to the open scientific community, including industry, through the Office of Science's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program with no requirement of DOE funding. INCITE projects, including those on the Leadership Computing Facilities, are characterized by substantial allocations for a small number of high-impact scientific applications and are selected through a fully open peer review and computational readiness review process.

As a result of the INCITE call for proposals issued July 27, 2006, eighty-eight proposals were received requesting over 184 million processor hours in 2007 allocations. Additionally INCITE renewal projects requested an additional 75 million processor hours for 2007. The proposals represented the following scientific disciplines: accelerator physics, astrophysics, chemical sciences, climate research, computer science, engineering physics, environmental science, fusion energy, life sciences, materials science, nuclear physics, and nuclear engineering. Following both readiness and peer reviews, over 95 million hours were awarded for 26 new and 19 renewal INCITE projects.

These changes were made to help ensure the continued quality, relevance, and performance of ASCR programs. All ASCR activities undergo prospective and retrospective merit reviews and our extensive use of partnerships with other SC programs ensures the relevance of our efforts to SC missions.

Interagency Environment

The activities funded by the MICS subprogram are coordinated with other Federal efforts through the National Information Technology Research and Development (NITRD) subcommittee of the National Science and Technology Council and its Technology Committee. The NITRD Subcommittee provides active coordination for the multiagency NITRD Program. The Subcommittee is made up of representatives from each of the participating NITRD agencies and from the Office of Management and Budget (OMB), OSTP, and the National Coordination Office for IT R&D (NCO/IT R&D). The Subcommittee coordinates planning, budgeting, and assessment activities of the multiagency NITRD enterprise. DOE has been an active participant in these coordination groups and committees since their inception. The MICS subprogram will continue to coordinate its activities through these mechanisms and will lead the development of new coordinating mechanisms as needs arise. While the DOE program solves mission critical problems in scientific computing, results from the DOE program benefit the Nation's information technology basic research effort. The FY 2007 program positions DOE to make additional contributions to this effort. In the area of high performance computing, ASCR has extensive partnerships with other Federal agencies and the National Nuclear Security Administration (NNSA). Examples include: participating in the program review team for the Defense Advanced Research Projects Agency (DARPA) High Productivity Computing Systems program; serving on the planning group for the Congressionally mandated Department of Defense (DOD) plan for high performance computing to serve the national security mission; co-chairing the Office of Science and Technology Policy (OSTP) High End Computing Revitalization Task Force; and extensive collaboration with NNSA-Advanced Simulation and Computing. In FY 2003, ASCR formalized many of these interactions by developing a Memorandum of Understanding with SC, NNSA, DOD's Under Secretary for Defense

Research and Engineering, DARPA, and the National Security Administration to coordinate research, development, testing, and evaluation of high performance computers.

At the direction of the Senate's Energy and Water Development Appropriations Committee, ASCR and the NNSA Advanced Simulation and Computing program co-funded a study by the National Research Council on the Future of Supercomputing. The final report of the study, *Getting Up to Speed: The Future of Supercomputing*, was issued in 2005 and assessed the state of U.S supercomputing capabilities and relevant research and development (*Getting Up to Speed: The Future of Supercomputing*, Susan L. Graham, Marc Snir, and Cynthia A. Patterson, Editors, The National Academies Press, Washington, D.C., 2005).

Scientific Discovery through Advanced Computing

The Scientific Discovery through Advanced Computing (SciDAC) program is a set of coordinated investments across all SC mission areas with the goal of achieving breakthrough scientific advances via computer simulation that were impossible using theoretical or laboratory studies alone. SciDAC has pioneered an effective new model of multidisciplinary collaboration among discipline-specific scientists, computer scientists, computational scientists, and mathematicians. The product of this collaborative approach is a new generation of scientific simulation codes that can productively exploit state-of-the-art computing and networking resources.

In FY 2006, ASCR recompeted its SciDAC portfolio, with the exception of activities in partnership with the Office of Fusion Energy that were initiated in FY 2005. In addition, in FY 2007 ASCR will continue the competitively selected SciDAC institutes which can become centers of excellence in high end computational science in areas that are critical to DOE missions. New SciDAC activities include Centers for Enabling Technologies, Science Applications and Scientific Applications Partnerships, and SciDAC Institutes.

Centers for Enabling Technologies (CETs), which replace the Integrated Software Infrastructure Centers (ISICs) from prior budgets, address the mathematical and computing systems software environment elements of the SciDAC scientific computing software infrastructure. The CETs are laboratory-university partnerships and address needs for: new algorithms that scale to parallel systems having hundreds-of-thousands of processors; methodology for achieving portability and interoperability of complex high-performance scientific software packages and libraries; operating systems and runtime tools and support for application execution performance and system management; and effective tools for analyzing, managing, visualizing and extracting scientific results from petabyte-scale scientific data sets obtained both from large-scale simulation and from laboratory experiment. CETs provide the essential computing and communications infrastructure for support of SciDAC applications.

Scientific Applications Partnerships (SAPs) are partnerships with other SC Programs and with some of the applied programs in the Department to integrate advanced applied mathematics and computer science technologies into specific SciDAC applications projects such as Genomics: GTL, Combustion, or the Fusion Simulation Project. Although the technical focus of SAPs is similar to that of CETs, the two program elements are complementary. First, the mathematicians and computer scientists funded by SAPs focus on the needs of specific science application teams and link these teams to the CET efforts which are larger and focus on software and mathematical tools that can be used by multiple applications teams. Second, SAPs provide the mechanism to supply application teams the computer science and mathematics expertise not covered by CET teams in order to fill important technical gaps.

SciDAC Institutes provide for the sustained infusion of new ideas and community focus to enhance the SciDAC program by building a broader community of researchers who understand the challenges of providing and using high-performance modeling and simulation capabilities and are willing to address these problems collaboratively. The SciDAC Institutes are university-led centers of excellence intended to complement the efforts of the other SciDAC program elements, and will provide a forum for discussion of fundamental computational issues affecting scientific discovery. SciDAC Institutes will be patterned on successful institute models in other scientific communities.

Scientific Facilities Utilization

The ASCR program's FY 2008 budget request includes support to the NERSC, ESnet, and the LCFs, located at ORNL's CCS and ANL. The investment in NERSC will provide computer resources for about 2,500 scientists in universities, DOE laboratories, Federal agencies, and U.S. companies. The proposed funding will enable NERSC to maintain its role as one of the Nation's premier unclassified computing centers, a critical element for success of many SC research programs. The investment in ESnet will provide the DOE science community with capabilities not available through commercial networks or the commercial Internet. ESnet provides national and international high-speed access to DOE and SC researchers and research facilities, including light sources, neutron sources, particle accelerators, fusion reactors, spectrometers, supercomputers, and other high impact scientific instruments. The investment in LCFs will deliver unclassified high performance capability resources to scientific researchers. The proposed funding will allow the high performance resources at the ANL LCF to be upgraded to a peak capability of 250–500 teraflops by the end of FY 2008. The ORNL-LCF will be on a path to one petaflop peak capability by the end of FY 2008.

	FY 2006	FY 2007 Estimate	FY 2008 Estimate
NERSC			
Maximum Hours	8,760	8,760	8,760
Scheduled Hours	8,585	8,585	8,585
Unscheduled Downtime	1%	1%	1%
ESnet			
Maximum Hours	8,760	8,760	8,760
Scheduled Hours	8,585	8,585	8,585
Unscheduled Downtime	1%	1%	1%
LCF-ORNL			
Maximum Hours	7,008	7,008	7,008
Scheduled Hours	7,008	7,008	7,008
Unscheduled Downtime	1%	1%	1%
LCF-ANL			
Maximum Hours	—	TBD[a]	6,000
Scheduled Hours	—	TBD	6,000
Unscheduled Downtime	—	1%	1%

[a] Inadequate basis for making reliable estimates at this time.

Workforce Development

The R&D Workforce Development mission is to ensure the supply of computational and computer science Ph.D. level scientists for the Department and the Nation through graduate student and postdoctoral research support. In FY 2008, this program will support approximately 415 graduate students.

ASCR will continue the Computational Science Graduate Fellowship Program with the selection of 20 new students in FY 2006 to support the next generation of leaders in computational science.

	FY 2006	FY 2007 Estimate	FY 2008 Estimate
# University Grants	135	150	170
Average Size (whole dollars)	$197,000	$197,000	$197,000
# Laboratory Groups	155	165	165
# Graduate Students	350	375	415
# Permanent Ph.D.s	625	670	720

Mathematical, Information, and Computational Sciences

Funding Schedule by Activity

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
Mathematical, Information, and Computational Sciences			
Mathematical, Computational, and Computer Sciences and Distributed Network Environment Research	109,631	117,122	129,910
High Performance Computing and Network Facilities and Testbeds	118,751	193,030	201,126
SBIR/STTR	—	8,502	9,162
Total, Mathematical, Information, and Computational Sciences	228,382	318,654	340,198

Description

The Mathematical, Information, and Computational Sciences (MICS) subprogram is responsible for carrying out the mission of the ASCR program: To deliver forefront computational and networking capabilities to scientists nationwide that enable them to extend the frontiers of science, addressing a range of science issues that include the function of living cells and the power of fusion energy.

Benefits

MICS supports ASCR’s contribution to DOE’s mission by providing world-class, peer-reviewed scientific results in mathematics, high performance computing and advanced networks and applying the potential of terascale computing to advanced scientific applications. Computer-based simulation enables us to predict the behavior of complex systems that are beyond the reach of our most powerful experimental probes or our most sophisticated theories. Computational modeling has greatly advanced our understanding of fundamental processes of nature, such as fluid flow and turbulence or molecular structure and reactivity. Through modeling and simulation, we will be able to explore the interior of stars and learn how protein machines work inside living cells. We can design novel catalysts and high-efficiency engines. Computational science is increasingly central to progress at the frontiers of almost every scientific discipline and to our most challenging feats of engineering. Accordingly, we must address the following questions:

- What new mathematics are required to more effectively model systems such as the earth’s climate or the behavior of living cells that involve processes taking place on vastly different time and/or length scales?
- Which computational architectures and platforms will deliver the most benefit for the science of today and the science of the future?
- What advances in computer science and algorithms are needed to increase the efficiency with which supercomputers solve problems?
- What operating systems, data management, analysis, model development, and other tools are required to make effective use of future-generation supercomputers?
- What tools are needed to make all scientific resources readily available to scientists, regardless of whether they are at a university, national laboratory, or industrial setting?

To answer these questions and develop the algorithms software and tools that are needed, MICS has developed four strategies (the strategy numbers refer to the SC Strategic Plan):

6.1 Advance scientific discovery through research in the computer science and applied mathematics required to enable prediction and understanding of complex systems.

6.2 Extend the frontiers of scientific simulation through a new generation of computational models that fully exploit the power of advanced computers, and through collaboratory software that makes scientific resources available to scientists anywhere, anytime.

6.3 Bring dramatic advances to scientific computing challenges by supporting the development, evaluation, and application of supercomputing architectures tailored to science.

6.4 Provide computing resources at the petascale and beyond, network infrastructure, and tools to enable computational science and scientific collaboration.

All MICS investments directly contribute to one or more of these strategies.

Supporting Information

To establish and maintain DOE's modeling and simulation leadership in scientific areas that are important to its mission, the MICS subprogram employs a broad, but integrated, research strategy. The MICS subprogram's basic research portfolio in applied mathematics and computer science provides the foundation for enabling research activities, which includes efforts to advance networking and to develop software tools, libraries, and environments. Results from enabling research supported by the MICS subprogram are used by computational scientists supported by other SC and DOE programs. This link to other DOE programs provides a tangible assessment of the value of the MICS subprogram for advancing scientific discovery and technology development through simulations.

In addition to its research activities, the MICS subprogram plans, develops, and operates supercomputer and network facilities that are available—24 hours a day, 365 days a year—to researchers working on problems relevant to DOE's scientific missions.

The Early Career Principal Investigator (ECPI) activity was initiated in FY 2002 for scientists and engineers in tenure track positions at U.S. universities. Since that time 62 awards have been made including six awards in FY 2006. The goal of the ECPI activity is to support SC mission-related research in applied mathematics, computer science, and high-performance networks performed by exceptionally talented university investigators, who are at an early stage in their professional careers.

FY 2006 Accomplishments

- ***NERSC to increase peak capacity by factor of 100.*** NERSC, through the competitive procurement process for NERSC-5, evaluated a number of vendors, using the NERSC Sustained System Performance (SSP) metric. The SSP metric was developed by NERSC to better gauge how well a proposed system will meet the needs of the Center's 2,500 users and measures sustained performance on a set of codes selected to accurately represent the Center's portfolio of challenging scientific applications. Based on the evaluations, NERSC selected a 100 teraflop Cray Hood system. The system will consist of over 19,000 AMD Opteron 2.6-gigahertz processor cores, with two cores making up one node. Each node has 4 gigabytes of memory resulting in aggregate memory capacity of 39 terabytes.
- ***Leadership Computing Facility doubles XT3 capability to 54 teraflops.*** The LCF at ORNL upgraded the Cray XT3 supercomputer to increase the system's computing power to 54 teraflops.

The LCF system is currently the largest high performance computing system in SC and will become a major computing resource for DOE's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. The upgrade involved replacing all 5,212 single core processors with Cray's dual-core processors, doubling the memory and increasing the bisection bandwidth resulting in a supercomputer that consists of more than 10,400 processing cores and 21 terabytes of memory. The upgrade will allow the LCF to provide additional resources for computationally intensive, large-scale projects with the potential of high scientific impact such as the design of innovative nanomaterials, predictive simulations of fusion devices and the understanding of microbial molecular and cellular systems.

- ***ESnet moves forward with new architecture to deliver cost effective, high reliability, high performance networks for science.*** Energy Sciences Network (ESnet) is implementing a new architecture that is a double core ring with interconnected metropolitan area networks (MANs). The new architecture is designed to meet the increasing demand for network bandwidth, high reliability, and advanced network services as next-generation scientific instruments and supercomputers come on line. In FY 2006, the second and third MANs were completed in the Chicago and New York-Long Island areas. They provide dual connectivity at 20 gigabits per second—10 to 50 times the previous site bandwidths, depending on the site using the ring—while reducing the overall cost. These MANs connect ANL, Fermi National Accelerator Laboratory (FNAL), and BNL to the ESnet backbone to address critical requirements such as Large Hadron Collider (LHC) data. By increasing bandwidth to these sites, DOE advances research in areas such as climate change, genetics, renewable energy, nanotechnology, national security, and basic science in physics and chemistry through support for the large-scale science and large-scale SC collaborations nationwide.
- ***Lambda Station enables High Energy Physics researchers to prepare for LHC.*** Lambda Station, a high-capacity software-based network technology device, which combines advanced optical networks technologies with ultra high-speed data-intensive applications, has enabled researchers at FNAL, bracing for an onslaught of data from LHC experiments, to develop ultra fast connections for moving US-CMS (the U.S. part of the Compact Muon Solenoid detector) data between LHC Tier1 and Tier2 centers. Initial test results using Lambda Station technology enabled FNAL, the US-CMS Tier1 center to transfer data at line rate (10 gigabits per second) to Caltech, a US-CMS Tier2 center. This transfer rate represents a 15 fold increase in file system to file system transfer speed.
- ***Simulations on Massively Parallel (32,000 Processor) Architectures Provide New Insights into Galaxies.*** ANL applied mathematicians have developed Nek5000, an advanced scientific simulation tool, that features high-order numerical discretizations and multigrid solvers capable of scaling to thousands of processors. Such extreme scalability is needed to simulate magnetohydrodynamics in complex domains. A major advance this year was the port of Nek5000 to the 32,000-processor Blue Gene platform at IBM Watson, where the researchers were able to identify an unexpected linear angular vector profile during their study of angular momentum transport in galaxies.
- ***Unified Parallel C implements one-sided messages to improve scientific software performance on high performance computers.*** Partitioned Global Address space languages offer an alternative to message passing programming on high end systems. LBNL and University of California groups recently demonstrated that the languages can effectively leverage modern network hardware to provide performance that is faster than the two-sided send/receive models for some machines and computations. One example is the communication-intensive 3D Fast Fourier Transform (FFT),

important to many scientific simulations. The compilers for these languages are highly portable and support interoperability with the Message Passing Interface, Fortran, and C/C++ languages.

Detailed Justification

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
Mathematical, Computational, and Computer Sciences and Distributed Network Environment Research	**109,631**	**117,122**	**129,910**
▪ **Applied Mathematics**	**32,022**	**29,495**	**36,900**

This activity supports research on the underlying mathematical understanding of physical, chemical, and biological systems, and on advanced numerical algorithms that enable effective description, modeling, and simulation of such systems on high-end computing systems. It directly supports SC Strategic Plan strategy 6.1. Research in Applied Mathematics supported by the MICS subprogram underpins computational science throughout DOE. Historically, the numerical algorithms developed under this activity have produced scientific advances through simulation that are as significant as those resulting from improvements in computer hardware. This activity supports research at DOE laboratories, universities, and private companies. Many of the projects supported by this activity involve research partnerships between DOE's national laboratories and universities.

The activity supports research in a wide variety of areas of mathematics, including: ordinary and partial differential equations and solution methods, including techniques to convert equations into discrete elements and boundary integral methods; advanced treatment of interfaces and boundaries (fast marching and level set methods, and front tracking); numerical linear algebra (advanced iterative methods, general and problem-specific preconditioners, sparse solvers, and dense solvers); fluid dynamics (compressible, incompressible, and reacting flows, turbulence modeling, and multiphase flows); optimization (linear and nonlinear programming, interior-point methods, and discrete and integer programming); mathematical physics; control theory (differential-algebraic systems, order reduction, and queuing theory); accurate treatment of shock waves; "fast" methods (fast multipole and fast wavelet transforms); mixed elliptic-hyperbolic systems; dynamical systems (chaos theory, optimal control theory, and bifurcation theory); automated reasoning systems; and multiscale mathematics; risk assessment and optimization of complex systems. This final area represents a new effort focusing on those mission-related applications involving control in complex systems.

In FY 2008, this activity is increased to support critical long-term mathematical research issues relevant to petascale science (+$2,000,000), research in optimization control and risk analysis in complex systems (+$1,900,000), and research in multiscale mathematics (+$2,505,000). Support for multiscale mathematics is $11,000,000 in FY 2008. The Computational Science Graduate Fellowship Program is also increased by $1,000,000, bringing the total to $5,000,000.

▪ **Computer Science**	**31,763**	**23,863**	**29,000**

This activity supports research in computer science to enable computational scientists to effectively utilize petascale computers to advance science in areas important to the DOE mission. This activity supports SC Strategic Plan strategies 6.1 and 6.3. DOE has unique requirements for high performance computing that significantly exceed the capability of software products from computer vendors. This activity supports computer science research in two general areas: the underlying software to enable applications to make effective use of petascale computers with hundreds or thousands of processors as well as computers that are located at different sites; and large-scale data management and visualization for both local and remote data analysis. Research areas include: scalable tools to diagnose and monitor the performance of scientific applications and enable users to improve performance and get scientific results faster; new programming models that scale to hundreds of thousands of processors to simplify application code development for petascale computing; advanced techniques for visualizing very large-scale scientific data; and efforts to improve petascale application performance through innovative next generation operating systems. Researchers at DOE laboratories and universities, often working in partnerships, propose and conduct this research.

All of the computer science research funded by this activity is reported to and coordinated through the High End Computing Interagency Working Group of the NITRD Subcommittee. The quality, relevance, and performance of the program is continually monitored through extensive peer review, interagency reporting and coordination, and interaction with end users to assist in the determination of impact and future research priorities.

Beginning in FY 2004, this activity incorporated the software research component of the implementation of the HECRTF plan to improve application performance and system reliability through innovative approaches to next generation operating systems. This activity is coordinated with other agencies through the High End Computing University Research Activity (HECURA), an outgrowth of the HECRTF. These activities were modestly increased to $5,363,000 in FY 2007, especially in areas such as performance analysis of innovative high-end architectures; frameworks for data intensive and visual computing; intelligent program development environments; application-specific problem solving environments; and common compile and runtime infrastructures and interfaces, where ASCR is the leader in the Federal agency research efforts. This research will play a key role in the interagency strategy for high-end software development.

Beginning in FY 2008, the Computer Science activity will have a focus on strengthening long-term research in computer science to ensure that scientific applications can fully exploit future hardware performance. In the software environment area, additional funding (+$4,137,000) will focus on developing software and tools (focused on integrated/intelligent software development environments and new generation debugging and performance analysis tools providing improved ease-of-use at the petascale) to enable both experienced and new researchers to make effective use of petascale scale systems at the national Leadership Computing Facilities (LCFs) and at the supercomputer facilities. In the data analyses, management, and visualization area (+$1,000,000), we will focus on accelerated visualization, uncertainty and user interface environments.

	FY 2006	FY 2007	FY 2008
▪ **Computational Partnerships**	**28,796**	**50,000**	**50,246**

This activity supports Scientific Discovery through Advanced Computing (SciDAC). The advanced computing software tools part of this activity supports research and development activities that extend key results from applied mathematics and computer science research to develop integrated software tools that computational scientists can use in high performance scientific applications (such as characterizing and predicting phase changes in materials). These tools, which enable improved performance on high-end systems, are critical to the ability of scientists to attack the complex scientific and engineering problems that can only be solved with such systems. This activity directly supports SC Strategic Plan strategy 6.2.

In FY 2008, this activity will support SciDAC Centers for Enabling Technologies (CET) and SciDAC Institutes that were competitively selected in FY 2006.

The CETs funded under this activity ($21,000,000), both university-led and national laboratory-led, will address the mathematical and computational systems software environment of the SciDAC computing software infrastructure. This infrastructure envisions a comprehensive, integrated, scalable, and robust high performance software environment, which overcomes difficult technical challenges to enable the effective use of terascale and petascale systems by SciDAC applications. CETs address needs for: new algorithms which scale to petascale computing systems having hundreds-of-thousands of processors; methodology for achieving portability and interoperability of complex high performance scientific software packages; operating systems and runtime tools and support for application execution performance and system management; and effective tools for feature identification, data management, and visualization of petabyte-scale scientific data sets. The CETs work closely with application scientists to develop and introduce software into application codes.

The SciDAC Institutes ($7,000,000) are university-led centers of excellence which complement the efforts of the SciDAC CETs but with a role in the development of the next generation of computational scientists. The SciDAC Institutes focus on application codes and are in turn dependent on the algorithms and software developed by the high-performance computer science community. The SciDAC Institutes activities will include: efforts to develop, test, maintain, and support optimal algorithms, programming environments, systems software and tools, and applications software; focus on a single general method or technique (for example, large scale optimization for engineering problems); be a focal point for bringing together a critical mass of leading experts from multiple disciplines to focus on key problems in a particular area of enabling technologies; and reach out to engage a broader community of scientists to advance in scientific discovery through advanced computation, collaboration, training of graduate students and postdoctoral fellows.

The FY 2008 request also includes $22,246,000 for Scientific Applications Partnerships (SAPs) that support collaborative research of applied mathematicians and computer scientists with domain scientists to develop and apply computational techniques and tools to address problems relevant to the SC mission. This effort tests the usefulness of advances in computing research, transfers the results of this research to the scientific disciplines and helps define opportunities for future research.

In the competitively selected FY 2006 SciDAC awards, partnerships have been formed with SC programs in Basic Energy Sciences (BES), Biological and Environmental Research (BER), Fusion Energy Sciences (FES), High Energy Physics (HEP), and Nuclear Physics (NP), and with the National Nuclear Security Administration (NNSA). The projects are part of the SciDAC activity and are coupled to the SciDAC CETs and Institutes. Areas under investigation include nuclear physics (HEP, NP, and NNSA); petascale data (HEP); accelerator physics and design (HEP); computational astrophysics (HEP, NP, and NNSA); quantum chromodynamics (NP); computational biology,

	(dollars in thousands)	
FY 2006	FY 2007	FY 2008

ground water modeling and simulation, and climate models (BER); plasma turbulence in tokamaks (FES); turbulence, materials science and chemistry (BES and NNSA). This activity directly supports SC Strategic Plan strategy 6.2.

The FY 2008 request for SAPs includes $16,000,000 to continue the competitively selected FY 2006 SciDAC awards, as well as the partnerships with the BER Genomics: GTL program, the BES program in nanoscale science, and the FES program for the Fusion Simulation Project (FSP).

	FY 2006	FY 2007	FY 2008
▪ **Distributed Network Environment Research**	**17,050**	**13,764**	**13,764**

This activity builds on the fundamental results of computer science to develop integrated software tools and advanced network services to enable large-scale scientific collaboration and make effective use of distributed computing and science facilities to advance the DOE science mission. The activity supports research and development in three areas: 1) distributed systems software, tools, and services to enable the discovery, management, and distribution of petabyte-scale data sets generated by simulations or by science experiments such the Large Hadron Collider (LHC) in HEP and ITER ($3,000,000) in FES, 2) advanced network protocols, optical network services, tools, and protocols to interconnect and provide access to LCFs and science facilities ($7,764,000); and 3) high-performance middleware to facilitate secure national and international scientific collaborations ($3,000,000). This activity will enable SC to exploit new capabilities being made available by ESnet and other national research and education networks to provide scientific data where it is needed at speeds commensurate with the new data volumes.

All research in this activity is reported to and coordinated with the Large-Scale Networking (LSN) Interagency Working Group of the NITRD Subcommittee. This activity builds the understanding that will enable ESnet as well as other Research and Education Networks such as the Internet2 Abilene network to fully take advantage of the opportunity to make optical networks tools for science. In much the same way that early scientific use of the Internet enabled today's worldwide infrastructure, the experience of scientists on these new optical networks is expected to influence the next generation of high performance networks for the country. For example, it includes standards-based network protocols and middleware that address challenging issues such as security, information location, and network performance that are encountered with ultra-high-speed data transfers, remote visualization, real-time remote instrumentation, and large-scale scientific collaboration. These tools provide a new way of organizing and performing scientific work, e.g., distributed teams and real-time remote access to SC facilities that offers the potential for increased productivity and efficiency. It will also enable broader access to important DOE facilities and data resources by scientists and educators throughout the country. It is particularly important to provide for efficient, high-performance, reliable, secure, and policy-aware management of large-scale data movement across the research enterprise.

	FY 2006	FY 2007	FY 2008
High Performance Computing and Network Facilities and Testbeds	**118,751**	**193,030**	**201,126**
▪ **High Performance Computing Facilities and Testbeds**	**94,985**	**170,294**	**176,790**

This activity directly supports SC Strategic Plan strategy 6.4 through a portfolio of capabilities that range from Research and Evaluation Prototypes (R&E Prototypes) to Leadership Computing

Facilities (LCFs) to High Performance Production Computing (HPPC). This activity integrates activities previously described separately as NERSC and ACRTs. It includes NERSC and resources at the ORNL and ANL LCFs. Related requirements for capital equipment, such as high-speed disk storage systems, archival data storage systems, and high performance visualization hardware are also supported at a reduced level in FY 2008.

	FY 2006	FY 2007	FY 2008
• **High Performance Production Computing**	**37,489**	**54,790**	**54,790**

This activity supports the National Energy Research Scientific Computing Center (NERSC), located at the LBNL. NERSC delivers high-end capacity computing services and support to the entire DOE SC research community and provides the majority of resources and services that are used to support SC SciDAC programs. The center serves 2,500 users working on about 400 projects. 56% of users are university based, 33% are in National Laboratories, 7% are in other government laboratories, and 4% are in industry. FY 2008 funding will support the continued operation of NERSC 3e at 10 teraflops peak performance, and the computer systems, NCSa and NCSb, with a combined peak performance of 10 teraflops and NERSC-5. NCSa and NCSb are focused on high performance production computing for scientific applications that do not scale well to more than 512 processors and are not well suited to the NERSC 3e. In addition, the next generation of high performance resources at NERSC, NERSC-5, scheduled to be delivered in FY 2007 will have a peak capacity between 100–150 teraflops. These computational resources are integrated by a common high performance file storage system that enables users to easily migrate to any of the resources. With the acquisition of NERSC-5, the capacity at NERSC increased by about a factor of 6.

In FY 2008, NERSC will continue to play a key role in the SC strategy for computational science because it enables teams to prepare to make the best use of the Leadership Computing Facilities (LCF) as well as to perform the calculations that are required by the missions of SC. In FY 2008, $29,435,000 is dedicated to hardware procurement, $4,836,000 to user support services, $4,506,000 to utilities, and $16,013,000 to other support costs.

	FY 2006	FY 2007	FY 2008
• **Leadership Computing Facilities (LCF)**	**53,630**	**102,504**	**105,000**

The LCF activity was initiated with a call for proposals in FY 2004. As a result of the peer-reviewed competition, the partnership established by ORNL, ANL, and PNNL was selected to provide capability computing resources for SC researchers. Eighty percent of LCF resources are made available to the open scientific community, including industry, through SC's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program with no requirement of DOE funding. INCITE projects, including those on the Leadership Computing Facilities, are characterized by substantial allocations for a small number of high-impact scientific applications and are selected through a fully open peer review and computational readiness review process.

	FY 2006	FY 2007	FY 2008
▸ **Leadership Computing Facility at ORNL**	**53,036**	**80,000**	**77,000**

The first LCF capability for science was established in late FY 2005 at ORNL with the acquisition of a Cray X1E, the most capable system available to scientific users in the U.S., and a complementary Cray Red Storm (XT3) system. In FY 2007, the ORNL LCF will upgrade the Cray XT3 to a peak capacity of 100 teraflops and will be on the path to one petaflop in FY 2008.

In FY 2008, the ORNL LCF will continue to provide world leading high performance sustained capability to researchers on a peer-reviewed basis. The acquisition of a 1 petaflop Cray Baker system in late FY 2008 will enable further scientific advancements such as simulations of diesel combustion that could lead to cleaner energy from coal and simulations of fusion devices that approach ITER scale devices and quantum Monte Carlo calculations of complex chemical reactions that extend over experimentally relevant times. The success of this effort is built on the enhancements to the research and evaluation prototype and computer science research activities elsewhere. In FY 2008, $37,195,000 is dedicated to hardware procurement, $9,906,000 to user support services, $4,892,000 to utilities, and $25,007,000 to other support costs.

- **Leadership Computing Facility at ANL** **594** **22,504** **28,000**

In FY 2007, further diversity with the LCF resources was realized with an acquisition by ANL of a high performance IBM Blue Gene P with low-electrical power requirements and a peak capability of up to 100 teraflops. The expansion of the Leadership Computing Facility to include the Blue Gene computer at ANL was an important element of the joint ORNL, ANL, and PNNL proposal selected in 2004.

In FY 2008, the IBM Blue Gene P at ANL LCF will be expanded to 250–500 teraflops. This capability will accelerate scientific understanding in areas that include molecular dynamics, catalysis, protein/DNA complexes, and aging of materials. In FY 2008, $17,741,000 is dedicated to hardware procurement, $4,822,000 to user support services, $1,788,000 to utilities, and $3,649,000 to other support costs.

- **Research and Evaluation Prototypes** **3,866** **13,000** **17,000**

The Research and Evaluation Prototype computer activity will prepare users for the next generations of scientific computers and reduce the risk of major procurements. This activity will be carried out in close partnership with the NNSA and the DARPA HPCS program. This effort is critical to address the challenges of the systems that will be available by the end of the decade. These systems will be ten times larger than those of today. Many of the issues that need to be addressed are shared with the computer science research effort described above. This activity includes the SC partnership in the DARPA HPCS Phase III program ($13,000,000) as well as support for SC's participation in the joint SC-NNSA partnership with IBM to explore low power density approaches to petascale computing ($4,000,000).

- **High Performance Network Facilities and Testbeds** **23,766** **22,736** **24,336**

This activity directly supports SC Strategic Plan strategy 6.4 to provide high capability networking services to support leading edge scientific research. This strategy integrates ESnet, a Wide Area Network (WAN) project that supports the scientific research mission of the DOE with a number of smaller Metropolitan Area Networks (MANs). ESnet provides high bandwidth access to the ESnet backbone to provide national and international high-speed access to DOE and SC researchers and

	(dollars in thousands)	
FY 2006	FY 2007	FY 2008

research facilities, including light sources, neutron sources, particle accelerators, fusion reactors, spectrometers, supercomputers, and other high impact scientific instruments.

In FY 2008, SC Networks will take advantage of the partnership between ESnet and the Internet2, which was announced in August 2006, to implement the next generation optical network infrastructure for U.S. science. At this funding level in FY 2008 ($24,336,000), ESnet will deliver a 10 gigabit per second (gbps) core Internet service as well as a Science Data Network with 20 gbps on its northern route and 10 gbps on its southern route. The success of this effort builds on the tools and knowledge developed by the Distributed Network Environment Research effort described above to enable SC to realize the promise of optical networks for DOE missions. $13,315,000 is dedicated to procuring data services, $7,211,000 to support services, and $3,810,000 to the research partnership with Internet2.

	FY 2006	FY 2007	FY 2008
Small Business Innovative Research (SBIR)/ Small Business Technology Transfer (STTR)	**—**	**8,502**	**9,162**

In FY 2006, $5,627,000 and $675,000 were transferred to the SBIR and STTR programs respectively. The FY 2007 and FY 2008 amounts shown are the estimated requirements for the continuation of the SBIR and STTR programs.

	FY 2006	FY 2007	FY 2008
Total, Mathematical, Information, and Computational Sciences	**228,382**	**318,654**	**340,198**

Explanation of Funding Changes

	FY 2008 vs. FY 2007 ($000)
Mathematical, Computational, and Computer Sciences and Distributed Network Environment Research	
▪ **Applied Mathematics**	
The increase will support critical long-term mathematical research issues relevant to petascale science, multiscale mathematics, and optimization control and risk analysis in complex systems as well as a $1,000,000 increase in the Computational Science Graduate Fellowship Program to $5,000,000.	+7,405
▪ **Computer Science**	
This increase will focus on strengthening long-term research in computer science to ensure that scientific applications can fully exploit future hardware performance. In the software environment area, additional funding will have a focus on developing software and tools to enable both experienced and new researchers to make effective use of petascale scale systems at the LCFs and supercomputer facilities. In data analyses, management and visualization, focus will be on accelerated visualization, uncertainty and user interface environments.	+5,137

	FY 2008 vs. FY 2007 ($000)
▪ **Computational Partnerships**	
Additional funds will continue the competitively selected FY 2006 SciDAC awards as well as the partnerships with the BER Genomics: GTL program, the BES program in nanoscale science, and the FES program for the Fusion Simulation Project (FSP).	+246
Total, Mathematical, Computational, and Computer Sciences and Distributed Network Environment Research	**+12,788**
High Performance Computing and Network Facilities and Testbeds	
▪ **High Performance Computing Facilities and Testbeds**	
• **Leadership Computing Facilities (LCFs)**	
The IBM Blue Gene P at ANL LCF will be expanded to 250–500 teraflops. This capability will accelerate scientific understanding in areas that include molecular dynamics, catalysis, protein/DNA complexes, and aging of materials. The ORNL LCF will operate the 250 teraflop Cray XT4 system and prepare to accept the 1 Petaflop follow on system.	+2,496
▪ **Research and Evaluation Prototypes**	
This activity will be expanded to support the DOE-DARPA HPCS partnership as well as the SC-NNSA Low Power Density petaflop computing partnership with IBM.	+4,000
▪ **High Performance Network Facilities and Testbeds**	
This increase will enable ESnet in FY 2008 to deliver a 10 gigabit per second (gbps) core Internet service as well as a Science Data Network with 20 gbps on its northern route and 10 gbps on its southern route.	+1,600
Total Funding Change, High Performance Computing and Network Facilities and Testbeds	**+8,096**
SBIR/STTR	
Increase in SBIR/STTR due to increase in operating expenses.	+660
Total Funding Change, Mathematical, Information, and Computational Sciences	**+21,544**

Capital Operating Expenses and Construction Summary

Capital Operating Expenses

	(dollars in thousands)		
	FY 2006	FY 2007	FY 2008
Capital Equipment	5,771	15,000	13,000