Advanced Scientific Computing Research

Funding Profile by Subprogram

(dollars in thousands)

	FY 2005 Current Appropriation	FY 2006 Original Appropriation	FY 2006 Adjustments	FY 2006 Current Appropriation	FY 2007 Request
Advanced Scientific Computing Research					
Mathematical, Information, and Computational Sciences	226,180[a]	237,055	-2,371[b]	234,684	318,654

Public Law Authorizations:
Public Law 95-91, "Department of Energy Organization Act"
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, leadership in scientific computation has become a cornerstone of the Department's 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 understand and 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 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. Computational science is increasingly central to progress at the frontiers of almost every scientific discipline and to our most challenging feats of engineering.

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[a] Total is reduced by $1,872,000 for a rescission in accordance with P.L. 108-447, the Consolidated Appropriations Act, 2005; $5,614,000, which was transferred to the SBIR program; and $674,000, which was transferred to the STTR program.
[b] Reflects a rescission in accordance with P.L. 109-148, The Emergency Supplemental Appropriations Act to Address Hurricanes in the Gulf of Mexico and Pandemic Influenza, 2006.

Strategic and Program Goals

The Department's Strategic Plan identifies four strategic goals (one each for defense, energy, science, and environmental aspects of the mission) plus seven general goals that tie to the strategic goals. The ASCR program supports the following goal:

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

The ASCR program has one program goal which contributes to General Goal 5 in the "goal cascade":

Program Goal 05.23.00.00: 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 Program Goal 05.23.00.00 (Deliver forefront computational and networking capabilities)

The ASCR program contributes to Program Goal 05.23.00.00 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 to deliver extraordinary science. Applied Mathematics enables scientists to build models of physical and natural systems with extraordinary fidelity, 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 critical to advance the frontiers of simulation. Shrinking the distance between scientists and the resources they need is also critical to 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 General Goal 5 by enabling research programs across SC, as well as other elements of the Department, to succeed. The following indicators establish specific long term (10 years) goals in Scientific Advancement that the ASCR program is committed to, and progress can be measured against:

- Develop multiscale mathematics, numerical algorithms, and software that enable 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 General and Program Goal

	(dollars in thousands)		
	FY 2005	FY 2006	FY 2007
General Goal 5, World-Class Scientific Research Capacity			
Program Goal 05.23.00.00, Deliver forefront computational and networking capabilities (Advanced Scientific Computing Research)..............	226,180	234,684	318,654

Annual Performance Results and Targets

FY 2002 Results	FY 2003 Results	FY 2004 Results	FY 2005 Results	FY 2006 Targets	FY 2007 Targets
Program Goal 05.23.00.00 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]	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]	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]	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 2006— >50%	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— >50%
	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]	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 2006— 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 2007— 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 leadership of the 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 Administration [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 Computing Information and Communications Research and Development (R&D) subcommittee of the National Science and Technology Council (NSTC), under the auspices of SC and Technology Policy. This coordination is periodically reviewed by the President's Information Technology Advisory Committee (PITAC). 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 Science 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)

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 FY 2005 PART review, OMB gave the ASCR program an overall rating of "Moderately Effective." 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 is 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 2007. 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. The Annual Performance Targets are tracked through the Department's Joule system and reported in the Department's Annual Performance Report. In response to PART findings, ASCR established a Committees of Visitors (COV) to provide outside expert validation of the program's merit-based review processes for impact on quality, relevance, and performance. ASCR has received the reports from the first COV, which focused on the research programs, and the second COV, which met April 5-6, 2005, to review the facilities and network research efforts, and is working on an action plan to respond to the recommendations. In order to address specific concerns ASCR has made plans in FY 2006 and future fiscal years to: engage advisory panel and other outside groups in regular, thorough scientific assessments of the quality, relevence, and performance of its research portfolio and computing/network facilities; engage 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; and to implement action plans to improve program management in response to past expert reviews.

For the FY 2007 Budget, OMB has developed PARTWeb – a new interface for PART that facilitates collaboration between agencies and OMB. PARTWeb will link to the website http://ExpectMore.gov and will improve public access to PART assessments and follow up actions. For 2006 there are three 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, ASCR will charge the Advanced Scientific Computing Research Advisory Committee to review progress toward the long term goals of the program before the end of FY 2006 and will continue to host Committees of Visitors (CoV) and other panels to review the quality, relevance, and performance of the program. ASCR will continue to publish responses to the COV's findings and will track improvements at http://www.sc.doe.gov/measures/FY06.html.

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.

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. As stated in the "Analytical Perspectives" of the FY 2004 Budget:

> Due to its impact on a wide range of federal agency missions ranging from national security and defense to basic science, high-end computing—or supercomputing—capability is becoming increasingly critical. Through the course of 2003, agencies involved in developing or using high-end computing will be engaged in planning activities to guide future investments in this area, coordinated through the National Science and Technology Council (NSTC). The activities will include the development of interagency R&D roadmaps for high-end computing core technologies, a federal high-end computing capacity and accessibility improvement plan, and a discussion of issues (along with recommendations where applicable) relating to federal procurement of high-end computing systems. The knowledge gained from this process will be used to guide future investments in this area. Research and software to support high-end computing will provide a foundation for future federal R&D by improving the effectiveness of core technologies on which next generation high-end computing systems will rely.

To address these issues the President's Science Advisor chartered the High End Computing Revitalization Task Force (HECRTF), which developed a plan for a Federal research program to address these issues. This task force was co-chaired by SC and the Department of Defense (DOD). ASCR's efforts in computer science, research and evaluation prototypes, high performance production computing (NERSC), and the Leadership Computing Facilities (LCFs) are important components of the interagency implementation of this plan.

How We Work

The ASCR program uses a variety of mechanisms for conducting, coordinating, and funding research in applied mathematics, network and computer sciences, and in advanced computing software tools. 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)—though inactive in 2005—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 Interagency Principals Group, chaired by the President's Science Advisor, and the Information Technology Working Group (ITWG). 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 the President's Science Advisor.

In addition, ASCR, both through ASCAC and independently, supported a number of workshops to support its planning. These include:

- Blueprint for Future Science Middleware and Grid Research and Infrastructure, August 2002;
- DOE Science Network Meeting, June 2003 (http://gate.hep.anl.gov/may/ScienceNetworkingWorkshop/);

- DOE Science Computing Conference, June 2003 (http://www.doe-sci-comp.info);
- Science Case for Large Scale Simulation, June 2003;
- Workshop on the Road Map for the Revitalization of High End Computing (http://www.cra.org/Activities/workshops/nitrd/);
- Cyber Infrastructure Report (http://www.nsf.gov/publications/pub_summ.jsp?ods_key=cise051203);
- "Federal Plan for High-End Computing, report of the High End-Computing Revitalization Task Force (HECRTF)" (http://www.itrd.gov/pubs/2004_hecrtf/20040702_hecrtf.pdf); and
- The Office of Science Data-Management Challenge, Report from the DOE Office of Science Data-Management Workshops (http://www.sc.doe.gov/ascr/Final-report-v26.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 2,000 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. Allocations of computer time and archival storage at NERSC are awarded to research groups based on a review of submitted proposals. As proposals are submitted, they 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, 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. A pioneer in providing DOE mission-oriented high-bandwidth, reliable connections, 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. The ESnet Steering Committee (ESSC) was established in 1985 to ensure that ESnet meets the needs of SC programs. All program offices in SC appoint a representative to serve on the ESSC. The ESSC is responsible for reviewing and prioritizing network requirements, for establishing performance objectives, and for proposing innovative techniques for enhancing ESnet capabilities. In addition to the ongoing oversight from the ESSC, ASCR conducts regular external peer reviews of ESnet performance. The last such review was chaired by a member of ASCAC and took place in September 2001. The next review is scheduled in 2006.

In FY 2002, ASCAC conducted a review of ASCR's high performance computing facilities. The charge to ASCAC, posed the following questions:

- What is the overall quality of these activities relative to the best-in-class in the U.S. and internationally?
- How do these activities relate and contribute to Departmental mission needs?
- How might the roles of these activities evolve to serve the missions of the SC over the next three to five years?

The essential finding of the Subcommittee was that these facilities are among the best worldwide. It was the opinion of the Subcommittee that these ASCR activities and the related spin-off research efforts contribute significantly to the mission needs of DOE, and profoundly and positively impact high performance computing activities worldwide. The complete report is available on the web. (http://www.science.doe.gov/ascr/ASCAC-sub.doc).

In FY 2004, ASCR conducted a peer review of the CCS evaluation of the Cray X1 computer. The results from this review validated the exceptionally 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 Leadership Computing Facility (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, the SC Project Assessment group conducted a formal Baseline validation review of the ORNL LCF.

Program Reviews

The ASCR program conducts frequent and comprehensive evaluations of every component of the program. Results of these evaluations are used to modify program management as appropriate.

In FY 2003, ASCR conducted a peer review of the Numerical Linear Algebra, Optimization, and Predictability Analysis areas within the Applied Mathematics activity. These areas represent 33% of this activity. In FY 2004, ASCR conducted a peer review of the Differential Equations and Advanced Numerical Methods for High Performance Computing areas within the Applied Mathematics activity, representing an additional 33% of this activity. In FY 2005, ASCR conducted a peer review of the remaining 34% of the Applied Mathematics activity, which consisted of Computational Fluid Dynamics and Meshing Techniques. Also, in FY 2003 ASCR completed reviews of all of the SciDAC Integrated Software Infrastructure Centers (ISICs). There are a total of seven such centers (three with a mathematics focus and four with a computer science focus), and this represents over 50% of the ASCR SciDAC budget.

In FY 2003, ASCR also conducted peer reviews of all the SciDAC Collaboratory Pilot and Middleware Projects. These reviews focused on accessing progress and the possible need for mid-course corrections.

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:

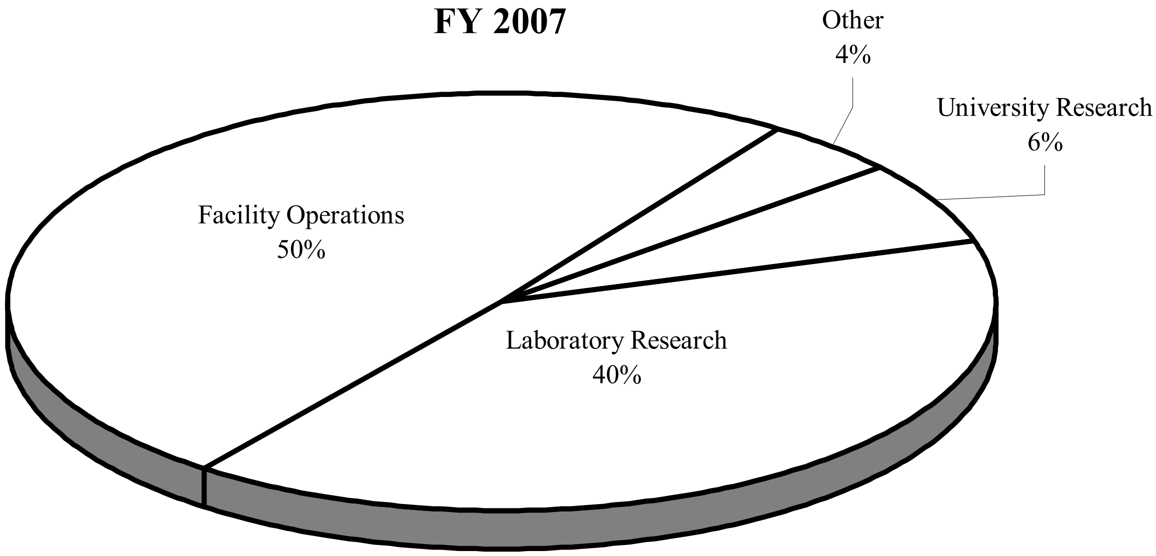
- The Department and SC Strategic Plan, as updated through program collaborations and joint advisory committee meetings (http://www.sc.doe.gov/Sub/Mission/mission_strategic.htm);
- SciDAC plan delivered to Congress in March 2000 (http://www.science.doe.gov/scidac/);
- ASCAC report on the Japanese Earth Simulator (http://www.sc.doe.gov/ascr/ascac_reports.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 2007 budget request continues the core and SciDAC research efforts and strengthens the research partnerships with other SC offices. Network operations expenditures account for 22% of the national laboratory research. The LTR subprogram was brought to a successful completion in FY 2004.

Advanced Scientific Computing Research Budget Allocation
FY 2007



Research

46 percent of the ASCR program's FY 2007 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. The division of support between national laboratories and universities is adjusted to maximize scientific productivity.

- ***University Research***: University researchers play a critical role in the nation's research effort and in the training of graduate students. During FY 2005, the ASCR program supported over 150 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 2005, CSGF activity selected 15 new graduate students representing 12 universities and 8 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 12 awards to early career principal investigators in FY 2005.

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. ASCR funds the best among the ideas submitted in response to grant solicitation notices (http://www.sc.doe.gov/grants/grants.html). 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 and novel applications of high performance computing 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 advances mathematics and computer science, and develops the specialized algorithms, the scientific software tools, and the software libraries needed by DOE researchers to effectively use high-performance computing and networking hardware for scientific discovery. The ASCR program has been a leader in the computational sciences for several decades and has been acknowledged for pioneering accomplishments. The FY 2007 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 are being recompeted in FY 2006, with attention paid to support for the long term maintenance and support 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. In addition, in FY 2006 ASCR is changing the way in which it manages its Genomics: GTL partnership with BER. The management of these efforts will be integrated into the portfolio of successful SciDAC partnerships. Finally, in FY 2007 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.

For the past two decades SC, and the worldwide scientific community, have been harvesting their success in building and developing the Internet. This has enabled roughly a doubling in bandwidth every two years with no increase in cost. However, the demands of today's facilities, which generate millions of gigabytes per year of data, now outstrip the capabilities of the Internet design. 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 possibility of exploiting these technologies to provide scientific data where it is needed at speeds commensurate with the new data volumes. However, to take advantage of this opportunity significant research is needed to integrate these capabilities, make them available to scientists, and build the infrastructure which can provide cybersecurity in this environment.

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 the NSTC and OSTP. This area has been identified as a priority within the overall Networking and Information Technology Research and Development (NITR&D) priorities of the Administration. In prior budgets some, but not all, of the activities related to the HECRTF plan were described as components of the Next Generation Architecture (NGA) effort. We have eliminated discussion of the NGA to enable a clearer description of how ASCR research and facilities contribute to the HECRTF plan.

In FY 2007, further diversity with the LCF resources will be 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. This capability will accelerate scientific understanding in areas that include materials science, biology, and advanced designs of nuclear reactors.

These changes were made to guarantee 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 NITR&D subcommittee of the National Science and Technology Council and its Technology Committee. The NITR&D subcommittee evolved through an interagency coordination process that began under the 1991 High Performance Computing Act as the High Performance Computing, Communications, and Information Technology (HPCCIT) Committee. The NITR&D Subcommittee provides hands-on coordination for the multiagency NITR&D Program. The Subcommittee is made up of representatives from each of the participating NITR&D agencies and from the Office of Management and Budget (OMB), the NSTC, and the National Coordination Office for IT R&D (NCO/IT R&D). The Subcommittee coordinates planning, budgeting, and assessment activities of the multiagency NITR&D 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. The DOE program solves mission critical problems in scientific computing. In addition, 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 and computation, ASCR has extensive partnerships with other Federal agencies and the NNSA. Examples include: participating in the program review team for the DARPA High Productivity Computing Systems program; serving on the planning group for the Congressionally mandated DOD plan for high performance computing to serve the national security mission; serving on the OSTP High End Computing Revitalization Task Force; and extensive collaboration with NNSA-Advanced Simulation 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.

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. The power of computers and networks is increasing exponentially. Advances in high-end computing technology, together with innovative algorithms and software, are being exploited as intrinsic tools for scientific discovery. SciDAC has also 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 terascale computing and networking resources. The program is bringing computation and simulation to parity with experiment and theory in the scientific research enterprise as demonstrated by major advances in climate modeling and prediction, plasma physics, particle physics, accelerator design, astrophysics, chemically reacting flows, and computational nanoscience.

The research focus of ASCR SciDAC activities includes Integrated Software Infrastructure Centers (ISICs). ISICs are partnerships between DOE national laboratories and universities focused on research, development, and deployment of software to accelerate the development of SciDAC application codes. Progress to date includes significant improvements in performance modeling and analysis capabilities that have led to doubling the performance on 64 processors of the Community Atmosphere Model component of the SciDAC climate modeling activity. The three Mathematics ISICs were begun in 2001 to bring a new level of mathematical sophistication to computational problems throughout SC. One of these, the Terascale Optimal Partial Differential Equations (PDE) Simulations (TOPS) Center, is combining the Hyper and Portable Extensible Toolkit for Scientific Computation (PETSC) libraries, together with newly developed algebraic multigrid solvers, to create fast algorithms for a variety of tough and important problems, including biochemical reaction diffusion equations and advection equations for combustion simulation. The Terascale Simulation Tools and Technologies Center is working to develop a framework for coupling different types of grids together in a single application. For example, in a simulation of engine combustion, one might want an unstructured grid for the complex geometry around the valves, but a regular grid in the rest of the cylinder. Finally, the Applied Partial Differential Equations Center is focused on using structured adaptive grids for simulation in a variety of application domains, including ground water flow, combustion chemistry, and magneto-hydrodynamics. Given the difficulty of magneto-hydrodynamic simulation, this center is having a strong impact on the design of new particle accelerators.

In FY 2006, ASCR is recompeting 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.

Scientific Facilities Utilization

The ASCR program's FY 2007 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 2,000 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 as described in the HECRTF report. The proposed funding will allow the high performance resources at the LCFs to be upgraded to a peak capability of 150 Teraflops in FY 2007.

	FY 2005	FY 2006 Estimate	FY 2007 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%

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 2007, this program will support approximately 800 graduate students and post doctoral investigators, of which 500 will be supported at SC user facilities.

ASCR will continue the Computational Science Graduate Fellowship Program with the successful appointment of 15 new students to support the next generation of leaders in computational science.

	FY 2005	FY 2006 Estimate	FY 2007 Estimate
# University Grants	140	135	150
Average Size	$197,000	$197,000	$197,000
# Laboratory Groups	165	155	165
# Graduate Students (FTEs)	354	350	375
# Permanent Ph.D.s (FTEs)	675	625	670

Mathematical, Information, and Computational Sciences

Funding Schedule by Activity

	(dollars in thousands)		
	FY 2005	FY 2006	FY 2007
Mathematical, Information, and Computational Sciences			
Mathematical, Computational, and Computer Sciences and Distributed Network Environment Research	108,105	105,275	117,122
High Performance Computing and Network Facilities and Testbeds	118,075	123,116	193,030
SBIR/STTR	—	6,293	8,502
Total, Mathematical, Information, and Computational Sciences	226,180	234,684	318,654

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, answering critical questions that range from the function of living cells to the power of fusion energy.

Benefits

MICS supports ASCR's contribution to DOE's mission to provide world-class scientific research capacity 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. The science of the future demands that we advance beyond our current computational abilities. Accordingly, we must address the following questions:

- What new mathematics are required to 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 for SC?
- What operating systems, data management, analysis, model development, and other tools are required to make effective use of future-generation supercomputers?

- Is it possible to overcome the geographical distances that often hinder science by making 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 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

Discussions of the extent to which the requirements of the Office of Science exceed current capabilities and capacity can be found in a number of reports including: “Federal Plan for High-End Computing, Report of the High-End Computing Revitalization Task Force (HECRTF)” May 10, 2004, Appendices A-1, A-2, and A-3, (http://www.sc.doe.gov/ascr/hecrtfrpt.pdf); “A Science-Based Case for Large-Scale Simulation,” Volume 1, July 30, 2003, (http://www.sc.doe.gov/ascr/Scalesreptvol1.pdf); “Theory and Modeling in Nanoscience, Report of the May 10-11, 2002 Workshop conducted by the Basic Energy Sciences and Advanced Scientific Computing Advisory Committees to SC, Dept. of Energy,” (http://www.sc.doe.gov/ascr/TMN_rpt.pdf); “Integrated Simulation and Optimization of Magnetic Fusion Systems, Report of the FESAC Panel,” November 2, 2002, (http://www.ofes.fusion.doe.gov/News/FSP_report_Dec9.pdf); and “High-Performance Networks for High-Impact Science, Report of the High-Performance Network Planning Workshop conducted August 13-15, 2002,” (http://www.sc.doe.gov/ascr/high-performance_networks.pdf). Furthermore, the algorithms and software tools, libraries, and environments needed to accelerate scientific discovery through modeling and simulation are beyond the realm of commercial interest. 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. Seventeen awards were made in FY 2002, twelve awards in FY 2003, sixteen in FY 2004, and twelve in FY 2005. Additional awards will be made in FY 2006 for this activity, pending the outcome of review of applications. 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 2005 Accomplishments

- Middleware collaboratory projects such as the Storage Resource Management project are providing the technology needed to manage the rapidly growing distributed data volumes produced as a result of faster and larger computational facilities. Over the past year, Storage Resource Manager software (SRMs) has been deployed in multiple High Energy Physics experiments as part of the Particle Physics Data Grid (PPDG) project, the Earth Science Grid (ESG), and the SciDAC Scientific Data Management Integrated Software Infrastructure Center (ISIC). SRMs are used by facilities such as BNL, NERSC, Fermilab, National Center for Atmospheric Research (NCAR) and ORNL for remote file access and intensive data movement between storage systems at different facilities. For example, SRMs have been setup to automate the movement of approximately 10,000 files per month (1 gigabyte each) between BNL and NERSC. Additionally sustained transfer rates between 40 and 60 megabytes per second have been achieved using SRM-to-SRM managed transfers from Castor at CERN to Fermilab's tape system. The benefit of using an SRM for these tasks is that error rates are reduced and human intervention is essentially eliminated.
- Energy Sciences Network (ESnet) is implementing a new architecture that is a core ring with interconnected metropolitan area networks (MANs). ESnet's current architecture consists of a national core network connecting six hubs with individual sites connected to the hubs in a single circuit, in spoke-like fashion. For reasons of both reliability and bandwidth, this architecture is insufficient to meet future demands. The new architecture is designed to meet the increasing demand for network bandwidth and advanced network services as next-generation scientific instruments and supercomputers come on line. The first MAN has been completed in the San Francisco Bay Area. It provides dual connectivity at 20 gigabits per second—which is from 10 to 50 times the previous site bandwidths, depending on the site using the ring—while reducing the overall cost. It connects six DOE sites—Stanford Linear Accelerator (SLAC), Lawrence Berkeley National Laboratory (LBNL), the Joint Genome Institute (JGI), the National Energy Research Scientific Computing Center (NERSC), Lawrence Livermore National Laboratory (LLNL) and Sandia National Laboratory (SNL) at Livermore. 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.
- UltraScienceNet Network (USNET) Testbed is a 20 gigabit per second highly reconfigurable optical network testbed developed to design and test advanced optical network technologies such as petabyte-scale data transfers, remote computational steering, collaborative high-end visualizations, and tele-instrumentation. A full deployment of USNET backbone was completed in August 2005. In the current configuration, it provides on-demand end-to-end guaranteed circuits with capacities ranging from 50 megabits per second to 20 gigabits per second within minutes of setup. Such

capability is in stark contrast with the Internet where the shared connections are statically provisioned and, as a result, the bandwidth is neither guaranteed nor stable. During the past year, USNET has enabled researchers at FNAL to develop and test advanced data transfer networking technologies capable of achieving data rates 15 times faster than with production ESnet networks and thousands of times faster than with traditional Internet connections. This achievement is very significant because it facilitates the efficient distribution of the high energy LHC data distribution between tier-1 and tier-2 centers. Upon maturation, the advanced networking technologies developed in USNET will be put into production in ESnet.

- Secure Group Collaborations – The SciDAC project "Security and Policy for Group Collaboration" has produced authentication and authorization algorithms and software that have been adopted by major distributed science projects. These projects have in turn profited from the availability of high-quality secure authentication and authorization mechanisms to achieve significant advances in distributed science. For example, the DOE Earth System Grid data portal has used Grid Security Infrastructure (GSI) mechanisms to register over one thousand climate researchers as users during the past year. These users have downloaded tens of terabytes of data from ESG sites and produced 250 publications from International Panel on Climate Change (IPCC) data alone. Thousands of scientists now access remote data and computational services on grid infrastructure securely thanks to Grid Security Infrastructure
- Performance Tools, Modeling and Optimization: Computer science researchers significantly enhanced the performance of several SciDAC applications, including,
  - a three-fold improvement of the fusion Gyrolcinetic Simulation model (GS2) on the IBM SP,
  - a two-fold improvement in the Community Atmospheric Model (CAM) on the Cray X1,
  - a 50% improvement in the Omega3P accelerator design code on an Opteron cluster.
- Using software components from NWChem, MPCQ, Tao Solver, Global Arrays, and PETSc, computer scientists and chemists have successfully performed quantum chemistry simulations obtaining a reduction in times up to 43% compared to the standalone chemistry packages.
- A novel, adaptive infrastructure for low-overhead monitoring for parallel applications on large-scale systems greatly reduces the volume of tracing data produced, and allows the user to specify constraints on the confidence and accuracy of monitoring. The Tuning and Analysis Utilities (TAU) parallel performance system is delivering state-of-the-art technology for performance instrumentation, measurement, and analysis of large-scale parallel computers to help application developers be more productive in achieving their optimization goals. The project is making important advances in application-specific performance evaluation, scalable performance tools, multi-experiment performance data management, and performance data mining. TAU has been ported to the IBM BG/L, Cray RedStorm, Cray XT3, and SGI Columbia systems, and TAU is used for performance analysis of important DOE production and research codes, including Flash, ESMF, KULL, VTF, Uintah, and S3D.
- Using lightweight one-sided communication in the Unified Parallel C (UPC) language, researchers demonstrated performance that was nearly double that of the standard NAS benchmark implementation in Fortran and MPI on an Itanium/Quadrics cluster and an Opteron/Infiniband cluster. These results were obtained using the Berkeley Open Source UPC compiler, and the UPC

code outperformed the MPI code on every platform and problem size tested. One of the evaluated benchmarks where performance doubled was a Fast Fourier Transform in 3D, a computation that is critical in climate modeling, fusion modeling, and many other SC applications.

- Researchers have developed an open-source compiler for Co-array Fortran (CAF), a model for parallel programming that consists of a small set of extensions to the Fortran 90 programming language. The prototype, multi-platform compiler was used in FY 2004 to develop efficient programs for a wide range of parallel architectures. Based on this work, in FY 2005 Co-arrays were officially adopted as part of the Fortran 2008 language standard. This is the first time the International Fortran Standards Committee has approved a parallel extension to the Fortran language.
- The Multi-Component-Multi-Data (MCMD) programming model was shown to be effective for improving scalability of real scientific applications on large processor counts. When combined with Global Arrays (GA), a computational scheme that supports three different levels of parallelism was implemented in the context of NWChem computational chemistry package. In particular, a factor of 10 reduction in the time needed to complete the numerical Hessian calculation was observed. This approach, is expected to be critical for running complex scientific applications on future massively parallel systems.
- The Scalable Linear Solvers project at LLNL has applied its Adaptive Smoothed Aggregation (αSA) method to Quantum Chromodynamics (QCD, currently funded under SciDAC). The αSA method is the only method ever to exhibit scalable convergence behavior on a QCD application independent of physics and discretization parameters, and αSA was shown to be faster than existing methods even on today's relatively small simulations. There were several new solver developments this past year that could have a similar impact on DOE applications in the future. A new variant of the adaptive multigrid idea has been developed and shown to be robust for difficult PDEs with large near null-spaces such as Maxwell's Equations on unstructured grids. Also, based on the new sharp convergence theory, a more predictive form of compatible relaxation has been developed that is aimed at further improving the robustness of algebraic multigrid (AMG). The co-principal investigators were invited to give eight talks at prestigious conferences such as the European Multigrid Conference, and included a Topical Lecture on AMG at this year's Society for Industrial and Applied Mathematics (SIAM) Annual Meeting. Their paper on αSA was selected by the editors of SIAM Journal on Scientific Computing (SISC) to appear as a SIGEST article in SIAM Review. The SIGEST section of the *SIAM Review* highlights excellent papers of broad interest from SIAM's specialized journals, making SIAM readers aware of outstanding work whose content and roots span multiple areas.
- As part of the Terascale Simulation Tools and Technologies (TSTT) applied mathematics Integrated Software Infrastructure Center (ISIC), researchers have developed and deployed advanced meshing and discretization technology to SciDAC application researchers in a diverse array of application areas. For example, PNNL scientists are applying TSTT tools to DOE bioremediation problems using the Virtual Microbial Cell Simulator (VMCS). The VMCS is one example where TSTT meshing and discretization technologies are being used successfully to construct a computational biology application. The main concept is to leverage this technology to provide a general biological application tool by providing common interfaces and interoperability among a set of computational biology tools.

- Argonne researchers have developed the Library for Automated Deduction Research (LADR), an evolving set of tools for constructing software for various automated deduction tasks. LADR greatly simplifies the task of building special-purpose systems for testing new theories and ideas in automated deduction—for example, programs that combine proof search with counterexample search and programs that automate the human-computer iterative processes typically used for difficult conjectures. Two production-quality programs have already been built with LADR. Prover9 searches for proofs of statements in first-order logic, and Mace4 searches for counter examples.
- Researchers at Argonne National Laboratory are providing a new modeling and solution paradigm for the design of efficient electricity markets. In a pilot project, they have used Stackelberg games to model the interactions between the producers and consumers in the Pennsylvania-New Jersey-Maryland electricity market and to investigate the implications of various delivery scenarios. The computational experience obtained with Argonne's large scale nonlinear optimization solvers will be useful to policy makers interested in simulating the complicated interactions among producers in imperfectly competitive markets. Future research will extend this modeling paradigm to games with more complex structure that will allow competition between two or more dominant producers in deregulated electricity markets.
- Argonne’s Portable, Extensible Toolkit for Scientific Computing (PETSc) project develops scalable numerical solvers and software that support high-performance simulations based on partial differential equations (PDE). The parallel computing infrastructure and scalable numerical solvers in PETSc enable scientists and engineers to focus on the science, thus, reducing implementation costs. For example, DOE applications from Fusion Energy to Geosciences have taken advantage of PETSc's unique structure. In particular, researchers in computational fusion have employed PETSc both in gyrokinetic simulations and in two plasma simulation codes—one using spectral methods, the other finite element methods. Fusion is a major potential major alternative energy source, and the plasma production efforts of the International Thermonuclear Experimental Reactor (ITER), planned around the year 2014, will require extremely accurate simulation.
- Sandia researchers have developed two new linear solver algorithms, S-LSC and NSA, which will improve the performance of many fluid flow simulations central to the advanced modeling performed at the national laboratories. Among the applications that currently use these solvers are chemical vapor deposition computations for semiconductor and Microelectromechanical Machines (MEMS) processing, aerodynamics calculations to determining flight characteristics, and combustion simulations to understand pool fires and validate weapon systems. Some of these simulations have been performed on equation sets with over 100 million unknowns on thousands of processors. These increased capabilities lead to more detailed and physically realistic studies over larger ranges of physical and temporal scales.

FY 2005 Awards

- R&D 100 Award to Argonne National Laboratory (ANL) Team—Every year, R&D Magazine recognizes the world’s top 100 scientific and technological advances with awards for innovations showing the most significant commercial potential. The Computer Science project “MPICH2” received an R&D 100 award for the year 2005. MPICH2 is a high-performance, portable implementation of community standards for the message-passing model of parallel computation. It enables scientists to write parallel programs that run efficiently on all major computers systems.

Companies such as Pratt and Whitney are using MPICH2 to design aircraft engines and the software is widely used in scientific applications.

- Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Program—Some of the most significant work done at NERSC in 2005 was made possible by the INCITE Program, which supports a small number of computationally intensive large-scale research projects that are expected to make high-impact scientific advances through the use of a substantial allocation of computer time and data storage at the NERSC Center. In December 2004, SC selected three computational science projects to receive a total of 6.5 million hours of supercomputing time at the NERSC Center—10% of the total computing time available in FY 2005 on NERSC's Seaborg system. One of the INCITE projects, "Direct Numerical Simulation of Turbulent Nonpremixed Combustion," performed detailed three-dimensional combustion simulations of flames in which fuel and oxygen are not premixed. The results of their simulations will provide insight into reducing pollutants and increasing efficiency in combustion devices.

Detailed Justification

	(dollars in thousands)		
	FY 2005	FY 2006	FY 2007
Mathematical, Computational, and Computer Sciences and Distributed Network Environment Research	**108,105**	**105,275**	**117,122**
▪ **Applied Mathematics**..	**29,577**	**29,354**	**29,495**

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. This final area represents our most recent effort at focusing on those mission-related applications which span wide ranges of interacting length- and time-scales.

	(dollars in thousands)	
FY 2005	FY 2006	FY 2007

The FY 2007 budget increases the Computational Sciences Graduate Fellowship activity by $500,000 to $4,000,000. The FY 2007 budget also includes $8,500,000 for the Atomic to Macroscopic Mathematics effort, the same as in FY 2006.

	FY 2005	FY 2006	FY 2007
▪ **Computer Science**	**21,590**	**24,271**	**23,863**

This activity supports research in computer science to enable computational scientists to effectively utilize high-performance 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 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 data analysis and for circumstances where key resources and users are geographically distributed. Research areas include: tools to monitor the performance of scientific applications and enable users to improve performance and get scientific results faster; new programming models to simplify application code development; advanced techniques for visualizing very large-scale scientific data; and efforts to improve 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 NITR&D 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 (HEC URA), an outgrowth of the HECRTF. These activities will be modestly increased 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.

	FY 2005	FY 2006	FY 2007
▪ **Computational Partnerships**	**35,769**	**38,052**	**50,000**

This activity supports the amalgam of those activities previously titled “Advanced Computing Software Tools” and “Scientific Applications Partnerships.” 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 2007, this activity will support the Integrated Software Infrastructure Centers (ISICs) SciDAC activities, that were competitively selected in FY 2006. The ISICs funded under this activity will focus on important computational infrastructure problems such as: structured and unstructured mesh generation for large simulations and high performance tools for solving partial differential equations on parallel computers; tools for analyzing the performance of scientific simulation software that uses thousands of processors; the development of data management and visualization software capable of handling terabyte scale data sets extracted from petabyte scale data archives; software for managing computers with thousands of processors; and software component technology to enable rapid development of efficient, portable, high performance parallel simulation software.

The ISICs are a fundamental component in DOE's SciDAC strategy. The ISICs are responsible for the entire lifecycle of the software that they develop. These software tools must be reliable, understandable, and well documented. Also, the scientific user community needs these tools to be maintained, bug-free, and upgraded as necessary. Since software tools for high performance scientific simulations have no commercial market, the ISICs provide the only means for developing and deploying these tools to the scientific community.

The scientific applications partnerships part of this activity, formerly titled Scientific Application Pilot Projects, supports collaborative research with computational scientists in other disciplines to apply the computational techniques and tools developed by other MICS activities 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. The FY 2007 funding for this activity will allow the continuation of the multidisciplinary partnerships that were competitively selected in FY 2006. These projects are part of the SciDAC activity and are coupled to the ISICs. Areas under investigation include design of particle accelerators with the High Energy Physics (HEP) and Nuclear Physics (NP) programs, plasma turbulence in tokamaks with the Fusion Energy Sciences (FES) program, global climate change with the Biological and Environmental Research (BER) program, and combustion chemistry with the Basic Energy Sciences (BES) program. This activity directly supports SC Strategic Plan strategy 6.2.

The FY 2007 request includes funds to continue the partnerships with the BER Genomics: GTL program, the BES program in nanoscale science, and the FES program for the Fusion Simulation Project (FSP).

The FY 2007 request also includes $7,000,000 to continue the competitively selected SciDAC institutes at universities which can become centers of excellence in high end computational science in areas that are critical to DOE missions.

(dollars in thousands)		
FY 2005	FY 2006	FY 2007

Finally, in FY 2007, this activity, as a part of the enhanced SciDAC effort, will begin a new investment in applied math and computer science to develop leadership class computing simulations for petascale computers in areas such as core collapse supernovae, molecular imaging of catalysis, combustion, tokamak experiments and the associated plasma physics, and expanding applied math and computer science in support of ultrafast science, lattice QCD, and simulation of nuclear reactions in collaboration with NNSA. This increment in SciDAC will enable the development of a suite of scientific software and science applications that can fully take advantage of petascale computers and build on SciDAC's initial success in enabling scientists to use those computers as tools for scientific discovery. This increment will enable SciDAC teams to prepare for 250 teraflop class computers in collaboration with applied mathematicians and computer scientists including focused efforts to transition early results from the basic research effort in Atomic to Macroscopic mathematics into multiscale algorithms in petascale scientific computing applications. This strategy for development of petascale applications to use petascale computers is critical for making further contributions to DOE science areas through modeling and simulation success.

- **Distributed Network Environment Research**.......................... **21,169** **13,598** **13,764**

This activity supported the integration of activities previously described under the titles: "Network Research," "Collaboratory Tools," and "Collaboratory Pilots." This integrated activity builds on results of fundamental research in computer science and networking to develop an integrated set of software tools and services to support distributed scientific collaborations and provide end-to-end network performance well beyond the levels that can be achieved today. For the past two decades the Office of Science (SC), and the worldwide scientific community, have benefited substantially from advances associated with the development and the building of the Internet. This has enabled roughly a doubling in bandwidth every two years with no increase in cost. However, the demands of today's facilities, which generate millions of gigabytes per year of data, now outstrip the capabilities of the Internet design. 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 an opportunity to exploit these technologies to provide scientific data where it is needed at speeds commensurate with the new data volumes.

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

	(dollars in thousands)		
	FY 2005	FY 2006	FY 2007

provide for efficient, high-performance, reliable, secure, and policy-aware management of large-scale data movement across the research enterprise.

High Performance Computing and Network Facilities and Testbeds	**118,075**	**123,116**	**193,030**
▪ **High Performance Computing Facilities and Testbeds**	**99,496**	**104,150**	**170,294**

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 Class Computers (LCCs) 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 Center for Computational Sciences (CCS). Related requirements for capital equipment, such as high-speed disk storage systems, archival data storage systems, and high performance visualization hardware are also supported. FY 2007 capital equipment requirements for these types of capital equipment are increased from FY 2006.

• **High Performance Production Computing**	**37,868**	**37,489**	**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 2,000 users working on about 700 projects. 35% of users are university based, 61% are in National Laboratories, 3% are in industry, and 1% are in other government laboratories. FY 2007 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. 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, in FY 2006, a procurement is planned for the next generation of high performance resources at NERSC to be delivered in early FY 2007. The resultant NERSC-5 peak capacity is expected to be 100–150 teraflops by the end of FY 2007. These computational resources are integrated by a common high performance file storage system that enables users to easily use all the resources. The FY 2006 oversubscription at NERSC is about a factor of 6-8. In FY 2007, we will increase the capacity by about a factor of 6.

NERSC plays 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.

• **Leadership Computing Facilities (LCF)**	**48,600**	**53,702**	**102,504**

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. The success of this effort is built on

	(dollars in thousands)		
	FY 2005	FY 2006	FY 2007

the enhancements to the research and evaluation prototype and computer science research activities described elsewhere.

▸ **Leadership Computing Facility at ORNL**	**48,600**	**53,702**	**80,000**

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 provide world leading high performance sustained capability to researchers on a peer-reviewed basis. The LCF will upgrade computers acquired in FY 2004 and FY 2005 to provide more than 250 teraflops peak capability by the end of FY 2007. These advancements will enable scientific advancements such as simulations of diesel combustion including realistic diesel fuel chemistry to minimize the processes that generate NO_x and soot, 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.

▸ **Leadership Computing Facility at ANL**	**—**	**—**	**22,504**

In FY 2007, further diversity with the LCF resources will be 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. This capability will accelerate scientific understanding in areas that include materials science, catalysis, protein/DNA complexes, and advanced designs of nuclear reactors. The IBM Blue Gene architecture is expected to deliver significantly greater performance per dollar for this class of applications than the computing at ORNL.

• **Research and Evaluation Prototypes**	**13,028**	**12,959**	**13,000**

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.

▪ **High Performance Network Facilities and Testbeds**..............	**18,579**	**18,966**	**22,736**

This activity supports SC strategy 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) that provide high bandwidth access to the ESnet backbone. The ESnet

(dollars in thousands)		
FY 2005	FY 2006	FY 2007

project/investment supports the agency's mission and strategic goals and objectives by providing DOE with interoperable, effective, and reliable communications infrastructure and leading-edge network services. ESnet supplies the DOE science community with capabilities not available through commercial networks or commercial Internet Service Providers. 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. ESnet provides the communications fabric that interconnects geographically distributed research facilities and large-scale scientific collaborations. ESnet supplies the critical infrastructure that links DOE researchers worldwide and forms the basis for advanced experimental research in networking, collaboratory tools, and distributed data-intensive scientific applications testbeds such as the national collaboratory pilot projects. This activity directly supports SC Strategic Plan strategy 6.4. ESnet provides network services through contracts with commercial vendors for advanced communications services including Asynchronous Transfer Mode (ATM), Synchronous Optical Networks (SONET) and Dense Wave Division Multiplexing (DWDM). ESnet interfaces its network fabric through peering arrangements to other Federal, education, and commercial networks, international research network connections, and the University Corporation for Advanced Internet Development (UCAID) Abilene network that provides high performance connections to many research universities. The MANs, which are developed by regional consortia of laboratories and other research institutions build on local knowledge of installed fiber optical infrastructure to provide an underlying DWDM fabric over which ESnet can manage high bandwidth end-to-end services.

In FY 2007, SC Networks will be upgraded dual backbone rings at 20 gigabits per second with fault tolerant connections of at least 10 gigabits per second to most major SC laboratories and higher bandwidth connections to selected laboratories to manage the increased data flows from petascale computers and the experimental facilities that are critical to the Nation's future. At this funding level the management of network facilities for SC will fully implement the transition to a partnership of high performance, fault tolerant backbone networks, which are entirely funded by ESnet, and regional or metropolitan area networks, where management responsibility is shared between ESnet and the laboratories in the region. ESnet's expertise in routing, cybersecurity, and public key infrastructure will have the maximum benefit for SC through an integrated management strategy. Connectivity to universities will be achieved through close partnerships with Internet2 and its networks. This increment 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.

	FY 2005	FY 2006	FY 2007
	(dollars in thousands)		
Small Business Innovative Research (SBIR)/ Small Business Technology Transfer (STTR)	**—**	**6,293**	**8,502**

In FY 2005, $5,614,000 and $674,000 were transferred to the SBIR and STTR programs respectively. The FY 2006 and FY 2007 amounts shown are the estimated requirements for the continuation of the SBIR and STTR programs.

	FY 2005	FY 2006	FY 2007
Total, Mathematical, Information, and Computational Sciences	**226,180**	**234,684**	**318,654**

Explanation of Funding Changes

	FY 2007 vs. FY 2006 ($000)
Mathematical, Computational, and Computer Sciences and Distributed Network Environment Research	
▪ **Applied Mathematics**	
Increase in funding for Computational Sciences Graduate Fellowship activity to train next generation of leaders in computational science.	+141
▪ **Computer Science**	
Modest decrease in support for Computer Science research due to completion of several small research efforts.	-408
▪ **Computational Partnerships**	
Increase in partnership activities resulting from recompetition of SciDAC activities and initiation of new university based competition for SciDAC Institutes which can become centers of excellence in scientific areas critical to the missions of DOE and enhancements to SciDAC to develop leadership class computing simulations for petascale computers. This increment in SciDAC will enable the development of a suite of scientific software and science applications that can fully take advantage of petascale computers and build on SciDAC's initial success in enabling scientists to use terascale computers as tools for scientific discovery	+11,948
▪ **Distributed Network Environment Research**	
Increase in support for Distributed Network Environment Research to enable support of one additional peer reviewed research project.	+166
Total Funding Change, Mathematical, Computational, and Computer Sciences and Distributed Network Environment Research	**+11,847**

	FY 2007 vs. FY 2006 ($000)
High Performance Computing and Network Facilities and Testbeds	
▪ **High Performance Computing Facilities and Testbeds**	
• **High Performance Production Computing**	
Requested funding for high performance production computing at NERSC will increase its peak capacity (NERSC-5) to 100-150 teraflop.	+17,301
• **Leadership Computing Facilities (LCF)**	
▸ **Leadership Computing Facility at ORNL**	
The ORNL LCF will deliver 250 teraflops of capability in FY 2007.	+26,298
▸ **Leadership Computing Facility at ANL**	
The ANL LCF will deliver 100 teraflops of capability in FY 2007.	+22,504
Total Leadership Computing Facilities	**+48,802**
• **Research and Evaluation Prototypes**	
Research and Evaluation Prototypes will be continued at the FY 2006 level. These investments in Research and Evaluation Prototypes help prepare scientists for petascale computing and reduce the risks associated with future ASCR computer acquisitions.	+41
Total High Performance Computing Facilities and Testbeds	**+66,144**
▪ **High Performance Network Facilities and Testbeds**	
Increases in funding to enable ESnet to meet current and near-term future network needs of SC. This increment builds on the tools and knowledge developed by the Distributed Network Environment research effort to enable SC to realize the promise of optical networks for DOE missions.	+3,770
Total Funding Change, High Performance Computing and Network Facilities and Testbeds	**+69,914**
SBIR/STTR	
Increase in SBIR/STTR due to increase in operating expenses.	+2,209
Total Funding Change, Mathematical, Information, and Computational Sciences	**+83,970**

Capital Operating Expenses and Construction Summary

Capital Operating Expenses

	(dollars in thousands)		
	FY 2005	FY 2006	FY 2007
Capital Equipment	9,942	9,964	15,000