## Advanced Scientific Computing Research

### Funding Profile by Subprogram

| | FY 2007 Current Appropriation | FY 2008 Original Appropriation | FY 2008 Adjustments | FY2 008 Current Appropriation | FY 2009 Request |
|---|---|---|---|---|---|
| Advanced Scientific Computing Research | | | | | |
| Mathematical, Computational, and Computer Sciences Research | 107,117 | 133,652 | — | 133,652 | 151,304 |
| High Performance Computing and Network Facilities | 168,617 | 220,746 | -3,225[a] | 217,521 | 217,516 |
| Total, Advanced Scientific Computing Research | 275,734[b] | 354,398 | -3,225[a] | 351,173 | 368,820 |

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

## Mission

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

## Strategic and GPRA Unit Program Goals

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

Strategic Theme 3, Scientific Discovery & Innovation
Strategic Goal 3.1, Scientific Breakthroughs: Achieve the major scientific discoveries that will drive U.S. competitiveness; inspire America; and revolutionize our approaches to the Nation's energy, national security, and environmental quality challenges.

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

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

[a] Reflects a reduction for the 0.91% rescission in P.L. 110–161, the Energy and Water Development and Related Agencies Appropriations Act, 2008.
[b] Total is reduced by $7,681,000: $6,858,000 of which was transferred to the SBIR program and $823,000 of which was transferred to the STTR program.

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

**Contribution to GPRA Unit Program Goal 3.1/2.51.00, Deliver forefront computational and networking capabilities**

The ASCR program contributes to this goal 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 both facilities and colleagues to enable scientific discovery.

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

The following indicators establish specific long term (ten year) goals in Scientific Advancement that the ASCR program is committed to, and progress can be measured against. The Advanced Scientific Computing Advisory Committee (ASCAC) was charged to review progress toward these long term measures and reported "good to excellent" progress to the Department in November, 2006. The long term measures are:

- Develop multiscale mathematics, numerical algorithms, and software that enable more effective models of systems such as the earth's climate, the behavior of materials, or the behavior of living cells that involve the interaction of complex processes taking place on vastly different time and/or length scales; and
- Develop, through the Genomics: GTL partnership with the Biological and Environmental Research (BER) program, the computational science capability to model a complete microbe and a simple microbial community. This capability will provide the science base to enable the development of novel clean-up technologies, bio-energy sources, and technologies for carbon sequestration.

## Funding by Strategic and GPRA Unit Program Goal

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2007 | FY 2008 | FY 2009 |
| Strategic Goals 3.1, Scientific Breakthroughs and 3.2, Foundations of Science | | | |
| GPRA Unit Program Goal 3.1/2.51.00, Deliver Forefront Computational and Networking Capabilities | | | |
| Advanced Scientific Computing Research | 275,734 | 351,173 | 368,820 |

## Annual Performance Results and Targets

| FY 2004 Results | FY 2005 Results | FY 2006 Results | FY 2007 Results | FY 2008 Targets | FY 2009 Targets |
|---|---|---|---|---|---|
| GPRA Unit Program Goal 3.1/2.51.00 (Deliver Forefront Computational and Networking Capabilities) | | | | | |
| Mathematical, Computational, and Computer Sciences Research | | | | | |
| 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] | Improved Computational Science Capabilities. Average annual percentage increased in the computational effectiveness (either by simulating the same problem in less time or simulating a larger problem in the same time) of a subset of application codes within the SciDAC effort. FY 2006—>50%. [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. FY 2007—>100% [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. FY 2008—>100% | 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. FY 2009—>100% |
| High Performance Computing and Network Facilities | | | | | |
| 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] | | | | |
| Focused usage of the primary supercomputer at the NERSC on capability computing. Percentage of the computing time used was accounted for by computations that required at least 1/8 of the total resource. [Goal Not Met] | Focused usage of the primary supercomputer at the NERSC on capability computing. Percentage of the computing time used that was accounted for by computations that require at least 1/8 of the total resource. [Goal Met] | Focused usage of the primary supercomputer at the NERSC on capability computing. Percentage of the computing time used that was accounted for by computations that require at least 1/8 of the total resource. FY 2006—40%. [Goal Met] | 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 (760 processors) of the total resource. FY 2007—40% [Goal Met] | Focus usage of the primary supercomputer at the National Energy Research Scientific Computing Center (NERSC) on capability computing. Thirty percent (30%) of the computing time will be used by computations that require at least 1/8 (2,040 processors) of the NERSC resource. FY 2008 goal 30%. | Focus usage of the primary supercomputer at the National Energy Research Scientific Computing Center (NERSC) on capability computing. Thirty percent (30%) of the computing time will be used by computations that require at least 1/8 (2,040 processors) of the NERSC resource. FY 2009 goal 30%. |

### 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 supports the following means:

- Ensure competitively selected, peer and merit reviewed basic research in relevant areas of mathematics, computer science, computational science, and network technology necessary to achieve program and Department goals.
- Deliver computing facilities and advanced networks necessary to advance research in the relevant areas of science and technology necessary to achieve program and Department goals.
- Ensure effective management processes for timely and cost effective investments resulting in desired deliverables.
- Utilize input from the scientific community to ensure progress is made and opportunities identified.
- Form mutually beneficial partnerships with programs sharing common goals.

ASCR utilizes the following strategies:

- Utilize external review to inform joint planning—In 2006, both the ASCR and Biological and Environmental Research (BER) advisory committees have been charged with reviewing progress toward the programs common goal for computational biology. Both committees recognized that excellent research was being supported toward this goal. However, the Advanced Scientific Computing Advisory Committee (ASCAC) expressed concern about progress toward the computational models described in the goal. A joint panel has been formed to recommend specific strategies for accelerating progress in model development and the programs will jointly implement the recommendations. This panel’s work will be greatly informed by several related reports of the National Academies of Science that were sponsored by the two programs.
- Utilize external review to prioritize program investments—In 2006, the ASCAC found excellent research was being supported toward the ASCR goal in Applied Mathematics and that excellent progress was being made toward this goal. However, the committee believes that opportunities in multiscale mathematics greatly outweigh resources and that increased investment in this area would have broad impacts on Department goals. ASCR has requested increases for this area of research in both FY 2008 and FY 2009.

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.

### Validation and Verification

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

## Program Assessment Rating Tool (PART)

The Department implemented a tool to evaluate selected programs. PART was developed by the Office of Management and Budget (OMB) to provide a standardized way to assess the effectiveness of the Federal Government's portfolio of programs. The structured framework of the PART provides a means through which programs can assess their activities differently than through traditional reviews. ASCR has incorporated feedback from OMB into the FY 2009 budget request and has taken the necessary steps to continue to improve performance.

In the FY 2005 PART review, OMB assigned 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. In addition, OMB found that the program supports world-class scientific user facilities, has demonstrated an improved level of interagency communication and cooperation, was then drafting a long-term strategic vision, and has been very successful with a major effort in interdisciplinary software. However, OMB was concerned that the program's external advisory committee, ASCAC, was underutilized. The assessment found that ASCR has developed a limited number of adequate performance measures which are continued for FY 2009 with a rewording of the NERSC measures to enhance the transparency of our progress in high performance capacity computing. 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. Roadmaps, developed in consultation with ASCAC, will guide reviews every three years by ASCAC of progress toward achieving the long-term performance goals of the program. In April 2006, ASCAC was charged to conduct the first such review of progress toward the long-term measures. ASCAC reported to the Department on November 10, 2006, with ratings of good and excellent. The committee reports are available at http://www.sc.doe.gov/ascr/ascac_reports.htm. The Annual Performance Targets are tracked through the Department's Joule system and reported in the Department's Annual Performance Report which is available at http://www.cfo.doe.gov/progliaison/part2005.htm.

For FY 2007, there were four new PART related actions and two continuing actions for ASCR.

- Engage advisory panel in an assessment of the strategic priorities for the program, focusing on the balance between "core" research and supercomputing hardware investments. (FY 2007)
- Engage 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. (FY 2006)
- Implement action plans for improving program management in response to past expert reviews. (FY 2005)
- Develop new annual measures to track how efficiently the program's supercomputers are operated and maintained on a unit per dollar basis by July, 2007. (FY 2007)
- Improve the quality of the supporting materials for the Office of Science IT Exhibit 300 business cases submitted to OMB, especially the alternative analysis, acquisition strategy, and risk management sections. (FY 2007)

- Participate in the development of a unified, action-based strategy for SC-wide collaboration in accelerator and detector R&D (including advanced accelerator concepts) by March 1, 2007. (FY 2007)

In response to these OMB recommendations ASCR has:

- Charged the ASCAC to assess the strategic priorities of the program focusing on the balance between the “core” research and facilities. Their report is expected in February 2008.
- Established a Committee of Visitors (COV) to provide outside expert validation of the program’s merit-based review processes for impact on quality, relevance, and performance. ASCR made changes in procedures and program manager training to respond to the recommendations of the first two COVs, which focused on the research programs and facilities, respectively. ASCR continues to host COVs and other panels to review the quality, relevance, and performance of the program. The most recent COV focused on the SciDAC program in July 2007. The report and program action plan is posted on both the PART website and at: http://www.sc.doe.gov/ascr/ASCAC/Reports.html
- Developed, in response to the recommendations of past expert reviews, a program manager manual and training course to improve the consistency and quality of program documentation. A “Management Model for Delivering High Performance and Leadership Class Computing Systems for Scientific Discovery”; and a new “Management Model for ESnet” were also developed.
- Revised the National Energy Research Scientific Computing Center (NERSC) facility measure to clarify progress in capacity computing. Experience has shown facility management efficiencies are best realized via a regular and detailed examination of operational procedures, so ASCR will require annual Facility Operations Review by a panel of independent external experts. The reviews will evaluate the performance and cost of operations of the facility; assess the level of resources needed to effectively support the facility’s mission and identify opportunities to optimize efficiency and performance of the facility.
- Performed annual program operations reviews of the ASCR facilities: NERSC and the Leadership Computing Facilities at both Oak Ridge National Laboratory (OLCF) and Argonne National Laboratory (ALCF). Operational assessments were conducted for NERSC and the LCFs in August, 2006 and May, 2007. As a guideline for these reviews, in FY 2007, ASCR developed a “Management Model for Delivering High Performance and Leadership Class Computing Systems for Scientific Discovery” and a corresponding “Operational Assessment Program Plan.” The reviews and plans will directly contribute to improving management of the facilities and will improve the quality and consistency of project documentation.
- Submitted a unified, action-based strategy for SC-wide collaboration in accelerator and detector R&D to OMB on February 26, 2007. A working group has been formed with regular meetings and updates. ASCR contributions in this area of research are focused on simulation and modeling efforts and include the FY 2007 SciDAC project entitled Community Petascale Project for Accelerator Science and Simulation (COMPASS) which is linked to seven other SciDAC Institutes and Centers.

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

### Basic and Applied R&D Coordination

Applied Mathematics for Optimization of Complex Systems, Control Theory, and Risk Assessment: The ASCR program is requesting $2,000,000 to support basic research in advanced mathematics for optimization of complex systems, control theory, and risk assessment. This R&D integration focus area was the subject of an ASCR workshop held in December 2006. The workshop recommended additional research emphasis in advanced mathematics could benefit the optimization of fossil fuel power generation, the nuclear fuel lifecycle, and power grid control. Such research could increase the likelihood for success in DOE strategic initiatives including FutureGen and the modernization of the power grid.

Applied technology offices within DOE that could benefit from this research integration effort include: the Offices of Electricity Delivery and Energy Reliability (for their research on electric power grid control and optimization); Nuclear Energy (for development of advanced design and simulation codes); Energy Efficiency and Renewable Energy (for development of first principles models with applications to biofuels, hydrogen storage, and vehicle technologies); and Fossil Energy (for FutureGen and advanced generation engineering).

Carbon Dioxide Capture and Storage: The ASCR program is requesting $976,000 to continue two projects, selected in the FY 2006 re-competition of the SciDAC portfolio and jointly funded by ASCR and BER. These projects are: a five-year “Modeling Multiscale-Multiphase-Multicomponent Subsurface Reactive Flows using Advanced Computing” project and a three-year “Hybrid Numerical Methods for Multiscale Simulations of Biochemical Processes” project. They were selected to advance modeling of subsurface reactive transport of contaminants across multiple length scales and have also been identified as directly relevant to carbon sequestration research efforts.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2007 | FY 2008 | FY 2009 |
| Applied Mathematics for Optimization of Complex Systems, Control Theory, and Risk Assessment | | | |
| Mathematical, Computational, and Computer Sciences Research | — | 1,900 | 2,000 |
| Carbon Dioxide Capture and Storage | | | |
| Mathematical, Computational, and Computer Sciences Research | — | 976 | 976 |
| Total, Basic and Applied R&D Coordination | — | 2,876 | 2,976 |

### Overview

Computational modeling and simulation has become a third pillar, along with experiment and theory, of scientific inquiry. Scientific computing is particularly important for the solution of research problems that are unsolvable through traditional theoretical and experimental approaches, or are too hazardous, 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’s research projects in applied mathematics, computer science, and networking provide key tools and techniques to help the other SC programs achieve their research objectives. The applied mathematics research program develops and implements the fundamental methods to allow scientists to effectively utilize high performance computers to accurately model complex physical, chemical, and biological processes and systems. ASCR’s computer science research efforts help scientists make the most efficient use of high-performance computing systems as they simulate, analyze, visualize, manage, and store massive amounts of data, gaining new insight from complex scientific modeling applications and on-line experimental facilities around the world. Networking research sponsored by ASCR enables scientists at research labs and universities to collaborate, access and share data, and effectively manage high-demand scientific resources.

ASCR's other main responsibility is to provide the DOE research community with the high-performance computing and networking tools required to support world-class scientific leadership. Dramatic advances in computational science—made possible, in part, by ASCR research programs and computing systems—underscore the importance of strengthening computational science as the Nation strives to maintain its global competitiveness in science, education, and commerce. The Administration has recognized the importance of high-end computing to the Nation. The President identified supercomputing as an important component of his American Competitiveness Initiative in the 2006 State of the Union Address. The High End Computing Revitalization Task Force (HECRTF) report was published in May 2004 and ASCR continues to implement that plan through this budget request.

The National Academies are conducting a study, which was described in the President's FY 2006 Budget Request, entitled "Toward Better Understanding the Potential Impact of High-End Capability Computing on Science and Technology" to "enable a better understanding of the potential scientific impact of high-end capability computing that identifies and categorizes important scientific questions and technology problems for which an extraordinary advancement in our understanding is difficult or impossible without leading edge scientific simulation capabilities." This study is expected to better inform decision makers about the potential impact of computational science in general and ASCR's approach in particular.

As we look to the next generation of computers, we anticipate hardware that is significantly more complex and difficult to use than current systems. These machines will contain significantly more (100–1,000 times more) possessors that will contain more processing units (for example, the Intel teraflop research chip implements 80 simple cores, each containing two programmable floating point engines). These processors will also likely move from horizontal two-dimensional designs to innovative three-dimensional chip stacking (for example, IBM's "*through-silicon via*" process to create 3-D integrated stacked chips). These changes will require multiple levels of memory hierarchy and interconnects which introduce other significant challenges. As a consequence, many of the tools, software, algorithms, and libraries that we have developed for today's computers will have to be revised or replaced to effectively operate at extreme scales. As was the case with terascale computing, success will be built on a decade of research effort focused on the challenges of hardware not yet available. Therefore, it is important for ASCR to carefully balance investments in facilities and research. To make this balance more transparent, ASCR has split the Mathematical, Information, and Computational Science (MICS) subprogram into two subprograms: Mathematical, Computational, and Computer Sciences Research and High Performance Computing and Network Facilities.

**Advisory and Consultative Activities**

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

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

The ASCR program must coordinate and prioritize a large number of goals from agency and interagency strategic plans; requests from other SC programs and the National Nuclear Security Administration (NNSA); demand for network and computing capacity and capability; and community identified research opportunities (from individual proposals to reports from workshops and the National Academies of Science); while also balancing immediate and long-term needs.

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 flexible to respond to developments in a fast paced area of research. In FY 2007, ASCAC was charged with assessing the priorities and balance of the ASCR portfolio. Their report is expected February 2008.

Also in FY 2007, a series of town hall meetings were held to gather community input to identify scientific opportunities that required more advanced computing capability than currently available. These meetings were very well attended, reflecting great excitement in the research community. The reports document the potential for significant contributions to the DOE missions in Energy, Ecology, and Security but they also document significant challenges to the effective utilization of the more powerful and complex machines currently envisioned.

The key planning elements for this program are:

- The Department and SC Strategic Plan, as updated through program collaborations and joint advisory committee meetings (www.sc.doe.gov/Sub/Mission/mission_strategic.htm);
- The HECRTF Plan (www.nitrd.gov/pubs/2004_hecrtf/20040702_hecrtf.pdf) (May 2004);
- The Federal Plan for Cyber Security and Information Assurance Research and Development (www.itrd.gov/pubs/csia/csia_federal_plan.pdf) (April 2006);
- The (Interim) Federal Plan for Advanced Networking Research and Development (May 2007);
- Intra- and inter-agency working groups, committees, and workshops; and
- Reports from ASCR sponsored workshops and town hall meetings.

### Mathematical, Computational, and Computer Sciences Research

### Funding Schedule by Activity

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2007 | FY 2008 | FY 2009 |
| Mathematical, Computational, and Computer Sciences Research | | | |
| Applied Mathematics | 28,804 | 36,900 | 43,164 |
| Computer Science | 23,020 | 29,000 | 34,618 |
| Computational Partnerships | 41,695 | 50,246 | 52,064 |
| Next Generation Networking for Science | 13,598 | 13,764 | 17,221 |
| SBIR/STTR | — | 3,742 | 4,237 |
| Total, Mathematical, Computational, and Computer Sciences Research | 107,117 | 133,652 | 151,304 |

## Description

The Mathematical, Computational, and Computer Sciences Research (Research) subprogram is responsible for carrying out the research elements of the ASCR program: To enable scientists nationwide to effectively utilize forefront computational and networking capabilities to extend the frontiers of science, addressing a range of science issues that include the function of living cells and the power of fusion energy. Computational science is increasingly central to progress at the frontiers of almost every scientific discipline and to our most challenging feats of engineering. Accordingly, we must address the following questions:

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

## FY 2007 Accomplishments

- *SciDAC Team Develops First Principles Simulations of Sawtooth Oscillations in Tokamaks.* Sawtooth oscillations are periodic events occurring near the center of tokamak plasmas under certain conditions and can have a significant impact upon the performance of burning plasmas. Researchers at the SciDAC Center for Extended Magnetohydrodynamic Modeling (CEMM) have performed self-consistent simulations of repetitive sawtooth cycles for the CDX-U tokamak using the two extended nonlinear MHD codes of the Center—NIMROD and M3D—obtaining excellent agreement between the two codes and good agreement with the experiment.

- *Employing SciDAC visualization tools to advance Fusion Energy science.* The SciDAC Institute for Ultrascale Visualization has developed a data exploration system that visualizes time-varying, multivariate point-based data from gyrokinetic particle simulations allows discovery of interesting features within the data. Another SciDAC team, the Visualization and Analytics Center for Enabling Technologies (VACET), is also working with PPPL to deploy tools for query based visualization of particle fusion data. The deployment of these tools allows fusion scientists to more fully explore their data as part of their verification and validation process which is a critical component in the development of simulation codes.
- *Multiscale Mathematics delivers more realistic models of Hanford contamination.* Research at PNNL and Brown University built a three dimensional (3-D) statistical conceptual model for Hanford site and conducted first of a kind 3-D stochastic flow simulations for the entire site. Previously, stochastic simulations were limited to the small domains within Hanford site. The PNNL team improved the underlying mathematics which allowed the researchers to build a more-realistic 3-D simulation of the Hanford site. This will inform field research and monitoring activities to improve remediation efforts.
- *Improving the mathematics of earthquake simulations*. A team of researchers at Lawrence Livermore National Laboratory have implemented the 3-D elastic wave equation in a code called “WPP”. It uses the Message Passing Interface (MPI) library for parallel computations on a Cartesian grid, with variable wave speeds and density throughout the domain with a free-surface boundary condition. They also implemented general point-force and moment-source terms to model the 1906 San Francisco Earthquake for the 100 year anniversary. This simulation covered a 550 km by 200 km by 40 km domain of northern California on a 125 meter grid, leading to roughly 2.2 Billion grid points and required about 24 hours of CPU time to simulate the first 300 seconds of the earthquake. The team has also applied their methods to problems in underwater acoustics and nondestructive evaluation. Many of these results have been implemented in the massively parallel, seismic simulation software, WPP, the first version of which was recently released as open source.

## Detailed Justification

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2007 | FY 2008 | FY 2009 |
| **Applied Mathematics** | **28,804** | **36,900** | **43,164** |

This activity supports the research, development, and application of applied mathematical approaches (algorithms) for translating physical, chemical, and biological processes into numerical libraries and tools that enable scientific computing applications to calculate and solve larger and more complex problems that may otherwise be unsolvable. This activity supports research at DOE laboratories, universities, and private companies, including partnerships between DOE’s national laboratories and universities.

| | (dollars in thousands) | |
|---|---|---|
| FY 2007 | FY 2008 | FY 2009 |

The Applied Mathematics activity supports research on vital areas important to creating and improving algorithms, including:

- Numerical methods for solving ordinary and partial differential equations, especially numerical methods for computational fluid dynamics. PDEs describe problems involving unknown relationships between several variables, enabling simulations of things like fluid flow, wave propagation, and other phenomena.
- Computational meshes for complex geometrical configurations, which seek to translate domains of mathematical values into discrete points to simulate continuous processes like combustion.
- Numerical methods for solving large systems of linear and nonlinear equations.
- Optimization, which seeks to minimize or maximize mathematical functions and can be used to find the most efficient solutions to engineering problems or to discover physical properties and biological configurations. This includes optimization, control, and risk assessment in complex systems with relevance for DOE missions in Energy, National Security, and Environment.
- Multiscale computing, which connects varying scales in the same problem, such as relating processes and properties at the tiniest scales of time and space to those at the largest scales.
- Multiphysics computations, which simulate physical processes of different kinds, such as a chemical reaction at its boundary with a material.
- Math software and libraries—modular codes that can be incorporated into programs from diverse science areas, allowing developers to quickly build software that performs difficult calculations efficiently and rapidly.

New for FY 2009 will be a joint Applied Mathematics-Computer Science Institute to focus on the challenges of computing at extreme scales that blur the boundaries between these disciplines. In addition, a new effort in the mathematics of large datasets will be initiated in FY 2009 to address the most fundamental issues in finding the dots (key features), connecting the dots (relationships between the key features), and understanding the dots (extracting scientific insights) in extremely large datasets.

Early Career Principal Investigator awards given to exceptionally talented university investigators in Applied Mathematics will continue to be supported. The Computational Science Graduate Fellowship Program, aimed at attracting the best graduate students in the scientific disciplines and helps educate them as the next generation of computational scientists, is continued at $6,000,000.

| | | | |
|---|---|---|---|
| **Computer Science** | **23,020** | **29,000** | **34,618** |

This activity supports research in computer science to enable computational scientists to effectively utilize computing at extreme scales to advance science in areas important to the DOE mission. DOE has unique requirements for high performance computing that significantly exceed the capability of software products from computer vendors.

The Computer Science activity supports research in two general areas: the underlying software to enable applications to make effective use of computers at extreme scales—many thousands of multi-core processors with complicated interconnections; and large-scale data management and visualization for both local and remote data analysis. Researchers at DOE laboratories and universities, often working in partnerships, propose and conduct this research in:

- Scalable software tools to diagnose and monitor the performance of software and scientific application codes to enable users to improve performance and get scientific results faster;
- new programming models that scale to hundreds of thousands of processors to simplify application code development for petascale computing;
- advanced techniques for visualizing and managing very large-scale scientific data; and
- efforts to improve application performance through innovative next generation operating systems.

Effective understanding and utilization for science, of computing at extreme scales will require dynamic behavior of system software (operating systems, file systems, compilers, performance tools) than historically developed due to the rapid introduction of these highly complex machines. Substantial innovation is needed to provide essential system software functionality in a timeframe consistent with the anticipated availability of hardware.

In FY 2009, the Computer Science activity will continue to support the most promising long-term efforts in software and data management, analysis and representation for computing at extreme scales. Early Career Principal Investigator awards to exceptionally talented university investigators in Computer Science, who are at an early stage in their professional careers, will continue to be supported. Computer Science will continue to support the Institute for Advanced Architectures and Algorithms with Centers of Excellence at Sandia National Laboratories and Oak Ridge National Laboratory, established in FY 2008.

New for FY 2009 will be direct support for science application "leading edge developers" willing to take on the risks of working with new and emerging languages and tools. Also new for FY 2009 will be a joint Applied Mathematics-Computer Science Institute to focus on the challenges of computing at extreme scales that blur the boundaries between these disciplines.

| | | | |
|---|---|---|---|
| **Computational Partnerships** | **41,695** | **50,246** | **52,064** |

This activity supports Scientific Discovery through Advanced Computing (SciDAC). 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 the reactive transport of contaminants through groundwater). 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 through simulation and modeling.

In FY 2009, this activity will support the SciDAC Science Applications and Partnerships, Centers for Enabling Technologies (CET), and SciDAC Institutes that were competitively selected in FY 2006. Some of the three year Science Application partnerships will be completed in FY 2008, resulting in a slight decrease in this program for FY 2009.

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

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

The Scientific Applications Partnerships (SAPs) support collaborative research of applied mathematicians and computer scientists with domain scientists to develop and apply computational techniques and tools to address the specific problems of a particular Science Application team. This effort tests the usefulness of advances in computational research, transfers the results of this research to the scientific disciplines and helps define opportunities for future research.

With 70 participating institutions and hundreds of researchers developing tools, techniques and software that push the state-of-the-art in high performance computing, ASCR needed to ensure that the SciDAC teams shared information across projects and, to leverage taxpayer investment, with others in industry, government and academia. A SciDAC Outreach Center was established as a pilot in FY 2007 at Lawrence Berkeley National Laboratory. The goal is to provide a single resource, knowledgeable with regard to the expertise and resources included in the SciDAC portfolio, to facilitate and accelerate the transfer of tools, techniques, and expertise to the broader research community. The SciDAC Outreach Center has become a resource for Innovative and Novel Computational Impact on Theory and Experiment (INCITE) applicants who need assistance in readying their application to effectively utilize leadership resources. This pilot will be peer reviewed in FY 2008 to evaluate the effectiveness of this approach in broadening the impact of SciDAC.

In the competitively selected FY 2006 SciDAC awards, partnerships have been formed with SC programs in Basic Energy Sciences (BES), Biological and Environmental Research (BER), Fusion Energy Sciences (FES), High Energy Physics (HEP), and Nuclear Physics (NP), and with the National Nuclear Security Administration (NNSA). These Science Application projects are coupled to the SciDAC CETs and Institutes and may include a dedicated SAP. Areas under investigation include nuclear physics (HEP, NP, and NNSA); petascale data (HEP); accelerator physics and design (HEP, NP, and BES); computational astrophysics (HEP, NP, and NNSA); quantum chromodynamics (HEP and NP); computational biology, ground water modeling and simulation, and climate models (BER); plasma

| | (dollars in thousands) | |
|---|---|---|
| FY 2007 | FY 2008 | FY 2009 |

turbulence in tokamaks (FES); Accelerator R&D (HEP, NP, and BES); chemistry (BES); and turbulence and materials science (NNSA). This activity also supports continuing partnerships with BES in nanoscience; with BER in Genomics: GTL, and with FES on the Fusion Simulation Project (FSP).

In FY 2009, the partnership with BER in climate models will be expanded to improve the representation of ice sheets in global circulation—a critical source of uncertainty in current Earth-systems models.

| | FY 2007 | FY 2008 | FY 2009 |
|---|---|---|---|
| **Next Generation Networking for Science** | **13,598** | **13,764** | **17,221** |

This activity, previously Distributed Network Environment, builds on the fundamental results of computer science to develop integrated software tools and advanced network services to enable large-scale scientific collaboration and make effective use of distributed computing and science facilities to advance the DOE science mission.

The Next Generation Networking for Science activity primarily supports research and development in three areas to enable SC to exploit new capabilities being made available by ESnet and other national research and education networks to provide scientific data where it is needed at speeds commensurate with the new data volumes:

- distributed systems software, tools, and services to enable the discovery, management, and distribution of extremely large data sets generated by simulations or by science experiments such the Large Hadron Collider (LHC) in HEP and ITER in FES,
- advanced network protocols, optical network services, tools, and protocols to interconnect and provide access to LCFs and science facilities; and
- high-performance middleware to facilitate secure national and international scientific collaborations.

In FY 2007, an interagency working group, led by ASCR, the Department of Defense and the National Science Foundation, developed a draft plan for Advanced Networking Research and Development to identify key research areas necessary to deliver future networking technologies that are critical for science but also for U.S. economic and national security. This interagency plan will provide a framework in which ASCR research can address key issues for science and leverage effectively on research sponsored by other agencies. The Next Generation Networking for Science activity will begin to implement key elements of that plan most relevant for open science networks in FY 2008.

For FY 2009, the Next Generation Networking for Science activity will initiate a basic research effort in cyber security focused on the unique needs of open science networks and computing facilities. This activity will be informed by the Federal Plan for Cyber Security and Information Assurance Research and Development and by two ASCR workshops on research needs for cyber security in open science held in FY 2007.

Early Career Principal Investigator awards given to exceptionally talented university investigators in Networking will continue to be supported.

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2007 | FY 2008 | FY 2009 |
| **Small Business Innovative Research (SBIR)/ Small Business Technology Transfer (STTR)** | **—** | **3,742** | **4,237** |

In FY 2007, $2,594,000 and $311,000 were transferred to the SBIR and STTR programs respectively. The FY 2008 and FY 2009 amounts shown are the estimated requirements for the continuation of the SBIR and STTR programs.

| | | | |
|---|---|---|---|
| **Total, Mathematical, Computational, and Computer Sciences Research** | **107,117** | **133,652** | **151,304** |

### Explanation of Funding Changes

| | FY 2009 vs. FY 2008 ($000) |
|---|---|
| **Applied Mathematics** | |
| This increase will support a new joint Applied Mathematics-Computer Science Institute to focus on the challenges of computing at extreme scales that blur the boundaries between these disciplines, a new effort in the mathematics of large datasets to address the most fundamental issues in finding the key features, understanding the relationships between those features, and extracting scientific insights in extremely large datasets, and increases in key areas of long-term research most relevant to meeting the challenges of computing at extreme scale and risk assessment in complex systems. | +6,264 |
| **Computer Science** | |
| This increase will support a new joint Applied Mathematics-Computer Science Institute, a new effort to provide direct support for science application “leading edge developers” willing to take on the risks of working with new and emerging languages and tools, and increases in key areas of long-term research most relevant to meeting the challenges of computing at extreme scale and risk assessment in complex systems. | +5,618 |
| **Computational Partnerships** | |
| Funding is reduced for Science Application Partnerships selected in FY 2006 which will be completed in FY 2008 (-$1,182,000). The partnership with BER in climate models will be expanded to improve the representation of ice sheets in global circulation—a critical source of uncertainty in current Earth-systems models (+$3,000,000). | +1,818 |
| **Next Generation Networking for Science** | |
| This increase will support a new basic research effort in Cyber Security for Open Science. Investment would be informed by ASCR workshops and elements of the Federal Plan for Cyber Security and Information Assurance Research and Development most relevant to open science. | +3,457 |

| | FY 2009 vs. FY 2008 ($000) |
|---|---|
| **SBIR/STTR** | |
| Increase in SBIR/STTR due to increase in operating expenses. | +495 |
| **Total Funding Change, Mathematical, Computational, and Computer Sciences Research** | **+17,652** |

## High Performance Computing and Network Facilities

### Funding Schedule by Activity

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2007 | FY 2008 | FY 2009 |
| High Performance Computing and Network Facilities | | | |
| High Performance Production Computing | 37,554 | 54,200 | 54,790 |
| Leadership Computing Facilities | 94,910 | 110,158 | 115,000 |
| Research and Evaluation Prototypes | 14,313 | 23,100 | 17,000 |
| High Performance Network Facilities and Testbeds | 21,840 | 24,336 | 25,000 |
| SBIR/STTR | — | 5,727 | 5,726 |
| Total, High Performance Computing and Network Facilities | 168,617 | 217,521 | 217,516 |

### Description

The High Performance Computing and Network Facilities (Facilities) subprogram is responsible for delivering forefront computational and networking capabilities to scientists nationwide that enable them to extend the frontiers of science, addressing a range of science issues that include the function of living cells and the power of fusion energy.

The Facilities subprogram contributes to DOE missions by providing the high performance computing facilities and advanced networks that advance DOE science. High performance computers carry out trillions or even quadrillions (a million, billion or a one with fifteen zeros) of calculations each second - powerful enough to simulate complex physical, biological and chemical phenomena. ASCR computing facilities help scientists understand these complex processes at unprecedented levels of detail - from individual atoms for nanoscale engineering to the entire planet for global climate studies or even the vast reaches of the Universe to understand the nature of dark energy. These computers, and the other research facilities of the Office of Science (SC), turn out many petabytes (a quadrillion bytes) of data each year. Moving this data to the researchers who need it requires advanced networks and related technologies also provided through the Facilities subprogram.

### Supporting Information

To maintain leadership in areas of scientific modeling and simulation important to DOE missions, the Facilities subprogram plans, develops, and operates high performance computing facilities and advanced networks that are available—24 hours a day, 365 days a year—to researchers nationwide. This includes High Performance Production Computing at the National Energy Research Scientific Computing (NERSC) facility at Lawrence Berkeley National Laboratory (LBNL), Leadership Computing Facilities (LCFs) at Oak Ridge and Argonne National Laboratories, and the Energy Sciences Network (ESnet) managed by LBNL. The Facilities subprogram also invests in long-term needs through the Research and Evaluation Prototypes activity.

The Facilities subprogram computing resources are partially allocated through the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program which provided 95 million hours of computing time in 2007. Eighty percent of the processor time on LCFs is allocated through INCITE to a small number of projects, each requiring a substantial amount of the available resources. A smaller percentage (~10%) of computing resources at NERSC and the Molecular Science Computing Facility at

Pacific Northwest National Laboratory, funded by the Biological and Environmental Research (BER) program, are also allocated through INCITE. These production computing facilities are more focused on the computing needs of the Office of Science and allocated through a competitive process reserved for researchers supported by the SC programs.

In 2007, INCITE research includes accelerator physics, astrophysics, chemical sciences, climate research, computer science, engineering physics, environmental science, fusion energy, life sciences, materials science, nuclear physics, and nuclear engineering. Practical applications of the research include designing quieter cars, improving commercial aircraft design, advancing fusion energy, studying supernova, understanding nanomaterials, studying global climate change, and the causes of Parkinson's disease.

Beginning in FY 2009, the ASCR computing facilities will develop and implement a unified approach to supporting and maintaining the software, languages, and tools that are critical to effective utilization of the machines.

**Scientific Facilities Utilization**

The ASCR program's FY 2009 budget request includes support to the NERSC, ESnet, and the LCFs, located at ORNL and ANL. The investment in NERSC will provide computer resources for about 2,500 scientists in universities, DOE laboratories, Federal agencies, and U.S. companies. The proposed funding will enable NERSC to maintain its role as one of the Nation's premier unclassified computing centers, a critical element for success of many SC research programs. The investment in ESnet will provide the DOE science community with capabilities not available through commercial networks or the commercial Internet. ESnet provides national and international high-speed access to DOE and SC researchers and research facilities, including light sources, neutron sources, particle accelerators, fusion reactors, spectrometers, supercomputers, and other high impact scientific instruments. The investment in LCFs will deliver unclassified high performance capability resources to scientific researchers. The proposed funding will allow the high performance resources at the ALCF to be upgraded to a peak capability of 250–500 teraflops by the end of FY 2008. The OLCF will be on a path to one petaflop peak capability by the end of 2008.

**FY 2007 Accomplishments**

- ***Leadership Computing Facility at Oak Ridge National Laboratory (OLCF) doubled XT capability to 119 teraflops.*** Users of the LCF's Cray XT3 supercomputer have recently received two substantial performance boosts, both linked to the arrival of a 68-cabinet Cray XT4 system capable of 65 teraflops. In December 2006, users were moved to the new system, gaining a 20 percent performance boost over the existing Cray XT3 system. The two systems were then connected, creating a system with a peak performance of 119 teraflops. Users were given access to this enormously powerful combined system in April 2007. Between the combined Cray XT system and the center's Cray X1E Phoenix supercomputer, users through DOE's Innovative and Novel Computational Impact on Experiment and Theory (INCITE) program were allocated 78.7 million processor hours in 2007 which more than doubled the processor hours available in 2006.
- ***Argonne Leadership Computing Facility established.*** The ALCF achieved significant progress in its major facility upgrade project at Argonne National Laboratory in FY 2007. Key milestones that were met include: successfully completing the cost and schedule review, validating the project plans, and establishing the project baseline. To meet DOE's scientific computing mission needs, the ALCF ordered a 100 teraflop Blue Gene/P system for delivery in 2007. To meet user support and operational needs, Argonne created a new Leadership Computing Facility division at Argonne, and

added staff—eleven by spring 2007—spanning computational science, applications performance, user services, operations and administration.

- ***National Energy Research Scientific Computer Center (NERSC) increased peak capacity by 500 percent.*** In 2007, NERSC, DOE's flagship high performance production facility at Lawrence Berkeley National Laboratory, accepted delivery of a 100 teraflop Cray Hood system consisting of over 19,000 AMD Opteron 2.6-gigahertz processor cores, with two cores making up one node. Each node has 4 gigabytes of memory resulting in an aggregate memory capacity of 39 terabytes. This computer will increase the resources available at NERSC for high performance capacity computing by 500%.
- ***Energy Sciences Network (ESnet) launched first segment of the next-generation nationwide scientific research network.*** The Department of Energy began operation of the first national ring of ESnet4 in September 2007. The first segment connects the Washington, D.C. area to New York and Chicago through a partnership between Internet2 and ESnet that was announced in August, 2006. The new network will initially operate on two dedicated 10 gigabit per second (Gbps) wavelengths on the new Internet2 nationwide optical infrastructure and will seamlessly scale over the next several years to meet the complex needs of large-scale DOE Office of Science research projects. Once completed, ESnet4 will be the most advanced and reliable, high capacity nationwide network supporting scientific research efforts of the DOE research community. By providing reliable high bandwidth access to DOE laboratories and other major research facilities, ESnet4 will enhance the capabilities of researchers and scientists across the country, and their international collaborators, to use large-scale instruments to advance the scientific mission of the Office of Science.
- ***Simulations on Cray XT4 Provide New Insights into Adsorption.*** Researchers from ORNL used the leadership supercomputers at Oak Ridge to significantly enhance our understanding of adsorption, the small-scale process by which one molecule attaches to another. The Oak Ridge team answered a question that has long vexed physical chemists, resolving the molecular structure of successive layers of methane as they attach to magnesium oxide. Their work was featured in January 2007 as the cover article in the *Journal of Physical Chemistry C*, a publication of the American Chemical Society that focuses on nanomaterials and surface science.

## Detailed Justification

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2007 | FY 2008 | FY 2009 |
| **High Performance Production Computing** | **37,554** | **54,200** | **54,790** |

This activity supports the NERSC facility located at LBNL. NERSC delivers high-end capacity computing services and support to the SC research community. Nearly 2,500 computational scientists, in about 400 projects, use NERSC to perform basic scientific research across a wide range of disciplines including astrophysics, chemistry, climate modeling, materials, analysis of data from high energy and nuclear physics experiments, investigations of protein structure, and a host of other scientific endeavors. NERSC users are primarily supported by the SC programs with 56% based in universities, 33% in National Laboratories, 7% in other government laboratories, and 4% in industry.

In 2007, the capacity of NERSC was expanded by 500 percent, with the acquisition of the 119 teraflop Cray XT4 system. FY 2009 funding will support the continued operation of the NERSC Cray XT4 system, and two clusters available for scientific applications that do not scale well to more than 512 processors and are therefore not well suited to the Cray architecture. These computational resources are integrated by a common high performance file storage system that enables users to easily migrate to any of the NERSC resources. With many petabytes of storage and an average transfer rate in the hundreds of megabytes per second this system also allows users to easily move data into and out of the NERSC facility.

In FY 2009, NERSC will continue to play a key role in the SC strategy for computational science because it enables teams to prepare to make use of the LCFs as well as to perform the calculations that are required by the missions of the SC programs. About 10% of the NERSC facility will be allocated through SC's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program.

| | FY 2007 | FY 2008 | FY 2009 |
|---|---|---|---|
| Maximum Hours | 8,760 | 8,760 | 8,760 |
| Scheduled Hours | 8,585 | 8,585 | 8,585 |
| Unscheduled Downtime | 1% | 1% | 1% |

| | FY 2007 | FY 2008 | FY 2009 |
|---|---|---|---|
| **Leadership Computing Facilities (LCF)** | **94,910** | **110,158** | **115,000** |

The LCF activity was initiated with a call for proposals in FY 2004. As a result of the peer-reviewed competition, the partnership established by ORNL, ANL, and PNNL was selected to provide capability computing resources for SC researchers.

| | FY 2007 | FY 2008 | FY 2009 |
|---|---|---|---|
| ▪ **Leadership Computing Facility at ORNL (OLCF)** | **77,000** | **83,716** | **85,000** |

The first LCF capability for science was established in late FY 2005 at ORNL. In FY 2007, the OLCF upgraded the Cray XT3 with 11,708 dual-core processors providing a peak capacity of 119 teraflops. The Facility will be upgraded to a peak capacity of 250 teraflops by the end of 2007 by replacing the dual-core processors with quad-core processors. This upgrade will provide applications with valuable experience using a multi-core architecture. By the end of 2008, the facility will operate a one petaflop (1,000 teraflops) Cray Baker system expected to contain over 22,000 quad-core processors.

In FY 2009, the OLCF will continue to provide world leading high performance capability to researchers on a peer-reviewed basis through INCITE awards. Some of these applications, particularly in fusion and climate research, are achieving sustained performance in excess of 80 teraflops or nearly 70% of the peak capability. The acquisition of a 1 petaflop Cray Baker system in late 2008 will enable further scientific advancements, such as simulations of fusion devices that approach ITER scale. The success of this effort is built on the gains made in research and evaluation prototypes and the SciDAC program and on years of research in applied mathematics and computer science.

| | FY 2007 | FY 2008 | FY 2009 |
|---|---|---|---|
| Maximum Hours | 7,008 | 7,008 | 7,008 |
| Scheduled Hours | 7,008 | 7,008 | 7,008 |
| Unscheduled Downtime | 1% | 1% | 1% |

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2007 | FY 2008 | FY 2009 |
| ▪ **Leadership Computing Facility at ANL (ALCF)** | **17,910** | **26,442** | **30,000** |

In FY 2007, further diversity with the LCF resources was realized with an acquisition by ANL of a high performance IBM Blue Gene P with low-electrical power requirements and a peak capability of over 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 facility provides many applications, including molecular dynamics and materials, with access to a system that is better suited to their computing needs.

In FY 2009 the ALCF will be operating the 500 teraflop IBM Blue Gene/P acquired in FY 2008. The facility will focus on utilizing the IBM Blue Gene architecture and assisting INCITE projects, pioneer applications, and tool and library developers. Strengthening the Argonne infrastructure in FY 2009 will be essential to prepare the facility, and the user community, for the more complex machine being developed through the joint research project with NNSA and IBM.

| | FY 2007 | FY 2008 | FY 2009 |
|---|---|---|---|
| Maximum Hours | 3,000 | 6,000 | 7,008 |
| Scheduled Hours | 3,000 | 6,000 | 7,008 |
| Unscheduled Downtime | 1% | 1% | 1% |

| | | | |
|---|---|---|---|
| **Research and Evaluation Prototypes** | **14,313** | **23,100** | **17,000** |

The Research and Evaluation Prototype activity addresses the challenges of the systems that will be available by the end of the decade. We anticipate that these systems will be significantly more complex than current systems. As a result, many of the tools and techniques we have developed will no longer be effective. By actively participating in the development of these next-generation machines, researchers will better understand the inherent challenges and can begin to work on overcoming those challenges. This activity will prepare researchers to effectively utilize the next generation of scientific computers and will also reduce the risk of future major procurements.

The Research and Evaluation Prototype activities will be carried out in close partnership with the NNSA and the DARPA HPCS program. This activity includes the DOE partnership in the DARPA HPCS Phase III program ($13,000,000) as well as support for SC's participation in the joint SC-NNSA partnership with IBM to explore and advance low power density approaches to petascale computing ($4,000,000).

| | | | |
|---|---|---|---|
| **High Performance Network Facilities and Testbeds** | **21,840** | **24,336** | **25,000** |

This activity supports operation and upgrades for the Energy Science network (ESnet) and a related research partnership with Internet2. The ESnet provides a high bandwidth network connecting DOE and SC researchers and research facilities, including light sources, neutron sources, particle accelerators, fusion reactors, spectrometers, supercomputers, and other high impact scientific instruments. Each year the amount of data generated by these facilities roughly doubles. To meet demand, ESnet has partnered with Internet2—the leading provider of university networks—to push the state-of-the-art and deliver next generation optical network technologies that greatly expand capacity in the core science networks.

| | (dollars in thousands) | |
|---|---|---|
| FY 2007 | FY 2008 | FY 2009 |

In FY 2009, ESnet, in partnership with Internet2, will continue to implement a next generation optical network infrastructure for U.S. science as announced in August 2006. ESnet will deliver 40–60 Giga (billion) bits per second (Gbs) connections to SC laboratories in FY 2009 on a path to achieving 160–400Gbs connectivity in FY 2010–FY 2011 when research efforts are expected to result in new technologies in the core network. Continued progress in high performance networks also builds on the tools and knowledge developed by the Next Generation Networks for Science research activity.

| | FY 2007 | FY 2008 | FY 2009 |
|---|---|---|---|
| Maximum Hours | 8,760 | 8,760 | 8,760 |
| Scheduled Hours | 8,760 | 8,760 | 8,760 |
| Unscheduled Downtime | 0.01% | 0.01% | 0.01% |

| | FY 2007 | FY 2008 | FY 2009 |
|---|---|---|---|
| **Small Business Innovative Research (SBIR)/ Small Business Technology Transfer (STTR)** | **—** | **5,727** | **5,726** |

In FY 2007, $4,264,000 and $512,000 were transferred to the SBIR and STTR programs respectively. The FY 2008 and FY 2009 amounts shown are the estimated requirements for the continuation of the SBIR and STTR programs.

| | FY 2007 | FY 2008 | FY 2009 |
|---|---|---|---|
| **Total, High Performance Computing and Network Facilities** | **168,617** | **217,521** | **217,516** |

## Explanation of Funding Changes

| | FY 2009 vs. FY 2008 ($000) |
|---|---|
| **High Performance Production Computing** | |
| The increase is due to increased operating costs for the NERSC facility. | +590 |
| **Leadership Computing Facilities (LCFs)** | |
| The increase will support the installation, testing, and operation of a one petaflop Cray Baker system at the OLCF and a 500 teraflop IBM Blue Gene system at the ALCF, including user support activities at both facilities. This capability will accelerate scientific understanding in an array of research areas including: astrophysics, biology, climate change, fusion energy, materials, and chemistry. | +4,842 |
| **Research and Evaluation Prototypes** | |
| The decrease is due to a decrease in the ASCR contribution to the DARPA HPCS program. In FY 2008, ASCR fully funded the DOE commitment to the DARPA HPCS program, including the NNSA portion of the effort. This budget request assumes that NNSA will resume participation in the DARPA HPCS effort in FY 2009. | -6,100 |

| | FY 2009 vs. FY 2008 ($000) |
|---|---|
| **High Performance Network Facilities and Testbeds** | |
| The increase will enable ESnet to deliver 40–60 Gbs connections to SC laboratories in FY 2009. The increase in bandwidth is critical to meeting the growing requirements for Department applications and facilities. | +664 |
| **SBIR/STTR** | |
| Decrease in SBIR/STTR due to small decrease in operating expenses. | -1 |
| **Total Funding Change, High Performance Computing and Network Facilities** | **-5** |

## Capital Operating Expenses and Construction Summary

### Capital Operating Expenses

| | (dollars in thousands) | | |
|---|---|---|---|
| | FY 2007 | FY 2008 | FY 2009 |
| Capital Equipment | 9,743 | 13,000 | 13,000 |